

**MATERIALS SCIENCE AND TECHNOLOGY
AND
CULTURE OF SCIENCE
IN THE ISLAMIC WORLD**

Mehmet Ergin
Moneef R. Zou'bi
Editors

Islamic Academy of Sciences
Amman, Jordan



**MATERIALS SCIENCE AND TECHNOLOGY
AND
CULTURE OF SCIENCE**

Materials Science and Technology and Culture of Science

Proceedings of the IAS Conference on Materials Science and Technology and
Culture of Science, organised in Islamabad, Pakistan
14-17 October 2002

Edited by

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and
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Preface

The science academies of today have a critical role to play as the public voice of science. A voice that promotes scientific excellence and science-based development. These academies, who some consider as the science advisors of their catchment areas, play a vital role in convincing the public that an intricate relationship exists between home-bred science and sustainable growth and sustainable development. In other words, it falls to the science academies in the various communities to cultivate a *Culture of Science* within the area in which they operate.

In response to the need for an international organisation that can play such a role and cater for the needs of the Islamic scientific community, the Islamic Academy of Sciences (IAS) came into being as a non-political, non-governmental scientific organisation of Muslim scientists of the various continents of the world.

The establishment of the Academy was recommended by the OIC Standing Committee on Scientific and Technological Co-operation (COMSTECH), and approved by the Fourth Islamic Summit, Casablanca, 1984.

The Academy, which commenced its activities in 1986, is an independent body that enjoys international status comparable to other international learned bodies of similar nature in the world.

Of the 'policy development' activities that the Academy undertakes is annually convening an international conference that addresses a major theme or themes of relevance to OIC and Developing countries in general. The twelfth such conference was held in Islamabad (Pakistan) during October 2002.

As well as addressing the frontier area of *Materials Science and Technology* and *Nanotechnology*, it also addressed the theme of *Culture of Science*.

The conference was the third in series organised by the IAS on *Transformational Technologies*; the first two being *Information Technology*, and *Biotechnology*; addressed in the preceding years by the IAS in Tunisia and Morocco, in 2000 and 2001, respectively.

A major objective of such activities is to bring certain scientific topics to the attention of political leaders and decision-makers in developing countries, and bridge this often-wide divide that exists between the science/academic community in any country and the decision-making/political echelon therein. Needless to say, that it sometimes falls to forces from outside a developing country to bring about this marriage of policies (scientists and planners) and politics (the craft of politicians).

Notwithstanding the vast experience of many universities and the work of a number of research centres, the frontier area of *Materials Science and Technology* and *Nanotechnology*, admittedly, is not a science priority area for

the majority of OIC-countries. It is partly for this reason that the IAS chose *Materials*, and the very exciting branch thereof... namely *Nanotechnology* as theme for its twelfth international conference.

This book, which carries the same, rather elaborate title as the conference, has been divided into six parts.

Part One is made up of the statements of the two IAS Patrons, and speeches of the various dignitaries, that were delivered during the inaugural session of the conference. **Part Two** contains a keynote paper entitled “Engineering Materials: The Driving Force of Technology in the Islamic World,” by the eminent Pakistani scientist, Dr A Q Khan, the then President of the Pakistan Academy of Sciences. **Part Three** presents, rather comprehensively, an assessment of *Nuclear Techniques in the Study of New Materials*, through four outstanding presentations by speakers from Pakistan, Kazakhstan, Germany and France. **Part Four** includes a paper that looks at Materials from the engineering standpoint, especially highlighting some the research work being done at universities in this field. **Part Five** includes papers that address the specific issue of the chemistry of materials, and the macro question of sustainability assessment of materials. *Nanotechnology* is the title of **Part Six** of the book with one overview paper on the subject, whereas **Part Seven** includes the various papers presented in the *Culture of Science Forum*, which was the second theme of the conference.

Part Eight of the book is the appendix that includes the list of participants in the conference, the conference scientific and organising committees, the names of IAS Fellows, IAS Council Members, as well as other details about the Islamic Academy of Sciences.

Overall, the book represents an effort by the Academy to bring the contemporary aspect of *Materials Science and Technology* and the research related thereto to the forefront, resulting in actions by decision-makers in OIC-member countries to start-up/strengthen existing research units working in the field, or to establish national commissions the task of which might be to assess how the new and exciting field of *Nanotechnology* can best be ventured into.

The *Culture of Science* element is part on a long-term effort by the IAS to link up science and scientific activities to the teachings of Islam, and cultivate awareness among the decision-making community and the public at large of the value of science as a means of attaining socio-economic development.

Mehmet Ergin
Moneef R. Zou’bi

Acknowledgements

The Islamic Academy of Sciences is grateful to His Excellency General Pervez Musharraf, President of the Islamic Republic of Pakistan, and Patron of the IAS, for his patronage of the Twelfth IAS Conference, and indeed the Academy. His Excellency Mr Justice Sheikh Riaz Ahmed, Acting President of Pakistan, deserves our gratitude for inaugurating the conference and also hosting a state dinner in honour of its participants. The support of His Royal Highness Prince Al-Hassan Ibn Talal of Jordan, Founding Patron of the IAS, is gratefully acknowledged.

The IAS extends its appreciation to all the organisations that sponsored the convening of the conference foremost among which are the Pakistan Academy of Sciences and its President Dr A. Q. Khan, the Islamic Development Bank (IDB), COMSTECH, UNESCO as well as the OPEC Fund for International Development.

We also wish to thank all the Pakistani organisations, institutions, and banks that sponsored and supported the convening of the conference.

We are very grateful to all the eminent speakers who participated in the conference and to all the specialists and the various participants who made the effort to take part in this international scientific activity.

The preliminary work done by the IAS Council and the efforts volunteered by Dr M. D. Shami, IAS-Vice-President; Dr M. Ergin, IAS Secretary General; and Mr Moneef R. Zou'bi, IAS Director General, during the meetings of the scientific committee and the conference itself are gratefully acknowledged.

The IAS Council headed by Dr A. S. Majali has done a lot too to help realise this activity.

The dedicated staff at IAS Secretariat including Ms Lina Jalal, Ms Taghreed Saqr, Ms Hind Bilbeissi, Mr Habis Majali, Mr Saleh Asa'ad, and Mr Khaled Abdul-Gahfoor; as well as the type - setting team of Mr George Anz, and Ms Amal Mizher, and Mr Khalil Adainat; who have all worked hard to produce this book, deserve our thanks.

Mehmet Ergin
Moneef R. Zou'bi

IAS Islamabad Conference
on
Materials Science and Technology
and
Culture of Science

Sponsor Organisations

- (1) Islamic Academy of Sciences (IAS), Amman, Jordan;
- (2) Pakistan Academy of Sciences, Islamabad, Pakistan;
- (3) OIC Ministerial Committee on Scientific and Technological Co-operation (COMSTECH), Islamabad, Pakistan;
- (4) Islamic Development Bank (IDB), Jeddah, Saudi Arabia;
- (5) OPEC Fund for International Development, Vienna, Austria;
- (6) Arab Potash Company, Amman, Jordan;
- (7) Islamic Organisation for Medical Sciences, Kuwait City, Kuwait;
- (8) Higher Council of Science and Technology, Amman, Jordan;
- (9) Arab Bank, Jordan;
- (10) National Centre for Human Resources Development, Amman, Jordan; and
- (11) Dar Al-Dawa' Pharmaceuticals Company, Amman, Jordan.

IAS Islamabad Declaration
on
Materials Science and Technology
and
Culture of Science

Adopted at Islamabad (Pakistan)

on

9 Sha'aban 1423

16 October 2002

PREAMBLE

- (1) *Allah* (God) *Subhanahu Wata'ala* has not only created man and endowed him with reason, but He has also made the pursuit of knowledge an (absolute) obligation. Accordingly the teachings of Islam emphasize the importance of carefully using the resources of the universe for the lasting well-being of man.
- (2) Concepts such as sustainability, and analytical tools such as human development indicators, provide conceptual frameworks for linking R&D to societal outcomes. This leads towards the implementation of an approach to R&D policy that addresses the complex interconnections between technological advance and societal response.
- (3) Recent decades have witnessed significant changes in knowledge-production systems, especially in scientific research and related applications. These changes are fuelled by the quickening pace of globalization and by new developments in Information and Communication Technologies (ICTs), Biotechnology and the field of Materials Science and engineering, including the new and exciting Nanotechnology.

PROPOSALS

- (4) For developing countries to be prepared for the transformational power of the Information Technology, Biotechnology and Nanotechnology, they need to develop the appropriate scientific capacity, knowledge and tools for more effectively connecting R&D inputs with desired societal outcomes, and ultimately for harnessing the powers of these technologies to realize socio-economic development. This would require the creation of a

dedicated intellectual, analytical, and institutional capability, focused on understanding the dynamics of science and the science-society interface.

Such a capability can include the following elements:

- (a) Analysis of past and current societal responses to transforming technologies;

A case-history approach could be used to investigate how society has responded to a range of technological advances. Understanding the roles and relations between the media, academia, policy makers, institutions, and cultural factors could be the basis for assessing the likely trajectories of technology-induced social change.

- (b) Biotechnology and Nanotechnology enterprises need to undergo comprehensive, real-time assessment and monitoring;

A database of important activities in Biotechnology and Nanotechnology should be built, and then track the evolution of these enterprises, in terms of directions of research and innovation, resources used, public and private-sector roles, publications and patents, marketed products, and other useful indicators.

- (c) A constructive technology assessment process, with participants drawn from representatives of the R&D effort, policy-makers, and the public can lead to a better understanding of the potential of Nanotechnology;

Technology assessment is both a process for bringing together a range of actors, and an evolving product that can lead to better understanding of the innovation and decision-making processes. Understanding the changing capabilities of both the Nanotechnology enterprise and various sectors and institutions likely to be affected by the enterprise can contribute to a healthy policy-making environment where innovation paths and social goals are compatible and mutually reinforcing.

- (d) Mapping out a Nanotechnology route;

Should Nanotechnology yield a small proportion of its anticipated advances, the impact on society can be far-reaching and profound - "as socially transforming as the development of running water, electricity, antibiotics, and microelectronics." We can allow these transformations to surprise and overwhelm us, or we can be smart about preparing for the coming changes, in order to enhance the benefits, and reduce the disruption, that accompanies any scientific revolution.

- (e) A thorough and objective review of the state-of-the-art Technology Trio; Information Technology, Biotechnology and Nanotechnology;

Economics-related yardsticks to evaluate the E-readiness, B-readiness and N-readiness scenarios in OIC and developing countries need to be formulated as a prerequisite to drawing the attention of the decision-maker, and investor to these vital sectors.

In Materials Science and Technology, this meeting calls for;

- (5) Formation of specialists groups in Advanced Materials Science and Technology in areas such as:
 - (i) Reactor based research in Materials Science and Technology;
 - (ii) Accelerator based research in Materials Science and Technology;
 - (iii) Nanotechnology of materials;
 - (iv) Materials for alternate or renewable energy technologies;
 - (v) Bio-materials;
 - (vi) Special materials for the aerospace industry;
 - (vii) Materials Science and Technology for Information Technology;
- (6) Establishment of collaborative centres for the OIC similar to CERN (Geneva), and ILL (Grenoble);

One current opportunity is the SESAME project, the Synchrotron Radiation Facility for the Middle East, "Bessy-1," donated by Germany and being set up in Jordan under the auspices of UNESCO. The facility is expected to go into operation in 2006. This is a very versatile facility for Materials Science research in a number of scientific disciplines including Physics, Biology, Chemistry, Medicine etc.
- (7) Undertaking training and education programmes in Materials Science and Technology:
 - (a) *Sharing of expertise in specific strong areas of research between OIC member countries; and*
 - (b) *Exchange of professors for short-term lectureships.*
- (8) Implementing joint projects between existing strong similar areas of expertise in OIC member countries;
- (9) Maintaining strong technical links and collaboration with researchers/centres of developed countries of Europe, United States, Japan as well as Korea and China, etc...;
- (10) Focussing on strong collaboration with scientists and research centres in central Asian states;
- (11) Cultivating strong linkages with decision makers and the media for expanding activities in Materials Science and Technology areas.
- (12) Publishing of a Journal on Materials Science and Technology in collaboration with OIC centres that are doing research in this area.

In Culture of Science, this meeting accordingly recommends that

- (13) A science-communication initiative is launched, within the context of the Culture of Science Initiative of the IAS, to foster dialogue among scientists, technologists, policy makers, the media, and the public.

Understanding, tracking, and enhancing the processes by which information about science and technology diffuses from the laboratory to the outside world is central to understanding the social-transformation process as it occurs. Of equal importance is the need to understand and monitor how public attitudes and needs evolve, and how they reach back into the innovation system.

- (14) Action is taken to set up an international multi-disciplinary group, to initiate and develop a dialogue and positive interaction between scientists, technologists and Islamic scholars, in order to:

- (i) *Lay down operating principles to resolve the moral and social issues that arise in the introduction of modern science and technology for the development of Muslim communities the world over;*
- (ii) *Develop such approaches to continuously determine appropriate responses to the so-called "Modernity," on the basis of the Qur'an and Sunnah, for the best implementation of maximum good for all;*
- (iii) *Undertake a programme for the integration of perennial knowledge with acquired knowledge, on the lines of the integrated curricula developed and being implemented in countries such as Malaysia and Indonesia; and*
- (iv) *Utilise the electronic and print media to bridge the gap between scientists and the public in OIC countries, and between OIC countries and Western countries.*

**Twelfth Conference of the
Islamic Academy of Sciences**
on
Materials Science and Technology
and
Culture of Science

14-17 October 2002
Islamabad, Pakistan

Conference Report

Under the patronage of His Excellency the President of Pakistan, the Islamic Academy of Sciences convened its twelfth international conference in Islamabad (Pakistan), during 14-17 October 2002. The conference addressed the themes of *Materials Science and Technology* and *Culture of Science*.

The conference, which was held at the Serena Hotel, was an open scientific activity in which over 100 participants representing over 25 countries participated. It was organised and sponsored by the following organisations:

- Islamic Academy of Sciences (IAS), Amman, Jordan;
- Pakistan Academy of Sciences, Islamabad, Pakistan;
- OIC Ministerial Committee on Scientific and Technological Co-operation (COMSTECH), Islamabad, Pakistan;
- Islamic Development Bank (IDB), Jeddah, Saudi Arabia;
- OPEC Fund for International Development, Vienna, Austria;
- Arab Potash Company, Amman, Jordan;
- Islamic Organisation for Medical Sciences, Kuwait City, Kuwait;
- Higher Council of Science and Technology, Amman, Jordan;
- Arab Bank, Jordan;
- National Centre for Human Resources Development, Amman, Jordan; and
- Dar Al-Dawa' Pharmaceuticals Company, Amman, Jordan.

The main objectives of the conference were:

- (1) To study some specific topics of importance to the field of new materials and future applications related thereto, and review the materials research activities undertaken in the various OIC countries;

- (2) To study the importance of materials science and technology to increasing wealth and enhancing the quality of life, especially how materials and materials science affect healthcare, the environment, sustainability, communications, innovation, education...;
- (3) To bring together those working at the cutting edge in new materials research in academia, industry and other research organisations, whether they are involved in materials science, chemistry, physics or engineering work;
- (4) To appraise some contemporary concepts in Nanotechnology with the aim of disseminating them in OIC and developing countries; and
- (5) To attempt to define a role for governments in materials research in terms of priorities, regulation, funding, private-public sector collaboration.

In addition to a keynote that overviewed recent developments in science and technology in Pakistan, which was presented by Prof. Atta-ur-Rahman (FIAS), Minister of Science and Technology in Pakistan; two other keynotes were presented. The first carried the title *Engineering Materials: Driving Force of Technology*, and was presented by Prof. A. Q. Khan (FIAS), President of the Pakistan Academy of Sciences; and the second on the *Culture of Science*, and that was presented by Dr Hussein Gezairy, WHO Regional Director for the Eastern Mediterranean.

A paper on *Nanotechnology Research in China* was presented by the director of the Centre of Nanoscience of the Chinese Academy of Sciences during a special session that was dedicated to Nanotechnology. That was followed by a video-conference presentation by Dr Alan Hewat of the Institute Laue-Langevin on *Neutron Diffraction and the Structure of New Materials*, in a specialised session that was dedicated to *Nuclear Techniques in the Study of New Materials*. A number of short introductory lectures were also arranged throughout the programme of the conference in order to introduce some specific aspects of the theme to the participants who generally belonged to a number of scientific disciplines.

At the conclusion of the three-day conference in which 25 papers were presented, the Academy adopted the IAS Islamabad Declaration on *Materials Science and Technology* and *Culture of Science*.

The declaration proposed the implementation of an approach to R&D policy that addresses the complex interconnection between technological advance and societal response. It highlighted that changes have been taking place in the knowledge production systems that were fuelled by globalisation and by new developments in Information Technology (IT), Biotechnology (BT) and Nanotechnology (NT).

The declaration proposed that for OIC and developing countries to be prepared for the transformational power of IT, BT and NT, they need to develop the appropriate scientific capacity, knowledge and tools for harnessing the powers of these technologies to realize socio-economic development.

The declaration made a specific mention of some joint collaborative research programmes that could be launched along the same lines as CERN (Geneva), and ILL (Grenoble), specifically highlighting the Unesco-sheparded SESAME project that involves the hosting by Jordan of the Synchrotron Radiation Facility.

On the theme of *Culture of Science*, the declaration emphasized that understanding, tracking, and enhancing the processes by which information about science and technology diffuses from the laboratory to the outside world is central to understanding social-transformation processes as they occur. Of equal importance, it elaborated, is the need to understand and monitor how public attitudes to science evolve, and how they reach back into the innovation system.

As part of the follow-up action to the conference, the Academy will circulate the IAS Islamabad Declaration to concerned individuals and relevant agencies throughout in OIC and developing countries, so that measures are taken to implement the ideas proposed at the conference.

The Academy will also publish the complete proceedings of the conference in a quality volume that will be distributed internationally. Such a book, like all other published IAS proceedings, will become a valuable reference for experts that are involved in *Materials Science and Technology* or undertake research in the field of science-society interaction.

**Address of
His Excellency Mr Justice Sheikh Riaz Ahmed
Acting President of the
Islamic Republic of Pakistan**

**Dr A. Q. Khan, President, Pakistan Academy of Sciences, and Advisor to the Chief Executive on Strategic Programmes and KRL Affairs;
Prof. Abdel Salam Majali, President, Islamic Academy of Sciences;
Prof. Atta-ur-Rahman, Minister of Science and Technology, and Coordinator General COMSTECH;
Excellencies;
Distinguished Delegates;
Ladies and Gentlemen**

السلام عليكم ورحمة الله وبركاته،،،

It is matter of great pleasure for me to extend to you a warm welcome at the 12th IAS Science Conference on “Materials Science and Technology” and “Culture of Science.” This assembly of eminent scholars is a testimony to our determination to introspect and find ways and means to strengthen the economic base of the *Ummah* through scientific and technological self-reliance. The events of last year have resulted in a radically changed global scenario and bred negative attitudes towards the Islamic world. This makes it all the more essential that we move ahead in our resolve to match adversities by accomplishments in the field of science with a renewed sense of urgency.

Muslim nations face unprecedented complexities of governance and economic turmoil. In the wake of the current international socio-political environment, floodgates of reactions have opened, implicitly if not overtly, with dire consequences for the Islamic world. Needless to say that such reactions are both unjust and unrealistic. It is an unassailable truth that in its universality, Islam stands for a culture of tolerance and places the highest premium on human rights, men and women included, and mutual respect for fellow beings. It is this very image of Islam that must emerge from our actions and must be shared with world communities. In the single concept of “Ilm,” Islam has taken in its grip both science and the broader pursuits of knowledge. Thus, the pursuit of knowledge in general and scientific knowledge in particular is both our duty and an obligation. The prophet of Islam (PBUH) said, “Seek knowledge from cradle to grave,” and “Seek knowledge even in China.” Attainment of scientific knowledge is an irrefutable prerequisite for its utilization by the self-reliant nations for the benefit of their peoples. The OIC region needs to make sincere

efforts in this respect. Fortunately, in this age of revolutionary breakthroughs in communication technologies, it has become much easier to share information in the field of science and technology with the privileged nations of the world and across institutional and national boundaries. We must remember that just as the nations of Europe benefited from their interaction with contemporary Muslim scientists, we too cannot work in isolation and must maintain a healthy liaison with the Western world in our scientific endeavours.

The Islamic Academy of Sciences has a very impressive tradition of organizing conferences on subjects of contemporary importance. We, in Pakistan, feel greatly honoured and privileged to host the current conference, which addresses the issues of “Materials Science and Technology” and “Culture of Science.” I must give credit to Dr A. Q. Khan for inviting the IAS on behalf of the Government of Pakistan and the Fellows of the Pakistan Academy of Sciences to hold this conference in Islamabad. This timely thought on his part speaks volumes of the dedication of the Pakistan Academy of Sciences to constantly contribute to building strong ties with scientists in the OIC region.

While the advances in technologies such as nanotechnology have opened up new avenues for researchers dealing with Materials Science, a number of other revolutionary developments in science have occurred at the close of the 20th century. These also invite our immediate attention and thus, I am hoping that your scientific deliberations would focus not merely on the immediate themes selected for this conference but also on the greater expectations of the *Ummah* in the scientific and technological fields. Pursuit of these scientific objectives demands that we proceed with wisdom and dedication. We ought to be able to rise above narrow political imperatives and generate a framework of policies based on pooling of our rich resources of skill and wealth through mutual cooperation and understanding. So far, we have somehow shied away from generating mutual confidence and hence failed to frame policies that could find unanimous favour among the governments and leaders of the Islamic world.

This conference provides a historical opportunity by bringing a large body of scientists from Pakistan and other Muslim countries to a common platform in Islamabad. It is a momentous opportunity that must not go to waste. Both the Pakistan Academy of Sciences and COMSTECH have been playing active roles in their own right in developing programmes of scientific cooperation in the OIC region. COMSTECH has initiated over the years exciting programs of cooperative research, exchange of scientists, training of technicians, maintenance of scientific equipment, supply of spare parts and in developing a culture of dedicated scientific efforts aimed at raising the infrastructure of science in Muslim countries. Continued collaboration of our educational institutions of higher learning and R&D organizations with COMSTECH promises to place the *Ummah* on the path of economic progress and prosperity. The IAS itself under the dynamic leadership of Dr Abdel Salam Majali is in a very strong position to lead the *Ummah* in sciences and in shaping its economic future. It can provide valuable guidance to scientists, the individual

governments of the OIC Member States and policy-makers of the Muslim world.

Whereas there is urgency to take measures for innovative changes in the scientific approach and to institutionalise a culture of science in Islamic countries, I also wish to highlight some of the serious ethical, moral and legal accompaniments of scientific and technological progress and their impact on societal development and our moral fabric. Specially relevant in this context are the ongoing debates on cloning, stem cell research, genetically engineered foods, environmental complications, and no less importantly, intellectual property rights. I am hopeful that the scientific community of the Islamic countries would actively engage in a dialogue on these issues in the light of universally shared principles and the question of quality of institutions that are destined to educate our youth on these issues.

There is no denying the fact that our survival as a Muslim *Ummah*, both in terms of economy and defence potential, depends entirely on the kind of science education we impart to our children. IAS can help develop a long-range perspective plan for promotion of scientific literacy in the Islamic world with special focus on quality, morals, and ethics. The dignity of nations in a highly competitive world depends on the quality of its educational institutions of learning as well as on productivity of knowledge - scientific knowledge and its applications in particular. We must, therefore, move with haste to develop a culture and a tradition of science that would facilitate development of the human resource that is both responsible and equipped with scientific ingenuity and foresight. In this process, scientific growth must occur hand in hand with moral growth, squarely in the light of Islamic teachings as well as in consonance with the needs of the society and the market. We have to overcome poverty and problems of cultural identity. Scientific and technological uplift of the *Ummah* holds the key in this regard.

It is heartening to note that the natural resources, with which the Muslim world is gifted, are immensely vast and precious. Their sustainable exploitation and utilization for the benefit of our peoples demand that we mobilize both the political will and earnest efforts to achieve excellence in all fields, in phases to begin with, by taking revolutionary steps in upgrading our educational system. It is the quality of educational opportunities that the *Ummah* promises to provide to its youth that will lead the Muslim world to compete successfully in areas of high technology in the 21st century. We must seriously address the question as to how long can the OIC peoples remain consumers of technology rather than producers of technology? The Muslim world can place its faith in IAS for guidance in these matters of utmost urgency and in coping with the compulsions of a global economy warranting new initiatives and strategies for progress. Our government during the recent years has taken a number of bold initiatives to strengthen our education system and scientific and technological activities in Pakistan. It is my earnest hope that similar revolutionary measures would be adopted elsewhere in the Islamic world.

In the end, I feel greatly honoured to have this opportunity to share with you some of my thoughts briefly and feel confident that this conference will generate a number of new ideas. I wish you all success in your deliberations and hope that your stay in Islamabad would be enjoyable and productive.

Thank you ladies and gentlemen.

**Message* of
His Royal Highness Prince Al-Hassan Ibn Talal of
Jordan, Founding Patron of the
Islamic Academy of Sciences**

بِسْمِ اللَّهِ الرَّحْمَنِ الرَّحِيمِ
وَالصَّلَاةِ وَالسَّلَامِ عَلَى نَبِيِّهِ الْأَمِينِ
وَعَلَىٰ صَحْبِهِ وَآلِهِ أَجْمَعِينَ

**Ladies and Gentlemen,
Distinguished Colleagues**

The topic of this important conference - materials science and the culture of science - seems particularly appropriate for discussion in Islamabad, where the International Symposium on Advanced Materials took place, and where so much human history lies behind the newly-created city. Our many thanks go to the organisers and sponsors of the conference who have brought together this distinguished gathering of thinkers at a time when the world needs new approaches.

The phrase ‘culture of science’ derives from Latin words that might also be interpreted as ‘caring about knowledge.’ As such, it recalls the Greco-English word ‘philosophy’ - the love of wisdom. Yet, our advances in the culture of science do not correspond with any philosophy, which allows us to understand the human heart and head. There are many clever people in our world but, sadly, few wise ones. Without some overarching principle or guide for our pursuit of knowledge, what separates a ‘culture of science’ from a mere ‘cult of technology?’

Knowledge for its own sake has been offered as a guiding principle. The Europe of the Enlightenment did not only separate Church from State. It also separated scientific knowledge (gained by empirical observation) from religious or philosophical knowledge (gained through personal experience and contemplation of supernatural possibilities beyond the material world.)

* Delivered by Mr Moneef R. Zou’bi, Director General, Islamic Academy of Sciences.

European thinkers such as Auguste Comte* defined new humanitarian and scientific agenda by excluding religious thought from the field. This approach led to rapid and rewarding advances in scientific disciplines.

However, we see that these advances have not solved the problems of the world – hunger, violence, abuse of the weak and environmental degradation. The secular culture of science, and especially advances in materials science and technology, have given us the *means* to feed everybody, protect everybody, and live in harmony with nature; but they have not given us the *will* to achieve these aims, nor an understanding of why we fail to find the will. The desire to gain knowledge for its own sake is probably necessary to drive individual thinkers towards new findings; but it is not sufficient to direct those findings towards promoting the greater good and minimising evil.

Materials science promises a great many further material advances for some of humankind - maybe all of us. Perhaps it is the oldest and most familiar of scientific fields. Archaeology is largely devoted to finding and studying the results of earlier industries and technologies in this field. Our constant research into the properties of ceramics, alloys, polymers, crystals and compound materials is bound up with our earliest development as tool-makers. The basics of materials science are, from birth, an integral part of each human being's understanding of the world. So it deserves to be taught and learnt as a discipline truly directed towards human welfare.

In February 2001, Professor Pervez Hoodbhoy of Qaid-e-Azam University addressed the Annual Meeting of the American Association for the Advancement of Science. Professor Hoodbhoy spoke on the topic of science teaching as a subversive activity; and I quote:

“... Science by itself is not enough to liberate humankind and create a better world. But, without science there is little chance of this. For it to be socially progressive, it must not be reduced to a mere functional and utilitarian tool or to a set of arbitrary rules and an endless number of facts. Science teaching should inspire reflection and enhance our capacity to wonder.”

To inspire reflection and wonderment concerning Creation is surely not to be regarded as a subversive activity. The Holy Qur'an admonishes us repeatedly to observe the variety and diversity of the world that God created, to seek learning, and to educate others thoughtfully.

However, Professor Hoodbhoy was also delivering a warning – that:

“As the pace of scientific discovery accelerates, even college-educated individuals will find it harder to deal with a bewilderingly complex environment. The temptation to opt for the simplistic solutions offered by various faiths will grow.”

In other words, we face a paradox. In defining a culture of science, we seek some higher moral order that will direct our findings towards worthy ends. It

* A French philosopher (1798-1857), was the founder of Positivism, which is a philosophical system of thought maintaining that the goal of knowledge is simply to describe the phenomena experienced, not to question if it exists or not (Editors).

has long been the task of religious faith and institutions to educate and preserve that higher moral order. At the same time, we cannot presume to destroy the complexity of Creation and mankind in the name of reductionist religious theories, which describe the richness and variety of life as perversions. No one has a monopoly upon the truth.

Science and technology are activities carried out by human beings. They are full of values and value-judgments. These values in turn form new fields: bio-ethics and info-ethics are recent examples. Scientists and technologists carry great moral responsibilities not just for their fields of research but for all humanity - just as religious leaders also carry great moral responsibility, not only for their co-religionists but also for all people, including those of other religions and no religion. In this context it is worth mentioning the conference on 'Health and Social Justice' which was held in Amman, Jordan, from the 1st to the 3rd of October 2003 - which addressed such topics as the provision of medicines to the poor, tracking of disease, interfaith perspectives on social justice, and trauma. There has never been such a great need to find the common ground between science and religion - to discover their common goals of bettering the human condition. There is a great need to develop and respect a universal code of conduct towards a global ethic of human solidarity.

The United Nations Human Development Report for the Arab World is by now familiar to many here. The authors reported three critical deficits across the Arab World, which need to be addressed urgently: freedoms, women's empowerment, and knowledge. These needs were recently repeated in the Mediterranean Development Forum. We need, in the words of the UN report, 'rapid growth from a strong knowledge base ... the way forward involves tackling human capabilities and knowledge.' I believe that even materials science has more to do with human capabilities and knowledge than it has to do with materials. Politics and economics today are not delivering justice and freedom. People are turning to religious extremism in the effort to promote changes in an unbearable status quo. Where is science?

The Electronic Engineering Times reported recently that a US and Jordanian partnership is investing in a major fibre-optic link between Jordan and Lebanon. This is planned to be the first phase of a high-capacity network that will supplement global communication networks by linking the Eastern Mediterranean and the Red Sea. The existing networks between Europe and India are already near capacity but there is expected to be a major increase in traffic over the next few years; and, clearly, Jordan's free-trade agreement with the United States makes this sort of investment attractive to US companies. In other words, we are being linked together by projects dedicated to profit - but should we not be linked by concepts, which develop the complementarities not only between the land and its resources but also between the peoples of our lands?

The culture of science is threatened by poverty and deprivation - not least because science has not succeeded in giving us the political will to address these problems effectively. The will to tackle those problems can make a huge

difference with little resources, and greatly benefit future science. In Brazil, we know of the Bolsa-Escola project, which successfully tackled poverty and education problems by enabling children from poorer families to go to school. One percent of the federal district budget made it possible for more than 50,000 children to attend school - about 10% of the enrolled students in the federal district - and obtain improved academic records because of better care and nourishment. Among those fifty thousand, is it not likely that a handful will make good scientists if their education continues - is it not possible that one of them will introduce a breakthrough in materials science which could lead to new and better ways of life?

Here in Pakistan, Tasneem Siddiqui has described new approaches to the issue of *Katchi Abadis*, or squatter settlements, in the cities of Karachi, Hyderabad, Sukkur and Larkana. The rejuvenation of the Sindh *Katchi Abadis* authority, with a simplified process of leasing, decentralisation, transparency of information and measures to make leasing affordable, made the authority more workable and the lifestyle of *Katchi Abadi* inhabitants more regular. The authority continues to provide an invaluable service. I suggest that success was due to the application of a truly scientific approach - observing and questioning the prescribed traditional method in order to improve conditions on the ground.

Ladies and Gentlemen

Surely, this is the culture of science that we want, not a culture of science driven by a culture of violence - in which arms spending overwhelms humanitarian assistance. Great imagination and innovation are devoted to the development and sales of weapons of mass destruction. Is it not the task of scientists to devote just as much if not more energy and imagination to the promotion of the centrist ground and common human aspirations? Is it not possible to make use of pragmatism and logical positivism - our inheritance from Auguste Comte and his successors - as scientific tools for material research, without abandoning the notion of a higher reality to which the human soul belongs?

What information will new memory chips store? Will it be the traditional knowledge of indigenous peoples about plant medicines, for use in developing cures for disease - or will it be gigabytes of data on every individual's movements and habits, in a clampdown on the 'war against terror?' What shapes will the new 'smart metals' be taught to recall - important parts for agricultural and irrigation machinery, or important parts for heavy weaponry? Would the mass-production of buckminsterfullerene deliver us new materials for cheap housing, or reinforced war defences?

Two years ago now, the chief scientific advisor to the UK government, Sir Robert May, argued in a lecture entitled 'Science and Politics: Melding Facts and Values,' that:

"We need to start a new debate at the international level, listening and learning from the values of countries from North and South, East and West, and pooling scientific knowledge, with a view to achieving some consensus on the

problems that face us and how best they might be solved. We have a model in the form of the Intergovernmental Panel on Climate Change, which collates the expertise of over 3000 scientists from around 170 countries, to delineate a landscape of scientific knowledge *and* uncertainty ...”

As the Holy Qur’an exhorts us: “Let a group emerge from amongst you which calls for that which is good, orders whatever is right, and prohibits whatever is wrong.” Materials science holds out great hope for the future. It is the task of scientists to make sure some of that hope is delivered. Otherwise, our culture of science will not only decay into servitude under commerce and violence; it will come into terrible conflict with other modes of knowledge and other human truths. Scientists and religious leaders alike as human beings can cultivate a common ethic of centrist human values which will enable us to meet not only the material needs of people but also their non-material needs.

Thank you very much.

والسلام عليكم ورحمة الله وبركاته.

**Address of
His Excellency Prof. Abdel Salam Majali FIAS
President of the
Islamic Academy of Sciences**

بِسْمِ اللَّهِ الرَّحْمَنِ الرَّحِيمِ

**Your Excellency Mr Justice Sheikh Riaz Ahmed, Acting President of the
Islamic Republic of Pakistan,
Eminent Fellows of the Islamic Academy of Sciences,
Excellencies,
Ladies and Gentlemen**

السلام عليكم ورحمة الله وبركاته

The Islamic Academy of Sciences convenes again this year, upon the gracious invitation of Pakistan and the Pakistan Academy of Sciences, in a spirit of brotherly interaction to define a scientific outlook concerning important scientific themes that affect our lives, namely Materials Science and Technology and Culture of Science. We meet in Islamabad, this beautiful city of open boulevards and flower gardens, with the same determined spirit that the towering figures of our Islamic history had, ... to address issues important to our present and to our future.

At a time when the smoke of war, aggression and terrorism, is still smouldering all around us, and the dark clouds of confrontation hanging heavily over this part of the world, and over the Middle East, we are signalling, through our meeting, our unwavering determination to focus on bettering ourselves, on building a future for the generations of tomorrow, a future in which man would like for his fellow man what he would like for himself, a future in which our great Islamic civilisation would again occupy its rightful place amongst the elite, a bright future for us as Muslims and as human beings.

The array and calibre of foreign guests gathered in this room today reflect the profound admiration that the Islamic scientific community has for the Islamic Republic of Pakistan. I take this opportunity to acknowledge the support of our eminent Patron, H E President Musharraf, and of COMSTECH and the very active participation of Pakistani scientists, educators and thinkers in the activities of the IAS. Many disciplines have contributed to this co-operation and

therefore, in keeping with the Academy's desire, and the famous Muslim tradition to promote interdisciplinarity, I have chosen "technology and societal transformation" as the theme of my remarks to you today.

**Your Excellency
Ladies and Gentlemen**

Technological innovation sustains a fundamental tension between humanity's quest for control over nature and the future, and our equally strong desire for stability and predictability in the present. Throughout history, sceptics were not against technology *per se*, but rather against losing their jobs, and so they smashed the power looms that had put them out of work. This transformational process is central to the dynamic that is commonly labelled "progress," and being the source of continual destabilization and dislocation as experienced by individuals, communities, institutions, nations, and cultures.

As scientists hailing from Muslim lands, we know what progress means; we know that a single technological innovation can have marked change on the world. Our Islamic civilisation is amply endowed with examples of prolific scientific achievements that had an impact on life. Al-Khawarizmi's Algebraic theories to Al-Zahrawi's surgical techniques are good examples. Indeed from the very early days of Islam when simple science was put to serve the cause of *Aqeedah*, concepts rose of how technology and technological advancement affected our lives. It is this ideology that provided a most powerful source of inspiration, especially for Muslims' quest for knowledge.

Such historical narrative is reinforced from more recent happenings that the Western civilisation had lived through. Many examples point to the power of new technologies to transform society, but to the comprehensive interconnectedness of technological change – and the complex social structure of society. More familiarly, a single class of technology, namely, nuclear weapons was a central determinant of geopolitical evolution after the end of World War II. Cars, television, air conditioning, and vaccinations have all stimulated deep changes in society during the past century.

Of course, new technologies rarely emerge in isolation. The industrial revolution is a story of technological revolutions in transport, communication, construction, agriculture, resource extraction, and, of course, weapons development. These technological systems penetrated the innermost niches of society and forced them to change. They also introduced completely new social phenomena, and stimulated the invention of completely new institutions. This is of course true, fundamentally so, in the case of our *Ummah*, for our famous scientists, scholars and thinkers of the past really blossomed at times when the *Ummah* enjoyed unity, stability and clarity of role and vision, when justice prevailed, and when our profound *Aqeedah* was understood by all for what it really is....

Recent decades have witnessed significant changes in knowledge production systems, especially in scientific research and related applications. And more

changes in knowledge production and systems of research and development (R&D) are in motion. These changes are fuelled by the quickening pace of globalization and by new developments not only in information and communication technologies (ICTs) but also in biotechnology and the field of materials science and engineering including the exciting world of Nanotechnology, which are primary manifestations of transformational technologies.

For us as developing countries, the impact of transformational technology cannot be but extreme. Either we move toward a process of technology-supported societal progress where different sectors and activities can continually coevolve or develop in response to the growth of knowledge production at a breathtaking rate, or we can simply watch wave after wave of transformational technologies pass by us without undue regard! The choice is really ours, as it has always been.

We thus must ride these Information Technology, Biotechnology and Nanotechnology waves with confidence and determination. We must salvage some controls over the transformational powers of these technologies, and not stand idly by, to be left behind other countries.

Your Excellency Ladies and Gentlemen

The birth of Nanotechnology can perhaps be traced back to the marriage of science and technology beginning in the latter part of the nineteenth century, which accelerated the process of innovation, and thus the process of societal transformation. If the industrial revolution played itself out in less than 200 years, the electronics revolution seems likely to have a working life of perhaps 75 years. The biotechnology revolution – which we addressed at last year's Morocco conference - although hardly yet on its feet, is already prophesied to be supplanted by the nanotechnology revolution in the first half of the new century. What type of transformations might this revolution have in store? Maybe we cannot predict the future of nanotechnology and its impacts, but we may predict the direction and scale of thinking that will be necessary if we are to successfully manage the interaction of new knowledge and innovation with society.

Some futurists predict that the promise of nanotechnology to remake our life is virtually infinite. Nanotechnology is likely to revolutionize manufacturing, health care, travel, energy supply, food supply, and warfare. It is going, as well, to transform labour and the workplace, the medical system, the transportation and power infrastructure, the agricultural enterprise, and the military. Each one of these technology-dependent sectors is operated by and for human beings, who act within institutions and cultures, according to particular regulations, norms, all of which may reflect decades or even centuries of evolution and tradition. Not one of them will be "revolutionized" without significant

difficulty. The current chaos in many developing countries' health care system is a manifestation of this type of difficulty.

The current state of knowledge may suggest that the first wave of useful nanotechnologies will lie in the area of detection and sensing. The capacity to detect, precisely identify, and perhaps isolate single molecules, viruses, or other complex, nanoscale structures has broad application in such areas as medical diagnosis, forensics, defense, and environmental monitoring. The potential for direct benefits is obvious; how might this evolving capacity influence society?

When detection outpaces response capability, ethical and policy dilemmas inevitably arise. For example, it is already possible to identify genetic predisposition to certain diseases for which there are no known cures, or to diagnose congenital defects in fetuses for which the only cure is abortion. In the environmental realm, new technologies that detect pollutants at extremely low concentrations raise complex questions about risk thresholds and appropriate remediation standards. These dilemmas may be expected to accelerate and proliferate with the advance of nanodetection technologies. These dilemmas may be further compounded by the fact that nanotechnology offers a dizzying range of potential benefits for military applications, where some of the earliest applications of nanotechnology will come in the military realm, as specific needs are well-articulated and customers already exist.

Such considerations are simple extrapolations of current trends in technological innovation and societal transformation. The question of public response to nano-innovation, however, should not be avoided, even at this early stage. The ongoing experience of public opposition to new technologies such as genetically modified foods, and prospective technologies such as stem cell therapies, needs to be viewed as integral to the relationship between innovation and societal transformation.

Three observations are particularly relevant here, and may be proposed for the consideration of our eminent participants:

- (1) The impact of rapid technological innovation on people's lives;
- (2) In the short term at least, the social changes induced by new technologies usually create both winners and losers; and
- (3) Rapid technological change can threaten the social structure, economic stability, and spiritual meaning that people strive in their lives to achieve.

If we wanted to prepare for the transformational power of a coming nanotechnology revolution, we would need first to develop the knowledge and tools for more effectively connecting R&D inputs with desired societal outcomes. This would require the creation of a dedicated intellectual, analytical, and institutional capability focused on understanding the dynamics of the science-society interface and feeding back into the evolving nanotechnology enterprise. This is where I see the science academies of the *Ummah* including the Islamic Academy of Sciences playing a role. We need to start talking about humans and humanity again. When we talk about society, then we talk about the human being. His welfare, well-being, needs and aspirations, fears and

ambitions, longing for security and stability, and freedom to fully realize his potential and use his God given capabilities to cultivate and harvest the fruits of his efforts.

Again, I would say without hesitation that we as an *Ummah* have the *dormant* capacity to achieve our potential. To build a vibrant society quite adaptable to the societal change brought about by scientific advancement.

**Your Excellency
Eminent Scientists
Ladies and Gentlemen**

The new millennium echoes with the familiar cries of anger and violence. Indeed as Muslims, we hear that some circles in the American administration claim - rather unwisely - that they want to transform the Islamic world. To such people, I say that if we continue to depend on the rule of force, on power, as a deterrent, we will eventually be unable to disable violence. We – all of us in the East and the West - must become more sensitive to the concept of consequences: the consequences of poverty, illiteracy, lack of opportunity, despair and injustice, which can all lead to the contemplation of violence. Intolerance, prejudice and bigotry can also be seen as forms of illiteracy and ignorance, eroding social values, eating away at our humanity and stamping on our sense of ethical obligations and duties - to one another and to the world as a whole.

The events of the last year or so, on the international arena, have produced a flood of reactions that are directed against Islam, most of which are unjust, unrealistic and unjustified. Our mission now as the science leaders of the *Ummah* is to address the world and project our pride in our Islamic civilisation and what it has achieved and how it contributed to Western civilisations, for we belong to a civilisation that believes in dialogue. The divine message that is the core of our civilisation, and indeed our existence, promulgates respect for human life and human rights and most of all justice.

We must open up to the world and point out to despair generating conflicts in our midst. We must activate our goodwill-based bilateral interaction, and jump-start our transitional thinking, in our quest to achieve commodity and natural resource security and thus national security. We must bridge science divides, digital divides, and maybe more importantly, we must aim to bridge the hope divide.

I am confident that our meeting here will give our stand on this subject a considerable boost. I thank all of you for being part of this gathering, whether in the chair or from the floor, in a spirit of open-mindedness.

Thank you.

والسلام عليكم ورحمة الله وبركاته

**Address of
Dr A. Q. Khan
President of the Pakistan Academy of Sciences,
and Advisor to the Chief Executive of Pakistan on
Strategic Programmes and KRL Affairs**

Mr Justice Sheikh Riaz Ahmed, Acting President of the Islamic Republic of Pakistan;

Prof. Atta-ur-Rahman, Minister for Science and Technology, and Co-ordinator General COMSTECH;

Prof. Abdel Salam Majali, President of the Islamic Academy of Sciences; Excellencies;

Distinguished Delegates;

Ladies and Gentlemen

I am immensely pleased to welcome you all to the 12th IAS Science Conference. I am particularly grateful to Mr Justice Sheikh Riaz Ahmed, Acting President of the Islamic Republic of Pakistan, for gracing this important gathering. Your presence here today, Sir, bears testimony to your personal interest in the advancement of science and technology.

This science conference gives me an opportunity to elaborate a little on academies in general and the academies of sciences in particular. Historically, academies, way back in the Greek period and those during the heydays of Islamic domination of philosophy and the sciences, used to be more like educational centres and universities where pupils used to gather from across national boundaries to quench their thirst for knowledge. The Academies of Sciences of today exclude the functions that universities are better disposed to fulfil, and function as supreme scientific organizations devoted to the promotion of science and its applications for the general welfare of humanity. They provide a forum for popularisation of science, advancement of scientific research and motivate scientists and technologists to cooperate with fellow scientists the world over. These academies elect scientists of the highest merit as Fellows with outstanding contributions to the advancement of scientific knowledge.

The Islamic Academy of Sciences too stands to foster and nurture the aspirations of the *Ummah* for scientific progress. I was indeed elated when my offer during the 11th IAS Science Conference at Rabat last year was received favourably by the Fellows of the Academy. Needless to say that the Pakistan Academy of Sciences, Islamic Academy of Sciences and COMSTECH take

boundless pride in jointly hosting this conference in Islamabad. I am confident that our deliberations during the days to follow will be productive in paving the way for further fruitful cooperation among OIC countries with focus on the scientific and economic well-being of the Islamic world.

As we prepare to engage in deeper discussions on the specific themes of “Materials Science and Technology” and “Culture of Science” for which we have gathered here, allow me to say that much of the economic progress achieved by the developed world would not have been possible without progress in the field of science, and the innovations and discoveries that have resulted from its application. This has never been more true than today.

At the beginning of this millennium, we live in an age when rapid developments are taking place in the fields of human and animal genome, biotechnology, bioinformatics, information technology, materials sciences and environmental sciences as well as in other areas. Scientific knowledge is being gainfully applied in industry, and the epoch-making global information highways have become accessible at affordable communication costs. Achievements of a country in the vital field of science are not only a measure of its prosperity but also of its respectability in the community of nations. Possession of scientific knowledge also ensures the sovereignty of nations. Advancements in science are thus the inescapable road to progress and freedom. Having said this, it is a lamentable fact that the Islamic nation, where natural resources on hand are immensely vast, has the lowest rating in terms of the Technology Achievement Index developed by the UNDP. Pakistan itself ranks 65th amongst 102 countries of the world. Apparently, this position of the Islamic world is due, among other reasons, to persistent low priority to investment in science. Such an unsustainable trend needs to be vehemently checked and reversed. This is possible only by strengthening our universities as well as research and development organizations.

The Islamic Academy of Sciences, in collaboration with national academies of sciences within the *Ummah*, can act as a catalyst in guiding the Islamic world towards rapid economic growth. The Pakistan Academy of Sciences, the distinguished body of eminent scientists of Pakistan, was founded at Lahore in 1953. Since then, it has been contributing to national scientific planning and policy development, and has been interacting with international scientists and academies by holding seminars and conferences. The present IAS Conference provides another unique opportunity to the Fellows of our Academy to share and exchange views on scientific strategies that the *Ummah* must adopt to ensure economic prosperity for its people.

The current century confronts us with very difficult times. It is abundantly obvious that the present international push towards globalisation and trade liberalization are some of the driving forces behind the emergence of a new economic order. Recent advancements in information and communication technology are compelling nations at large to be ever more competitive in seeking shares in the global market. In a globalised economy, knowledge alone promises to raise productivity of capital through education, training of

manpower, technological developments and creation of management structures and organizations. Thus, knowledge is the engine that drives nations towards a prosperous future. As the *Ummah* nations seek to mobilize their social and economic systems to harness contributions from science and technology, there is a need to ensure a suitable S&T delivery system and an enabling environment. The challenge for our policy makers, thus, is to facilitate an environment that is conducive to the creation of scientific knowledge and its application for technological innovations. In the present day environment of stiff competition, partnerships must be created involving the public and private sectors in tandem with industry and academia. Research and development activities must be performed to meet market demands. Frameworks are needed to promote linkages among universities, engineering and technology institutions.

There is no denying the fact that there was a time in the remote past when the world turned for knowledge to Islamic Centres and Academies such as Al-Ghazali's Nizamiyah Academy at Baghdad in the 11th Century, while Europe was still desperately poor in comparison with the great civilizations of the East. However, I hasten to add here that instead of merely revelling in our glorious past, the task on hand is to work for institutionalising a culture and environment of science in the Islamic world. We are fully cognizant of the fact that the foundations of the present day Europe's wealth were laid down by industrial revolution. Its roots lay in a single philosophical idea, which today is called Science and Technology. Having consistently ignored the blandishments of western science beyond the 15th/16th centuries, the Islamic nations have fortunately started to at least absorb, though in a somewhat undigested form, the so-called blessings of modern science. While most nations continue to simply rely on imported S&T with little concern for innovation and self-reliance, there nevertheless are some lessons for the *Ummah* to learn from the experiences of countries such as Indonesia, Korea and Malaysia. The recent economic crisis faced by Indonesia had its origin in heavy dependence on foreign investment and multinational ventures, apart from other reasons. Immediate preventive measures, however, involving major focus on provision of training in basic sciences and technology are now beginning to bear fruit through stress on equipping the youth with scientific skills for dealing with complex technological demands of the agriculture and medical sectors, to name a few.

In this paradigm, basic sciences hold centre stage as the fountainhead for goal-oriented training and R&D. The university system is also rising to the occasion by offering guidance in scientific entrepreneurship for shouldering responsibility in times of crisis. The Indonesian crisis reminds us of the value of sound economic system, social justice, national security and national pride. Self-reliance, the very ingredient of inner strength, is by no means a narrow national goal that aims at protecting and developing the yet poorly exploited but abundant natural resources at the disposal of the *Ummah*.

A simultaneous look at the Korean miracle is no less an eye opener. Confronted with adversities, the Korean nation lost little time in launching a

Programme for Promotion of Science and Technology Development. Beginning in 1972, this programme encouraged the private sector to adapt and improve imported technology and to develop domestic technology through R&D effort. The Government freely provided appropriate incentives to R&D enterprises and industries. In 1977, it introduced follow-up steps by granting further financial incentives, made R&D activities mandatory for strategic industries, ensured protective measures to create demand for domestic technologies, and launched a movement for the popularisation of science and technology as an integral part of its economic development policies. The basic goal of this movement was the reorientation of the public's attitude and creation of a scientific environment in the country.

The Malaysian model too is a success story in its own right and a befitting indicator of how crises can be overcome, with resolve.

With these thoughts and without further testing the patience of this august gathering, I wish to simply express my hope that the eminent scientists participating in the conference will ponder and strive to develop strategies of scientific cooperation among the Islamic nations that would lead us towards self-reliance and sustainable economies in the Islamic community of nations.

In the end, I feel highly obliged to the Government of Pakistan, its various Ministries, specially the Ministry of Science & Technology, International bodies, national scientific organizations and private agencies for their unrestrained sponsorship, moral and financial support for the conference. Indeed the conference would not have been possible without the generous financial input from the Islamic Development Bank, COMSTECH, Dr A. Q. Khan Research Laboratories, Pakistan Atomic Energy Commission, Pakistan Science Foundation, Pakistan Council of Scientific and Industrial Research, COMSATS, Hamdard Foundation, Pakistan Agricultural Research Council, National Bank of Pakistan, Askari Bank Ltd and Habib Bank Ltd.

I also owe immensely to the local organizing committee, headed by Prof. M. D. Shami, for making all necessary arrangements for the conference. The hard work put in by Eng. Moneef R. Zou'bi, Director General, IAS, and his staff, to make this scientific event a success is indeed praiseworthy.

Lastly, I am confident that the eminent delegates would find their stay in Islamabad comfortable and enjoyable. Any inadvertent lapse of duty on our part may please be overlooked and excused.

Engineering Materials: The Driving Force of Technology in the Islamic World

A. Q. KHAN*

*President, Pakistan Academy of Sciences
Islamabad, Pakistan*

I consider it appropriate to open this keynote address by the words of Sir George Thompson, the Nobel Laureate, who said:

We have for some time labelled civilizations by the main materials they have used: The Stone Age, The Bronze Age, and The Iron Age. A civilization is both developed and limited by the materials at its disposal. Today, mankind lives on the boundary line of the Iron Age and a new Materials Age.

Curiosity and inventiveness are two of the fundamental defining characteristics of homo sapiens and these have driven civilizations through many transitions from The Stone Age to present time. Interestingly, anthropologists, historians and social scientists have chosen materials to define old and modern civilizations: we have had The Stone Age, The Bronze Age, The Iron Age, The Silicon Age, and the contemporary advanced Materials Age. Men and Materials are thus synonymous in the eyes of the intelligentsia and in the scheme of nature, if I may say so.

Around 1250 BC, corresponding to the Late Bronze Age and Early Iron Age in the Middle East, the Prophet Moses said:

*For the Lord your God is bringing you into a good land..... a land where the rocks are iron and you can dig copper out of the hills.
[Bible, Deuteronomy (8:7-9)].*

These biblical words spoken by Moses about the ‘promised land’ of Canaan are perhaps the oldest recorded statement underlying the strategic importance of materials to attain a significant competitive advantage and prosperity.

The importance of materials, especially that of Iron, is also highlighted in the holy Qur’an in Surah Al Hadid, Ayeh 25:

* Research Professor of Metallurgy, and Fellow of the Islamic Academy of Sciences.

We verily sent our messengers with clear proofs, and revealed to them the Scriptures and the Balance that mankind may observe right measure; and He revealed iron wherein is mighty power and many uses for mankind, and that Allah may know him who helped Him and His messengers, though unseen. Lo! Allah is Strong, Almighty.

The later part of the industrial revolution around 1800 AD was of great technological and economic importance owing to the emergence of steel, a new material at that time. The Silicon Age followed The Steel Age – silicon may be regarded as the steel of the semiconductor industry, and just as the steel enabled the industrial revolution to transform the developed world at that time, so silicon underpinned and enabled the information technology (IT) revolution to transform our present world. The developments of steels and semi-conducting materials illustrate the fact that Materials Science and Technology (MST) is a key enabling subject promising and producing new sets of products and industries that in turn have profound influence upon society. The Silicon Age perhaps represents the last age based on a single material. The Advanced Materials Age (AMA), covering a wide range of materials, has dawned with enormous potential for economic growth & development. It is significant that going from The Stone Age to the present day, each materials revolution has occurred more quickly than the previous. For example, The Iron Age took about 500 years to spread throughout the world. The industrial revolution took about 100 years to spread, but The Silicon Age took about 10 years to spread from the USA to Japan.

It is now recognized by most developed nations that materials research is of key national importance. For example, in 1990, Allan Bromley, the science advisor to President Bush Sr, said:

Materials Science is by far the most important subject in the USA.

The economic importance of materials research was discussed in a 1986 issue of Scientific American entirely devoted to materials. Let me quote from that issue:

Advanced materials are essential to the future growth of aerospace, electronic devices, automobile and other industries. Progress in Materials Science and Technology sets ultimate limits on the rate at which key sectors of the economy can grow.

The reason for the Age of Advanced Materials was neatly summarized in the same issue as follows:

A fundamental reversal in the relationship between human beings and materials is taking place. Its economic consequences are likely to be profound. Historically humans have adapted natural materials..... Recent advances have made it possible to start with a need and then develop a material to meet it, atom by atom.

Thus new and improved materials enable new technologies to develop, which results in new industries and an increase in national wealth and employment. Being man-made and not existing in nature characterize the new or advanced materials themselves. They are based upon our understanding of the physics and chemistry of materials. The vitality and the usefulness of the field of Advanced Materials are becoming evident everywhere. The award of prizes for fundamental advances in materials research by The Nobel Committee for three consecutive years – 1985, 1986 and 1987 – is a clear reflection of this recognition. A variety of Advanced Materials – rapidly solidified alloys, synthetic structured materials on modulated structures, nanocrystalline metals, superconductors, shape memory alloys – are emerging from laboratory curiosity status to new device applications. In short, success in translating advances in Materials Science and Engineering into new and improved materials is unparalleled. They are designed and tailor-made for specific needs and they are essential for economic growth.

Science-fiction-like inventions, like computers and robots, supersonic aircrafts and space shuttles, satellites, space communication and nuclear energy, represent super-sophisticated technologies which would not have been possible had metallurgists not invented new materials. Whether it is a sewing needle or a satellite, nothing can be made without a proper understanding of materials. Of all the 'M's viz, manpower, materials, machines, methods and money, involved in the industrial and technological development of a country, materials and how to shape and use them, is the most important factor.

The impact of new materials is absolute in every sphere of modern-day technology. Already, scientists all over the world are talking of the possibilities of replacing glass fibres in polymer matrix composites with natural fibres, which are renewable, cheap, abundant, recyclable, and safe to handle. Planners and scientists in the USA are eager to give fibreglass a try to replace about half of the 600,000 U.S. steel-concrete bridges that need repair. Fibreglass composite bridges could last four times longer than the previous material. The material costs roughly five times more, but they are five times lighter, faster to build, and possibly self-maintained, which means more economical overall.

Another dazzling achievement in the field of materials is the arrival of Nanomaterials. Regarded as a new class of materials with astounding properties and a truly universal set of potential applications, Nanomaterials are commonly defined as materials with an average grain size less than 100 nanometers (one billion nanometers equals one meter). The average width of a human hair is of the order of 100,000 nanometers and a single particle of smoke is of the order of 1,000 nanometers.

Nanomaterials are no longer a laboratory curiosity. This class of materials has now reached the initial stages of commercialisation and is fast emerging to take over world markets. In fact, there are now over 50 domestic companies in the USA alone involved in the production of nanocrystalline materials and many more looking to utilize these materials for market advantage. Present applications include ultraviolet absorption in high end cosmetics and sun block

creams, thin film coatings to increase the wear resistance of vinyl flooring and as catalysts in energy applications. These materials are revolutionizing the functionality of material systems. From multiple functionality to increased performance, nanomaterials are the face of modern materials technology.

The US Department of Commerce published a document in 1994, translated from an earlier work originally published by Japan's Economic Planning Agency, which summarizes 101 future technologies from 10 fields ranging from:

- Information and Electronics;
- New Materials;
- Life Sciences;
- Energy;
- Automation;
- Communication;
- Transportation;
- Space Utilization;
- Environment; and
- High Pressure Processed Food.

The New Materials list include:

- Superconducting materials;
- Ceramic gas turbine engines;
- Semiconductor super lattice elements;
- Amorphous alloys;
- Hydrogen occluded metal alloys;
- Magnetic materials;
- Organic non-linear photoconductive elements;
- Photochemical hole burning memory;
- Molecular devices;
- High performance composite materials; and
- Nanomaterials.

The global market size of these new materials is projected to be about 200 to 500 billion dollars by the year 2010. These technologies, it is believed, will have great impact on world economy from the late 1990s through the year 2010.

In order to plan for the future, an accurate assessment of the present is needed. It is surprisingly difficult to achieve this, given the prevalent apathy in the Muslim world. There are many amongst us who genuinely believe that there is nothing wrong with us and if there is, it will be set right by the divine power of *Allah* Almighty. There are others who, without denying the divine power of *Allah*, think that there are serious problems associated with the weaker knowledge and technology base of the Muslim world and that the situation is worsening rapidly.

As scientists, engineers, and intellectuals we are aware of the fact that, in addition to physical boundaries, there are also "technology boundaries" in our contemporary world, which separate technologically advanced countries from those knocking at the doors of technologies. Recent events suggest the emergence of religious ideological boundaries, adding another dimension to an already complex global situation. The Muslim world comprises 57 countries, has an approximate population of about 1.3 billion people living over about 27% of the total global territory. It is currently producing 60% of world crude oil, 40% of the natural gas, 80% of natural rubber, 75% of Jute, and 40% of various raw materials etc. The Muslim world, despite being the major provider of the world's most precious raw materials and other important resources, remains in the sidelines when the rest of the world, especially the industrialized and semi-industrialized nations, marches forward on the paths of development and progress. In the contemporary world of science & technology, where the rate of change of knowledge is phenomenal, the Muslim world is in a terrible state as it is stranded mostly in an outmoded knowledge base. Sadly, it is widely believed, especially in the prosperous countries of the Muslim world, that R&D should have a low priority because new materials developed in industrialized countries can always be procured. This thinking was valid twenty years ago but it is not true today - especially in the aftermath of the unfortunate event of September 11, 2001. The message for the Muslim world is thus very loud and clear:

The Muslim world cannot rely on even buying materials and materials expertise; it has to have its own materials expertise if it wants to survive honourably in the contemporary world. Unless the seed of R&D is planted today, the harvest of production and profits cannot be reaped tomorrow.

It is important for the Muslim world to have a strong Materials Science and Engineering research base in its technical universities over a wide range of new and improved materials if it is to survive and develop progressively in a competitive world. World-class scientists and engineers with vision must be provided with state-of-the-art equipment and literature in order to contribute towards the general welfare of Muslims in particular and the world community in general.

A substantial investment in materials research is essential to strengthen the industrial base in the Muslim world. Such investments should be directed to establish and upgrade existing R&D facilities and manufacturing plants. A pan-Islamic centre of excellence for advanced materials should be established through a materials research fund based on contributions from all the Islamic countries. Such contributions from each Muslim country should be roughly the same fraction of GDP as being spent currently by the industrialized nations.

From the foregoing it becomes evident that the multi-faceted process of overall development is driven by the engine of technology and more precisely

by the engine of materials and associated technologies. The Muslim world must also conduct a comprehensive materials research and technology assessment for the next decade. In the first instance we must have an initial recognition of Materials Science and Engineering as a distinct area of endeavour. Then we must work out our national goals – keeping in view our natural resources, energy and the environment, as well as defence – by dealing with materials issues related to strategic materials. The fruit for a successful implementation of advanced materials program in the Muslim world is nothing less than its economic survival, and a first step towards the revival of its past glory. The names of Abu al-Nasr al-Farabi, Ibn Sina (Avicenna), Ibn Rushd, Mohammad Bin Musa al-Khawarizmi, Mohammad Ibn Zakariya al-Razi, Adul Hasan Ali al-Masu'di, Abul Wafa Mohammad al-Buzjani, Abu Raihan al-Biruni, Nasir al-Din al-Tusi, Ibn-e-Tufail, Yaqub Ibn Ishaq al-Kindi, to mention only a few, reverberate through the ages.

I personally take great pride in acknowledging the fact that I have been trained in the field of Materials Science and Metallurgy and it was mainly because of my wide experience in the application of materials to nuclear and missile technology that I, together with my colleagues, guided the nuclear and missile programmes of Pakistan to successful completion in a very short span of time. Pakistan has been lucky to have a reasonably large number of scientists and engineers specializing in the field of materials science and metallurgy who are making invaluable contribution in the development of the country.

Before I conclude, I would like to quote the famous warning of Professor Alfred North Whitehead given almost a century ago to the western nations but which is now more appropriate for Islamic countries. If we do not pay heed to these prophetic words we are doomed forever.

In the conditions of modern life the rule is absolute: the race that does not value trained intelligence is doomed. Not all your heroism, not all your social charm, not all your wit, not all your victories on land or at sea, can move back the finger of fate. Today we maintain ourselves, tomorrow science will have moved over yet one more step and there will be no appeal from the judgment that will be pronounced – on the uneducated.

Prof. Alfred North Whitehead

Nuclear Techniques in the Study of Materials Science

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1 ABSTRACT

Material properties on micro and now on nano-scale have gained special importance in recent years both from the point of view of basic knowledge as well as from the point of view of economic and human utility. The physical and thermal properties of the same material turn out to be extremely different when these materials are used on micro and nano scale of physical dimensions. The improvement of strength of metals and alloys with decrease in grain size is very well known. The properties of heat resistance of fine particles as compared to bigger particle size of same material are also well known.

To investigate the properties of materials on micro and nano scale, the use of nuclear techniques has been extensively made, since the advent of the nuclear science. As the nuclear radiation and nuclear particles are dealt with at the smallness of atomic levels, the techniques used to study their properties are inherently dealing with materials at that small scale of dimensions. This lends a great importance to the use of nuclear techniques in the study of Materials Science and Technology.

2 INTRODUCTION

Today's high technology society is entirely dependent on the materials that have been developed and optimised. Materials science and engineering provides the key to future technologies, economic wealth and sustainable growth. They are also the keys to mastering many of the future challenges such as the development of new energy sources and pollution control. Because of these

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many aspects, materials scientists use a large number of experimental techniques.

Since the advent of nuclear science, nuclear methods have played a vital role in the study of materials. Material characterization is an essential aspect of material research and quality control in production processes, while chemical composition of the material is of paramount importance. Nuclear techniques such as neutron diffraction and scattering and reflection, neutron activation, gamma-ray scattering, radiation processing of materials, nuclear imaging, Mossbauer spectroscopy, and the recent techniques of synchrotron radiation and the applications of ions-beams have been found to present the basis for increasingly productive and more sensitive techniques than traditional methods.

Neutron scattering is playing an increasingly important role in materials technology. Neutrons being highly penetrating provide information on structure and dynamics of materials. Information obtained by neutrons is unique in the sense that it represents the bulk properties. Furthermore, neutron diffraction can give structural information that cannot be obtained with other techniques, for example, location of light atoms in the vicinity of heavy elements. Another distinct advantage of using neutrons is the study of magnetic properties of materials because of the fact that neutron has a magnetic moment and can thus have magnetic interaction. Neutron scattering is therefore a strong tool for investigating magnetic materials.

The neutron activation method is widely utilized for trace elements analysis to the sensitivity of parts per million and even parts per billion in a host material. The techniques of imaging with nuclear radiation have extensive applications for studies of defects in major components such as engines and turbine blades etc.

Ions beams from nuclear accelerators have been extensively used directly both for materials characterization and for materials modification. Mostly, the accelerator-based techniques such as Rutherford Back scattering, PIXE, PIGE and ERD are implemented for trace element analysis whereas Ion Implantation is used for modifying the properties of a given material. On the other hand, synchrotron radiation emitted from the high speed rotating electrons in the nuclear accelerators is being employed to explore sub-surface regions, interfaces, thin films, surface spectroscopy, microscopy and a host of surface physics investigations of materials.

The Mossbauer gamma-ray spectroscopy is being utilized for determination of micro-magnetic properties of materials such as determination of magnetic fields at the nucleus, investigation of isomer shift and quadruple splitting in materials and ionic properties in metals and alloys.

3 REACTOR BASED TECHNIQUES

3.1 Neutron scattering

3.1.1 General

The neutron is a subatomic particle with zero charge, mass 1.0087 atomic units, spin $\frac{1}{2}$, and magnetic moment $\mu_n = -1.9132$ nuclear magnetrons. Combination of these properties makes the neutron a unique probe of condensed matter. There are numerous aspects that make neutron scattering a valuable tool in material science.

Firstly, as the neutron has no charge it can penetrate deep into matter, thus the scattering depends on the bulk of the sample, and not merely on the surface properties. Measurements in special sample environment, for example, high-temperature furnaces, low-temperature cryostats and high-pressure cells can be performed. Secondly, the neutron energy and wavelength simultaneously match characteristic phonon energies and inter-atomic distances. Making neutron a principal tool for the study of crystal structure and lattice vibrational spectra of materials. Thirdly, due to its spin, when the neutron is scattered by a nucleus with non zero spin, the strength of the interaction depends on the relative orientation of the neutron and nuclear spins. This makes the neutron a unique probe of nuclear spin correlation and ordering at low temperatures. Finally, the neutron possesses a magnetic moment and interacts with the magnetic fields within the material. This makes neutron a unique probe of magnetic ordering in solids.

Utility of neutron has been demonstrated in a wide variety of applications. These range from conventional crystal structure and lattice dynamics to high resolution studies of atomic spacing in glasses and amorphous materials, biological structures, long chains polymers, defects in solids, phase transitions, magnetic structures, liquid crystals, ionic and colloidal solutions and protein crystallography. While its use in industries range from neutron radiography to microstructure determination, crystallographic phase determination, texture measurement, and residual stress measurement [1].

3.1.2 Neutron production

Although there are various ways for extraction of neutrons from the nucleus, only two produce sufficient intensity to be useful for neutron scattering research. First and most widely used method is the fission chain reaction of ^{235}U or ^{239}Pu . Second approach to neutron production is that used in spallation neutron sources.

Fission process in which the nucleus (of ^{235}U or ^{239}Pu) splits into two massive parts with the absorption of a slow neutron occurs in nuclear reactors. Each fission event produces approximately 2.5 neutrons. The neutrons produced by fission have a distribution of kinetic energies ranging from a maximum of about 14 MeV to almost zero. The peak of the distribution is about 0.8 MeV.

These fission neutrons are slowed in the moderator (typically H₂O or D₂O) through successive collisions to a Maxwellian distribution, which for room temperature peaks at about 60meV (1.2Å). Some of these thermal neutrons diffuse outward from the reactor core. The neutrons are transported from the reactor core to the experiment in evacuated or Helium filled beam tubes or neutron guide tubes. In order to shift the peak in the neutron spectrum to higher or lower energies, high temperature (hot source) or low-temperature (cold source) moderators can be placed in front of the beam tube near the reactor core. The most powerful of this type of neutron source in the world today is the 57 MW HFR (High-Flux Reactor) at the Institute Laue-Langevin (ILL) in Grenoble, France [2].

Spallation refers to the nuclear reactions which occurs when high-energy particles usually protons (500 to 800 MeV) collide with a heavy metal target. Particle accelerators and synchrotrons are used to generate intense, high-energy proton beam. Approximately 5 to 30 neutrons per proton are produced. These neutrons are moderated in a fashion similar to that of reactor neutrons. However, the proton beam is normally pulsed, leading to pulsed neutron production, and experiments are usually performed in the time-of-flight mode. The most powerful spallation neutron source in the world is the ISIS Facility near Oxford in the United Kingdom [3]. Figure 1 shows the historical development in the available thermal neutron fluxes projected up to year 2020.

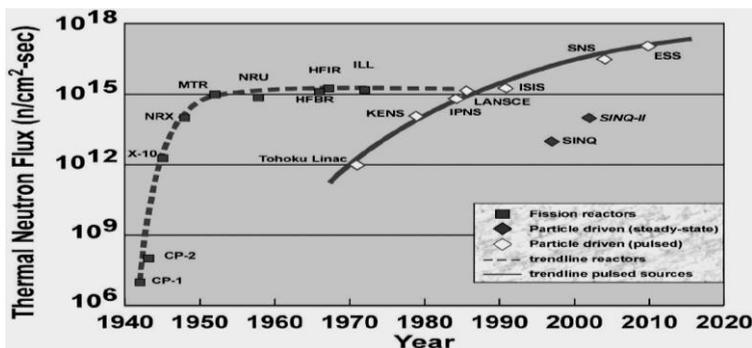


Figure 1. Year wise development in thermal neutron flux.

3.2 Neutron powder diffraction

3.2.1 Background

The fundamental equations governing neutron powder diffraction are essentially the same as for x-rays, except that the neutron scattering length b replaces the x-ray form factor f . The most fundamental difference between neutrons and x-rays is the mechanism by which it interacts with matter. X-rays are scattered by the electrons surrounding atomic nuclei, but neutrons are scattered by the nucleus itself. This single fact has several important consequences.

The scattering factor of nuclei for neutrons varies randomly across the periodic table (see Table 1). Consequently, contrast between nearby elements in

the periodic chart may be extremely good, and “light” atoms are almost always observable even in the presence of “very heavy” atoms, which would dominate in x-ray or electron scattering. The range of scattering amplitude for neutrons varies only by a factor of approximately 4 (with a few exceptions) compared to a factor of nearly 100 between hydrogen and uranium for x-rays. Thus, the neutron scattering length, b , for hydrogen ($b_H = -0.374 \times 10^{-12}$ cm) is a significant contributor in a neutron diffraction of Ta_2H [4], where $b_{Ta} = 0.691 \times 10^{-12}$ cm, but produces almost no measurable diffraction contribution of x-rays due to the presence of heavier Ta. Of particular importance for neutrons is the difference in scattering for isotopes of the same element because this permits scattering patterns to vary without changes in chemistry. This allows the extraction of partial scattering factors for each element, which is particularly useful for studying amorphous materials, but also has applications in crystalline systems. Some of the most important isotope effects are those for hydrogen ($b_H = -0.37 \times 10^{-12}$ cm, $b_D = +0.67 \times 10^{-12}$ cm), chlorine ($b_{35Cl} = 1.17 \times 10^{-12}$ cm, $b_{37Cl} = 0.31 \times 10^{-12}$ cm), and nickel ($b_{58Ni} = 1.44 \times 10^{-12}$ cm, $b_{60Ni} = 0.28 \times 10^{-12}$ cm), but many other elements show significant (if smaller) effects with isotopic substitution.

Table 1. Neutron scattering lengths and scattering cross-sections for some elements [5]

Atomic Nucleus	b_{coh} (fm)	σ_{coh} (barns)	σ_{inc} (barns)	σ_{abs} (barns)
1H	- 3.741	1.8	80.3	0.3
2D	+ 6.671	5.6	2.1	0.0
B	+ 5.304	3.5	1.7	767.0
C	+ 6.646	5.6	0.0	0.0
N	+ 9.362	11.0	0.5	1.9
O	+ 5.803	4.2	0.0	0.0
Na	+ 3.580	1.6	1.7	0.5
Si	+ 4.153	2.2	0.0	0.2
P	+ 5.131	3.3	0.0	0.2
S	+ 2.847	1.0	0.0	0.5
Cl	+ 9.577	11.5	5.3	33.5
Ti	- 3.438	1.5	2.9	6.1
V	- 0.382	0.0	5.1	5.1
Cd	+ 5.130	3.3	2.5	2520.5
Gd	+ 6.550	29.4	151.2	49700.1

The neutron form factor is essentially constant with diffraction angle, unlike those for x-ray or electron diffraction.

Peak shapes from steady-state neutron sources (reactors) are essentially Gaussian, and no complications due to the $K\alpha_1$, $K\alpha_2$ doublet are present as for x-rays. This makes peak fitting simpler and more accurate than in the x-ray case. The situation is more complicated for the spectrum of neutrons necessary for measurements made at pulsed neutron sources. Therefore more reliable structural information can be obtained from neutron diffraction data as compared to x-ray data.

3.2.2 Instrumental Aspects

Neutron powder diffraction is carried out in one of two modes: (1) a fixed-wavelength mode in which the scattering is observed as a function of angle 2θ or (2) a fixed-angle mode with the scattering observed as a function of wavelength λ . In principle, either method can be used with steady state or pulsed neutron sources. However, constant-wavelength data is the preferred method at the former, while constant-angle data are collected in the time-of-flight mode at pulsed neutron sources. For reactors, data are generally collected in Debye-Scherrer geometry with a highly collimated, monochromatic beam impinging on the sample from a Bragg reflecting monochromator crystal (Figure 2). With crystal monochromator, the resolution depends on collimation, the Bragg angle, and the mosaic spread of the monochromator [6]. Time-of-flight instruments generally utilize long distances between source and sample to give a large time spread between differing neutron wavelengths, which travel at different velocities. One advantage of pulsed-source compared to fixed-wavelength diffraction is that the resolution ($\Delta d/d$) is approximately constant with d -spacing (d being the distance between the lattice planes) which permits data collection to very small d -spacing ($<0.5\text{\AA}^{-1}$). This is further enhanced by the relative richness of short-wavelength neutrons available at pulsed neutron sources compared to reactors.

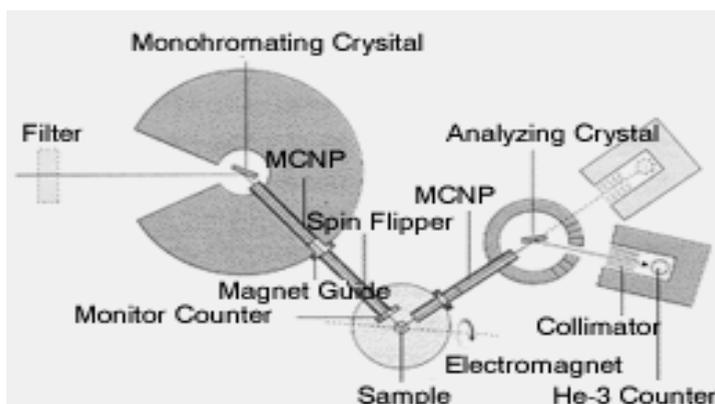


Figure 2. Schematic diagram of triple-axis neutron spectrometer.

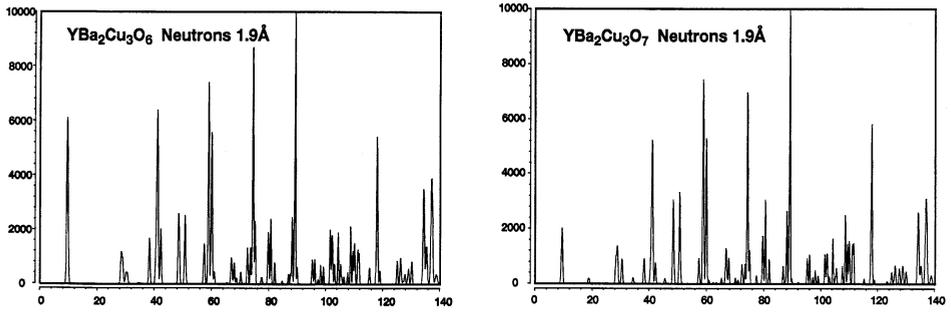


Figure 4. Neutron diffraction patterns of $\text{YBa}_2\text{Cu}_3\text{O}_6$ and $\text{YBa}_2\text{Cu}_3\text{O}_7$.

3.2.3.3 Lattice dynamics studies of mixed crystal $\text{K}_{0.5}\text{Rb}_{0.5}\text{I}$

The inelastic slow neutron scattering method has been extensively used to determine the frequencies of vibrations of atoms in a crystal lattice what is commonly known as lattice dynamics. Single crystals are often used on a particular type of neutron instrument known as Triple-axis neutron spectrometer. Slow neutrons from a research reactor are made mono-energetic through a single crystal monochromator. Such neutrons of wavelength of about $1\text{-}5\text{\AA}$ are scattering from the atoms of the mixed crystal $\text{K}_{0.5}\text{Rb}_{0.5}\text{I}$ under study. The wavelength (or energy) of the scattered neutrons is changed after interaction with the lattice vibrations (phonons). Measurement of energy changes of the scattered neutrons gives the frequencies of the lattice vibrations. The frequency spectrum as a function of the wave vector of the incident neutron is given in Figure 5 [13]. The lattice dynamics studies of materials are of practical use for reactor moderators in the fabrication of research and power reactors.

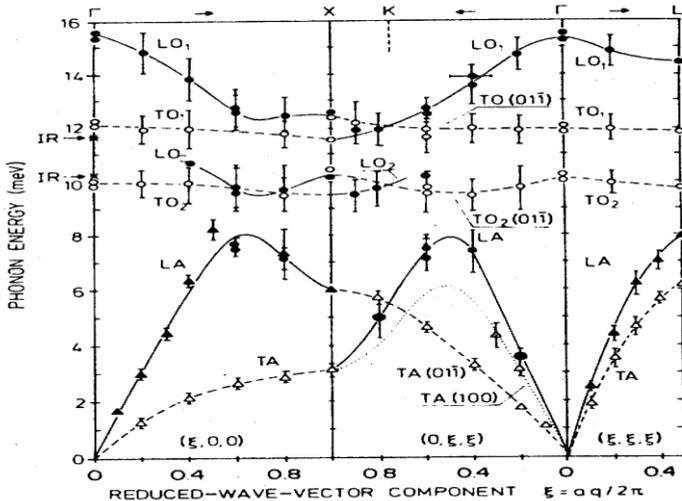


Figure 5. Phonons dispersion curves of $\text{K}_{0.5}\text{Rb}_{0.5}\text{I}$.

3.2.3.4 Thermal atomic displacement parameters B

Information about the temperature factor or the atomic displacement parameter is vital for a thorough understanding of the microscopic mechanism responsible for the structural and thermal properties of materials. This information can be obtained from x-ray or neutron scattering experiments [14]. In some cases, for example light elements in the vicinity of heavier ones, the information obtained by x-rays becomes unreliable. Rietveld refinement of high-resolution neutron diffraction data provides reliable information in such cases. Figure 6 shows the neutron diffraction pattern of SrO [15]. The vertical bars are the peak positions and the line at the bottom is the difference in the observed and calculated pattern. Rietveld refinement yields $B_{\text{Sr}} = 0.55 \text{ \AA}^2$ and $B_{\text{O}} = 0.60 \text{ \AA}^2$, while single crystal x-ray measurements [16] gives $B_{\text{Sr}} = 0.43 \text{ \AA}^2$ and $B_{\text{O}} = 1.93 \text{ \AA}^2$, which is anomalously large compared to the theoretical estimates [17]. Powder neutron diffraction is a powerful tool for such investigations.

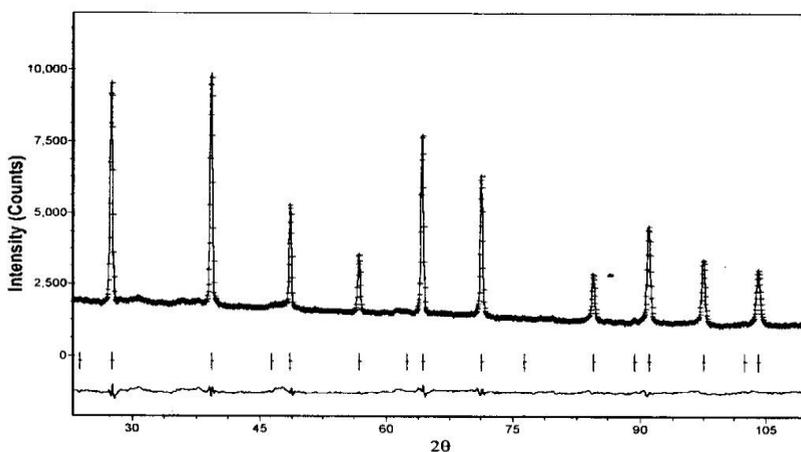


Figure 6. Observed (+) and calculated (-) neutron diffraction pattern of SrO.

3.2.3.5 Real time reaction kinetics

With the development of analysis programs capable of handling multi phase systems and data acquisition systems using position sensitive detectors on high flux neutron sources, it is now possible to study the real time chemical reaction kinetics using neutron diffraction techniques. Pioneering work was performed at ILL Grenoble, France [18]. Ca_3SiO_5 is a main component of ordinary Portland cement. In order to study the hydration process in cement Christensen and co-workers investigated the reaction of Ca_3SiO_5 with heavy water [19]. The results on the reaction are shown in Figure 7. As the reaction proceeds, diffraction peaks from $\text{Ca}(\text{OD})_2$ phase which is the only crystalline product, grows with time. Integrated intensity of the peaks from Ca_3SiO_5 and $\text{Ca}(\text{OD})_2$ as a function of time are shown in Figure 8.

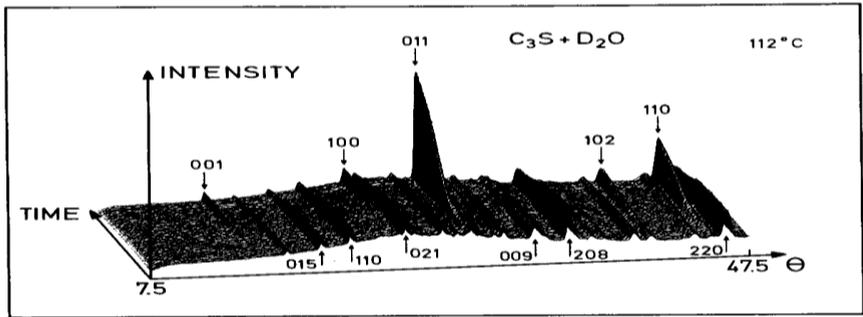


Figure 7. Time dependent neutron diffraction pattern of $\text{D}_2\text{O} + \text{Ca}_3\text{Si}$ at 112°C . Miller indices refer to CaSiO_5 (up) and Ca(OD)_2 (down).

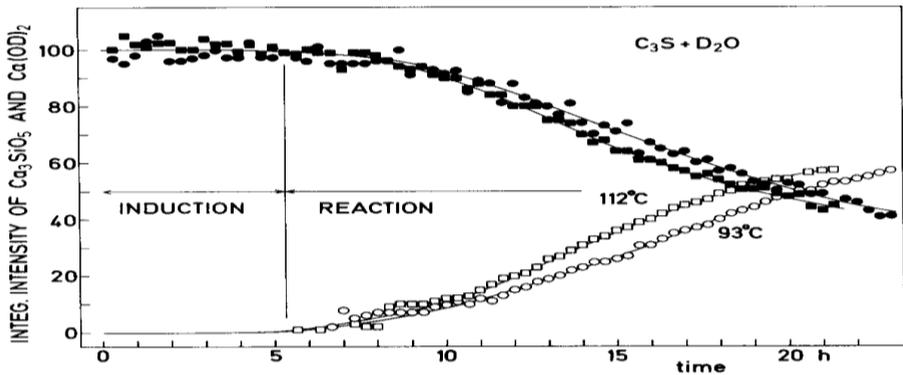


Figure 8. Integrated intensities of Ca_3SiO_5 (solid points) and Ca(OD)_2 (open points) with time for reaction of CaSiO_5 with D_2O at 93 and 112°C .

3.2.3.6 Characterization, authentication, and interpretation of manufacturing processes of metals

Materials change their microscopic structure as a result of mechanical or thermal treatments during manufacturing. This implies that a structural analysis by neutron diffraction may give valuable information about ancient production processes. This has been demonstrated [20] by TOF neutron diffraction analysis in the case of an Etruscan bronze olpe (Figure 9). The compositions of the bottom and the wall of the object were determined to be typical for classical bronzes with 90% copper and 10% tin.

Interestingly, a significant amount of lead was found in the handle, and a repair patch at the base of the vessel revealed a considerable degree of corrosion as indicated by the detection of a substantial amount of cuprites (copper oxide). Furthermore, from detailed analysis of the diffraction peak profiles it was possible to distinguish the underlying original bronze from the patch material, which is almost pure copper.

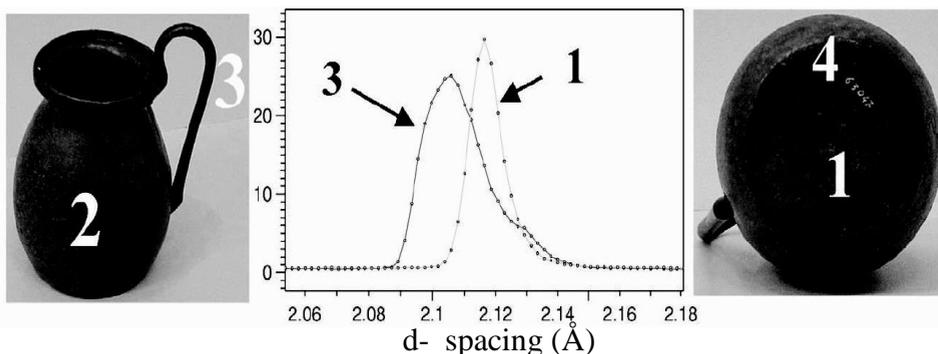


Figure 9. Etruscan bronze olpe and its TOF neutron diffraction patterns.

3.3 Neutron activation analysis (NAA)

Neutron activation analysis (NAA) involves irradiation of sample by neutrons followed by γ -spectroscopic measurements for determination of trace constituents in the sample. NAA is capable of non-destructive simultaneous multi-elemental analysis of trace level in various materials and provides detailed information about the elements in the sample. The neutron is captured by the nucleus of an element present in the sample and makes it radioactive, resulting in later decay through γ -ray activity, giving a γ -ray spectrum. Different γ -ray energies in the spectrum correspond to different elements in the sample while the varying intensities of the γ -ray peaks correspond to the relative amounts of various elements in the sample. Traces of parts per million impurities can easily be detected in main material by this powerful method.

The sample preparations involved are very simple and very small (typically 0.1 to few grams) sample in any form is required for complete analysis. Wide range of elements can be determined with the use of thermal, epithermal and fast neutrons [21]. As thermal neutron activation cross section for many elements is very high, therefore majority of the analysis is performed with thermal neutrons from the nuclear reactors. The intensity of a particular γ ray peak in the spectrum depends strongly on the half-life of its associated radioisotope and must be taken into account. At early time after neutron irradiation of a multi-element sample, the short-lived activities dominate the γ spectrum. Thus in true evaluation of complex samples, the γ spectrum must be recorded at several decay times to detect the full set of observable elements. Figures 10(a) and 10(b) show example of the changes that can occur in the γ -ray spectrum as a function of time [22].

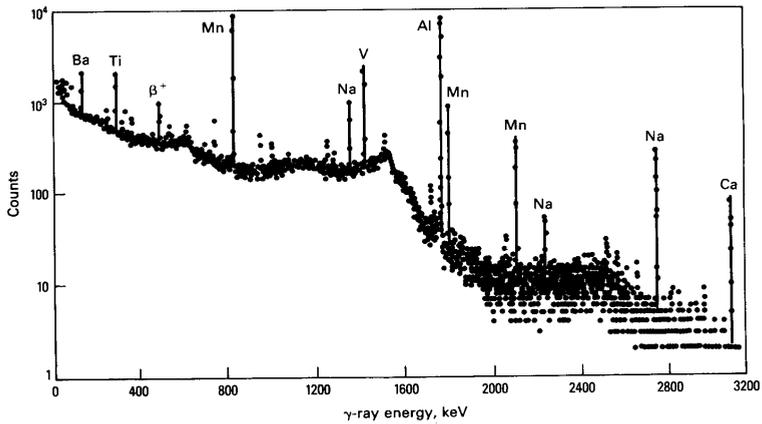


Figure 10(a). γ -ray spectrum of a neutron irradiated fly ash sample recorded 20 minutes after neutron irradiation.

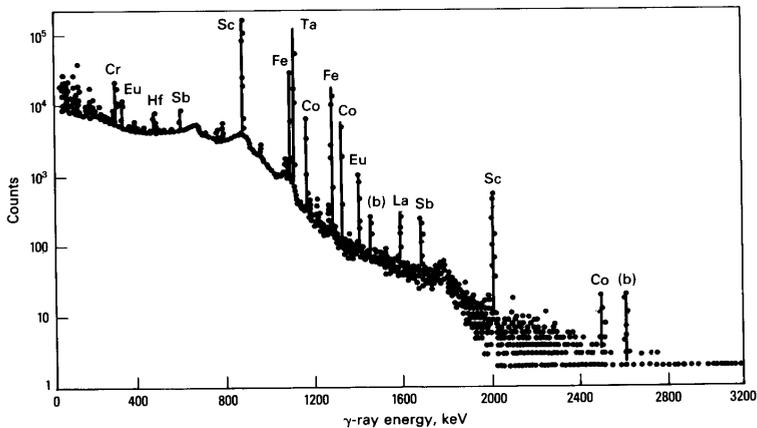


Figure 10(b). γ -ray spectrum of a neutron irradiated fly ash sample recorded 20 days after neutron irradiation.

3.4 Neutron Radiography

Neutron Radiography is an imaging technique, which provides images similar to x-ray radiography. The neutron beam penetrating a specimen is attenuated by the sample and detected by a two-dimensional imaging device. The imaging device can be a combination of a film and a neutron-sensitive converter foil, combination of a light-emitting scintillator screen with a CCD camera or neutron sensitive image plate. Schematic arrangement of a neutron radiography facility is shown in Figure 11.

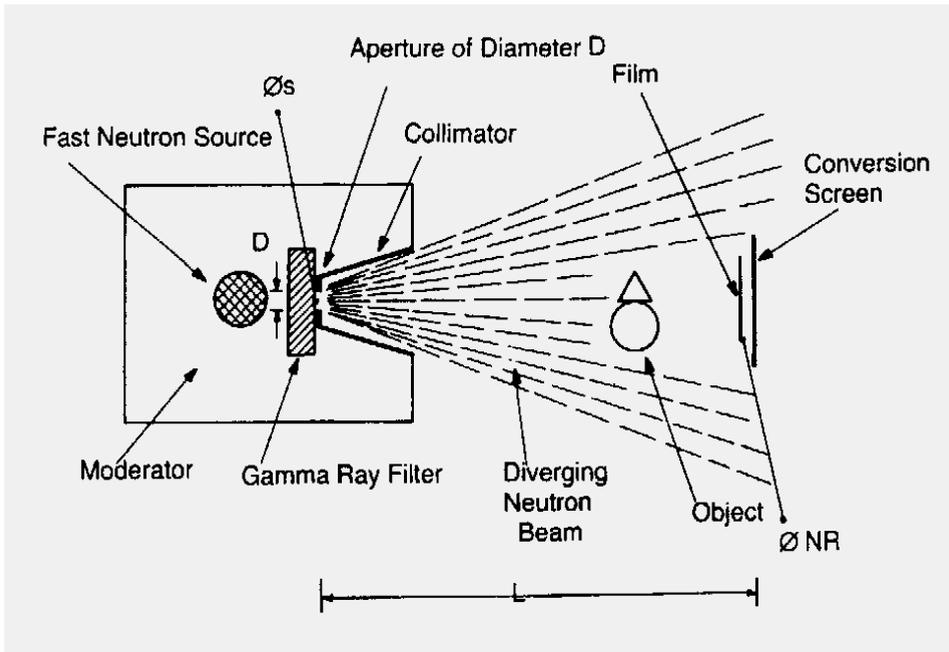


Figure 11. Schematic arrangement of a neutron radiography facility.

Macroscopic structure of the sample interior is represented by the radiographic image. The essential difference between x-ray and neutron radiograph is due to the mechanism by which they interact with matter. X-rays interact with electrons of the atom while the neutrons interact with the nucleus of the atom. Thus the density of the material dictates x-ray attenuation, while neutron attenuation depends on nuclear cross-section. Therefore many structural materials such as aluminum or steel are nearly transparent to neutrons while water and organic materials are clearly visible in neutron radiograph. Because of the deep penetration of neutrons in many structural materials it is well suited for imaging embedded features. Due to its ability to image hydrogenous materials, it is the main Non-Destructive Technique (NDT) used in quality control of explosive devices.

The following radiographs show some applications and demonstrate the difference between x-ray and neutron radiography. Figure 12 is the radiographic image of a camera, obtained both by x-rays and neutrons. Plastic parts, which are not visible in x-ray image, can clearly be seen in the neutron radiograph. Similarly Figure 13 shows radiographic image of a telephone set. Taking radiographs in different orientations, tomographic images can be formed. Figure 14 shows a tomographic image of an engine part.

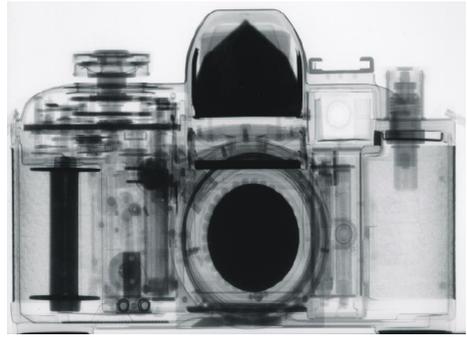
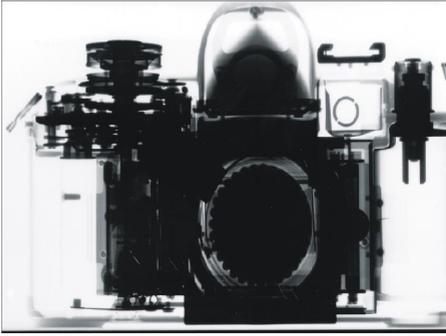


Figure 12. X-ray (left) and Neutron (right) radiographs of a camera.

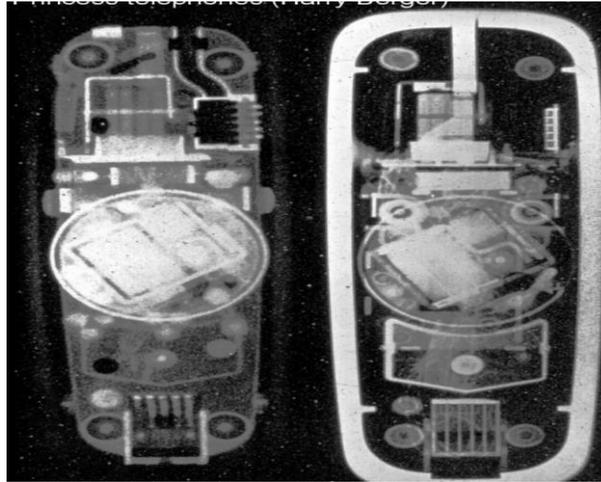


Figure 13. X-ray (right) and neutron radiographs of a telephone apparatus.

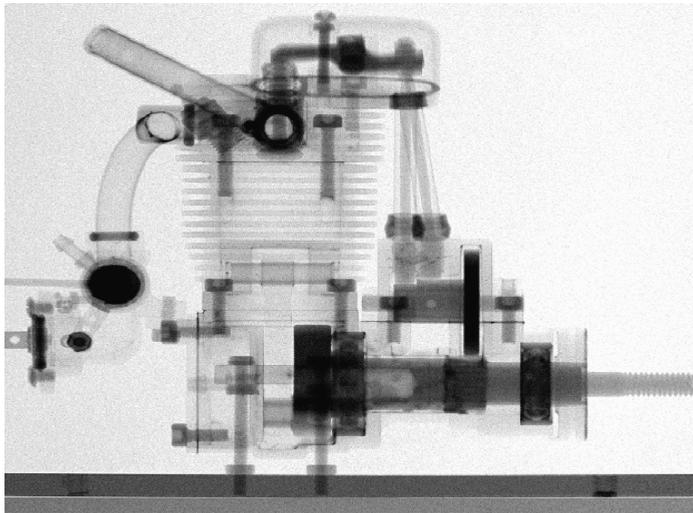


Figure 14. Neutron tomographic image of an engine part.

4 ACCELERATOR BASED ION BEAM METHODS

4.1 General

When ion beam passes through matter, radiation is emitted as a result of interaction of charged particles with the electrons or nuclei of the target atom. These emitted radiations are characteristic of the atomic number Z or atomic mass A of the target atom. Analysis of emitted radiation thus provides useful information about the target material. There are several such processes, which are being used for material characterization. Figure 15 depicts summary of such processes [23]. A brief description of these methods is given below.

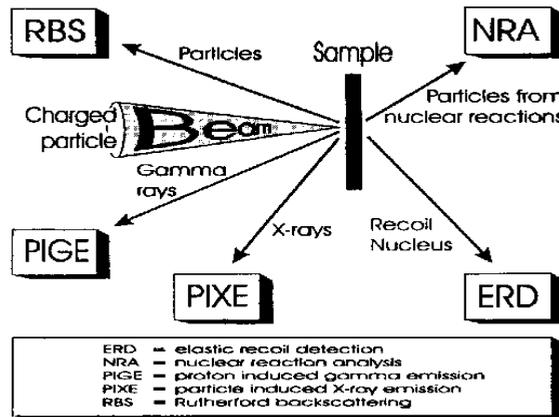


Figure 15. Possible processes by interaction of charged particles with matter.

4.2 Rutherford backscattering spectroscopy (RBS)

4.2.1 Background

Rutherford backscattering spectroscopy is a quantitative, non-destructive method to study the composition of thin films, layered structures or bulk materials [24]. This technique can provide information on surface impurities of heavy elements on substrates of lighter elements, defect distribution, depth profile and lattice locations of impurities in single crystals, and is mostly used to study thin films, ion implanted materials and the processes like diffusion.

RBS is based on two-body elastic collision kinematics. It involves measuring the number and energy of ions in a beam, which backscatter after collision with the atoms in the sample. Energy of the scattered particle determines the mass of the target atom while their number enables quantitative analysis of atomic composition. An incident ion loses energy in a medium through interactions with electrons. This energy loss depends on the elements in the sample and the

density of the sample material and allows RBS analysis to perceive depth distribution of masses, a process called depth profiling.

Basic equipment in RBS is a small accelerator capable of generating 2MeV helium ions, which after passing through a short drift tube enter the analysing magnet that selects ion species and energies for given experiment. After passing the magnet, the ion beam is directed to the sample. A small fraction of ions backscattered from the sample are detected and analysed using silicon surface barrier detector. A schematic sketch is shown in Figure 16.

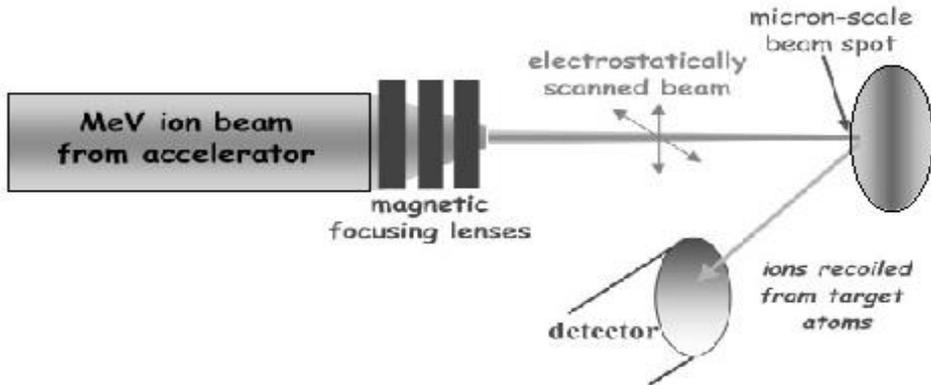


Figure 16. Schematic diagram for Rutherford back scattering (RBS) Spectroscopy.

4.2.2 Application

Impurity profiles

Depth profiles of heavy element impurities in a light substrate can be obtained easily using RBS. Figure 17 depicts RBS profiles of arsenic in silicon on three ion-implanted silicon samples, showing the energy spectrum of 2.0-MeV ^4He ions backscattered from a silicon sample implanted with 2×10^{15} As/cm² at 50, 150, and 250 keV. The peak positions are below the surface by an energy ΔE that corresponds to the projected range R_p of the arsenic distribution. The surface position of arsenic is defined by calculations or by scattering from a GaAs calibration sample. The full width at half maximum (FWHM) of the arsenic spectrum corresponds to a FWHM of a depth distribution after subtraction from detector resolution and energy straggling. A detailed analysis of this example is given in [25]. A substitutional portion of arsenic can be obtained by channelling process. Peak concentration can be obtained from the scattering cross-section ratio of arsenic to silicon and from comparing peak heights of arsenic to silicon.

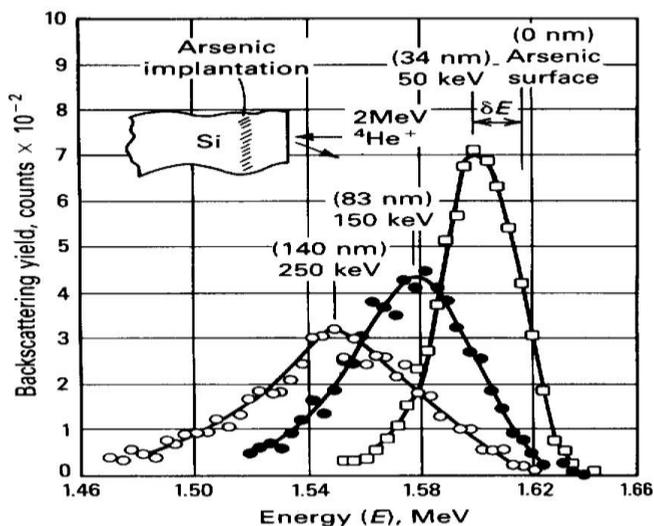


Figure 17. 2.0 MeV 4He RBS spectra of As implanted Silicon samples.

4.2.3 Particle induced x-ray emission (PIXE)

PIXE is an analytical technique capable of trace element detection in parts per million concentrations. When a charge particle moves through matter, it loses energy primarily by exciting electrons in the matter. Electrons in the inner shells (K and L), which gain enough energy, are ejected from their shells and vacancies are created. To fill these vacancies electrons from higher shells in the atom drop down. During this process an x-ray photon is emitted. The energies of these x-rays are characteristic of the elements and are used to identify elemental composition. While intensities of the characteristic x-ray lines determine concentration of elements All elements from $Z=11$ to 92 in a relative limit as low as $0.1\mu\text{g/g}$ can be quantified in a single analysis. Furthermore, PIXE with microbeams can provide information on lateral elemental distribution in the sample [23]. Proton beams of 1-2 MeV energy with $0.4\ \mu\text{m}$ diameter and 100 pA currents are normally used for PIXE. Schematic diagram of the PIXE system is shown in Figure 18.

The PIXE technique can be applied to a wide variety of materials, and has found many applications in geology, archaeology, biology, material science and environmental studies.

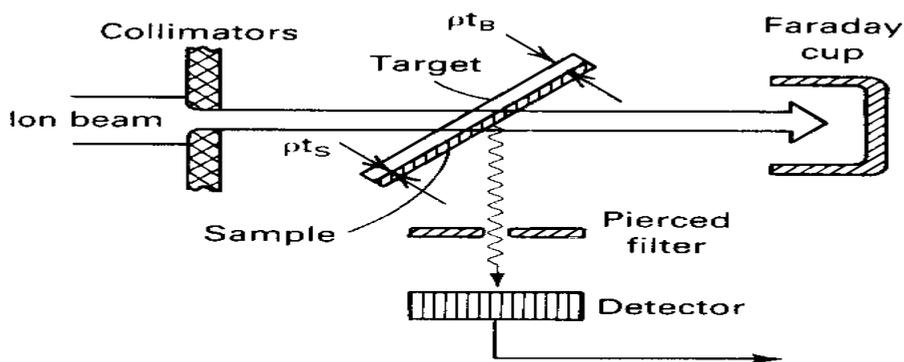


Figure 18. Schematic diagram for PIXE analysis.

4.2.4 Elastic recoil spectrometry (ERS)

When an ion beam incident on a sample, atoms lighter than the incident ions recoils in the forward direction and the resulting spectrum allows determination of concentration and depth profiling of these atoms. Normally few MeV ^4He ions are used for measurements of H and D profiles. Profiles of other lighter atoms like T, He, Li, B, C can be measured by using appropriate heavier ions. ERS provides a unique method for measuring the H and D content in thin films with detection limit ~ 0.01 at%. Because of the relatively small energy loss of H in solid, the depth resolution of this method is typically $\sim 300\text{-}600\text{\AA}$ [26]. ERS is also called elastic recoil detection (ERD) or forward recoil spectrometry (FRS).

4.3 Non-Rutherford backscattering spectrometry (n-RBS) (Nuclear resonance scattering)

In RBS one assumes a pure Coulomb process in which scattering occurs between two completely unscreened nuclear point charges. When the collision diameter is very small and becomes comparable to the sum of the nuclear radii of the projectile and the target atom, the finite sizes of the nuclei and the nuclear force interactions lead to deviations from the Rutherford scattering cross section. For MeV ion beams, this phenomenon can be observed in low Z projectile/target system where the Coulomb barrier is small. The cross-section for such nuclear resonance scattering can be many times greater than the Rutherford values. Non-Rutherford scattering has been used to some extent for the detection of light elements (C, N, O, Si) in heavy matrixes.

4.4 Nuclear reaction analysis (NRA)

When a charged particle of well-defined energy hits a nucleus in a target material, a variety of final products may form. These products depend on the specific combination of the ions and target nucleus. Thus by measuring the reaction products with good resolution, quantitative determination of the

concentration of specific nuclide can be obtained. Depth profiling of a specific nuclide can be achieved by recording the yield as a function of incident particle energy.

RBS is a special case of NRA in which the reaction products are the same as those before reaction. In cases where the incident beam energy exceeds a certain threshold value, other energetic particles appear in the spectrum. The detection of these particles usually provides information, which is not obtainable from RBS. The NRA technique is very useful as a tool for the detection and profiling of light elements in heavy matrix.

4.5 Ion channelling

When an ion beam is well aligned with a low index crystallographic direction of a single crystal, e.g $\langle 100 \rangle$ of Si, the incident ions can follow open channels by a succession of small angle scattering events and penetrate deep into the specimen before undergoing a large angle scattering event. The result is a $>95\%$ reduction in the yield of small impact parameter interaction processes, namely RBS, PIXE and NRA. Detailed theory and application of channelling in material science can be found in reference [27].

RBS and PIXE measurements in the channelling orientation are therefore, ideal for providing crystallographic information on radiation damages, crystal defects, impurity locations and strains in superlattice structures. This technique has been applied for the study of damage in ion-implanted crystals, lattice location of impurities in semiconductors, solid phase epitaxial regrowth of amorphous layers and to check the crystalline quality of epitaxial thin films.

Brief comparison of various ion beam methods is presented in Table 2.

Table 2. Comparison of various ion beam analysis methods

Technique	Elements detected	Depth Probed (mm)	Depth resolution (\AA)	Detection limit (at%)	Depth Profiling
RBS	B - U	1 - 2	20 - 200	1-10 ($Z < 20$) 10^{-2} - 10^{-3} ($Z > 70$)	Yes
PIXE	Al - U	Up to 10	Poor	10^{-4}	No
ERS	H, D	1	500	10^{-2}	Yes
Non-RBS	B, C, N, O, Si	Up to 10	200	0.1	Yes
NRA	H, B, C, N, O, F	Up to a few mm	500-1000	10^{-3} - 1	Yes
Channelling	B-U	1 - 2	20-200	10^{-4}	Yes

5 MOSSBAUER SPECTROSCOPY

5.1 General

Mossbauer spectroscopy is concerned with the phenomenon of nuclear gamma-rays resonant absorption and fluorescence, which was established and explained by R.L. Mossbauer [28]. The Mossbauer source is a radioactive isotope that decays into an excited state of the isotope under study, which returns to its ground state by the emission of a gamma ray or electrons. For example, ^{57}Co in Rh which decays to ^{57}Fe in its $I=5/2$ excited state is used to study ^{57}Fe . This decay scheme is shown in Figure 19. Source and absorbing nuclei must be incorporated in solid matrix, to make emission and absorption recoil free. The energy levels in the absorbing nuclei can be modified by their environment in three main ways, namely isomer shift, quadruple splitting and magnetic splitting. Oscillating the source results in shifting the energy of gamma rays (Doppler shift) which, when resonantly absorbed in the sample reduces the gamma ray count in the detector.

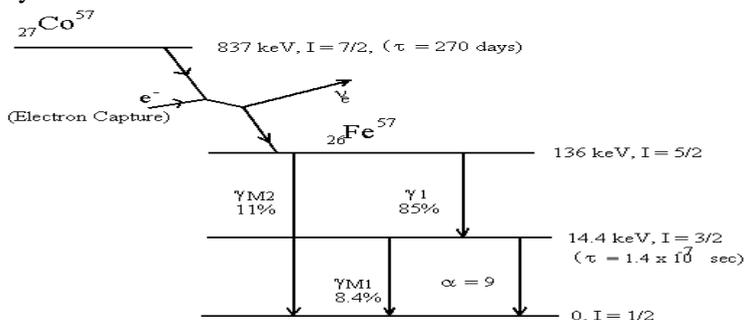


Figure 19. Decay scheme of ^{57}Co .

Mossbauer spectrometer (transmission geometry) consists of a Mossbauer source, a sample to be analysed, a master oscillator, which controls both the source velocity and the address of the active channel of the multi-channel analyser (MCA) and counting system with MCA. Schematic diagram of the Mossbauer spectrometer is shown in Figure 20.

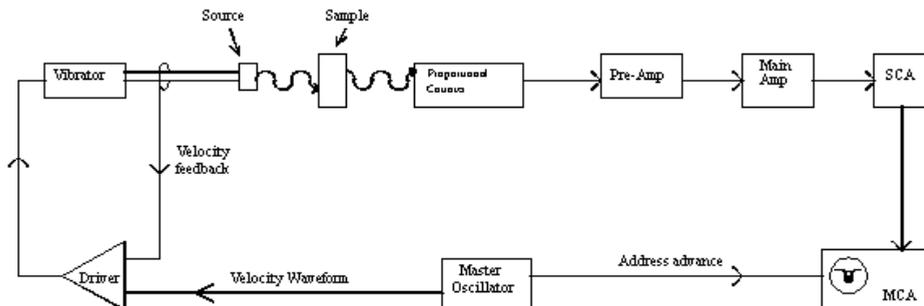


Figure 20. Schematic diagram of Mossbauer spectrometer.

5.2 Isomer shift

If the source and absorber differ chemically, due to difference in the electron densities at nuclear sites in the source and absorber, a shift is produced in the resonance energy of the transition atoms. This shifts the whole Mossbauer spectrum from relative zero velocity position, as is illustrated in Figure 21.

Isomer shift cannot be measured directly and is quoted relative to a known absorber. For example ^{57}Fe spectra is quoted relative to alpha-iron at room temperature.

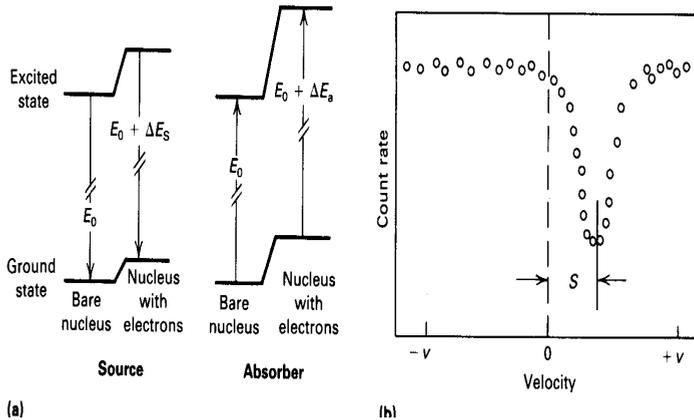


Figure 21. Illustration of isomer shift. The ground – and excited state energies are shifted by different in source and absorber (a), spectra from such situation (b).

5.3 Quadruple splitting

Nuclei in states with an angular momentum quantum number $I > 1/2$ has a non-spherical charge distribution, which produces nuclear quadrupole moment. The interaction of nuclear quadrupole moment with an asymmetric electronic charge distribution gives a splitting of nuclear energy levels. For example in ^{57}Fe , an isotope with $I=3/2$, the excited state is split into two substates as is shown in Figure 22.

This parameter offers an opportunity to detect variations in crystal structure, local atomic environment, lattice defects and conduction electron states. Further, angular dependence of the quadruple splitting can be used to determine the orientation of the spins in the structures.

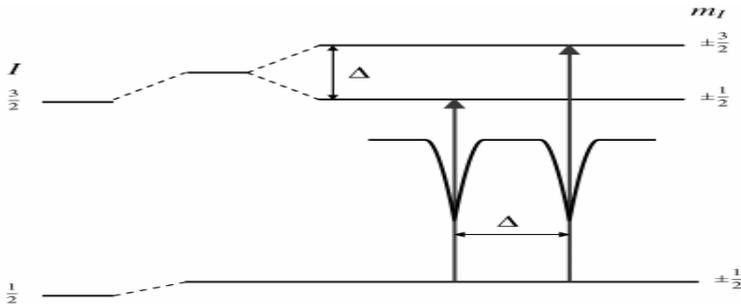


Figure 22. Illustration of quadruple splitting in ^{57}Fe .

5.4 Magnetic Splitting

The hyperfine interactions between the nuclear magnetic moment and a magnetic field at the nuclear site gives rise to the lifting of degeneracy of nuclear states with angular momentum quantum number I into $2I+1$. Transitions and relative line intensities for the familiar case of ^{57}Fe are given in Figure 23 and Figure 24. Ground state ^{57}Fe with $I=1/2$ splits into two and excited state $I=3/2$ splits into four substates. The line intensities are related to angle between the Mossbauer gamma ray and the nuclear spin moment.

This parameter is useful for phase identification in magnetic materials, magnetic phase transitions and for studying the local atomic environment.

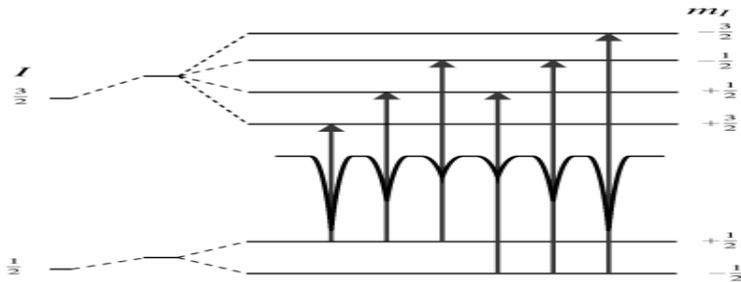


Figure 23. Illustration of magnetic splitting in ^{57}Fe .

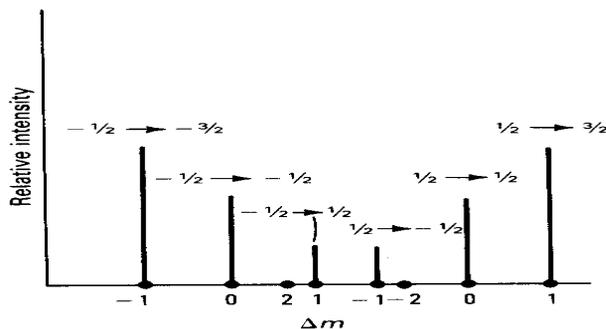


Figure 24. Relative line intensities for magnetic interactions in ^{57}Fe .

5.5 Applications

5.5.1 Mossbauer study of cation distribution in ferrites

Mossbauer spectroscopy is a very useful technique to study the cation distribution at tetrahedral/octahedral sites in ferrites. At PINSTECH we have studied the cation distribution in Zn-substituted $\text{Mn}_{1-x}\text{Zn}_x\text{Fe}_2\text{O}_4$ ferrites [29]. The variation in Mossbauer parameters indicates that the Zn^{2+} ions prefer tetrahedral site. It is also observed that Fe^{2+} ions show a sign of spin fluctuation for $x=0.50$ (Figure 25).

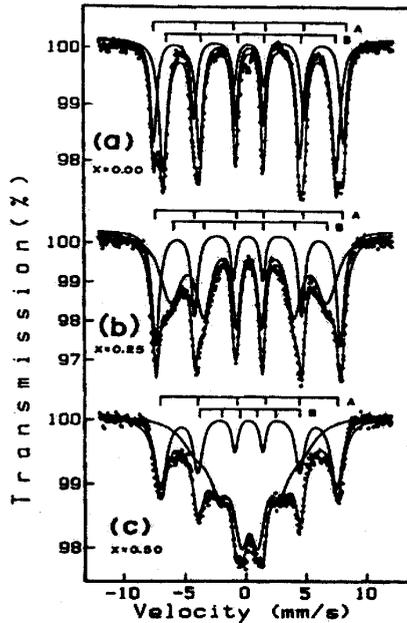


Figure 25. Mossbauer spectra of $\text{Mn}_{1-x}\text{Zn}_x\text{Fe}_2\text{O}_4$ for various concentrations (a) $x=0.00$, (b) $x=0.25$ and (c) $x=0.50$.

5.5.2 Phase transition in melt-spun alloys

Mossbauer effect technique is widely used to study the phase transition in melt-spun alloys. Mossbauer spectroscopy along with resistivity measurements is used to study the phase transition in $\text{Fe}_{88}\text{B}_{12}$ and $\text{Fe}_{72}\text{B}_{28}$ alloys [30]. O- Fe_3B and t- Fe_3B phases were found to be metastable and transferred into t- Fe_2B and Fe while t- Fe_2B was stable upto 825K (Figure 26).

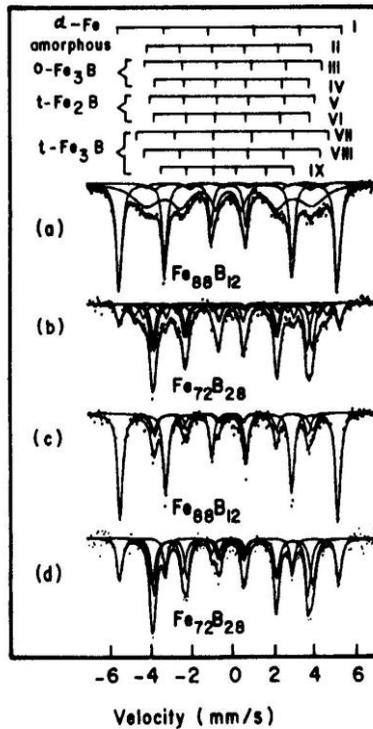


Figure 26. Mossbauer spectra of melt-spun $\text{Fe}_{88}\text{B}_{12}$ and $\text{Fe}_{88}\text{B}_{12}$ alloys, (a) and (b) as quenched, and (c) and (d) heat treated.

5.5.3 Hydrogen storage device

The intermediate compound TiFe has application as a hydrogen gas storage device. It forms TiFeH_x phases with the absorption of hydrogen. Mossbauer spectroscopy was used to study the phases formed [31]. Figure 27 shows the results of Mossbauer measurements for $x=0.1$, 0.9 and 1.7 . For $x=0.1$ (spectrum A) the spectrum has single peak of $\text{TiFeH}_{0.1}$, for $x=0.9$ (spectrum B) the spectrum is resolved into two phases while for $x=1.8$ (spectrum C) three different phases have been identified.

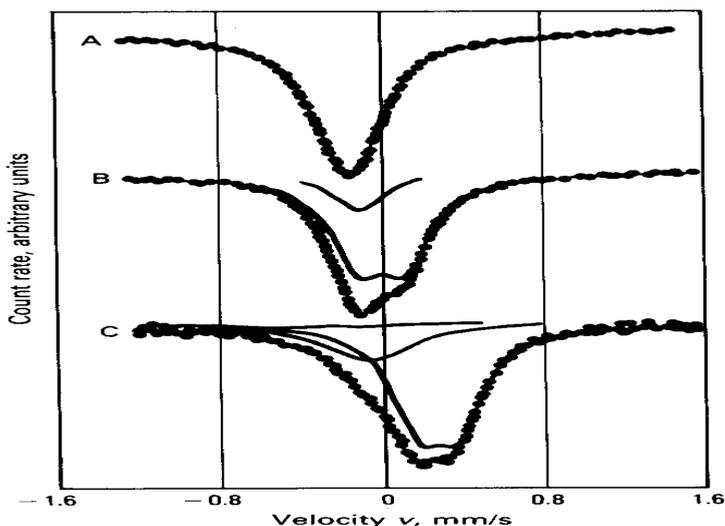


Figure 27. ^{57}Fe Mossbauer spectra for TiFeH_x for $x=0.1$ (A), 0.9 (B) and 1.7 (C)

5.5.4 Weathering of pyrite

From the data obtained from the spacecraft it is known that there is a reduced level of sulphur gases at the surface of Venus, and it is supposed, in particular, that this is connected with the chemical weathering of pyrite (FeS_2). A detailed experimental Mossbauer study [32] of the mechanism of the chemical weathering of pyrite under Venus surface conditions has shown that pyrite is unstable under on the Venus surface. The Mossbauer spectroscopy results are illustrated in Figure 28.

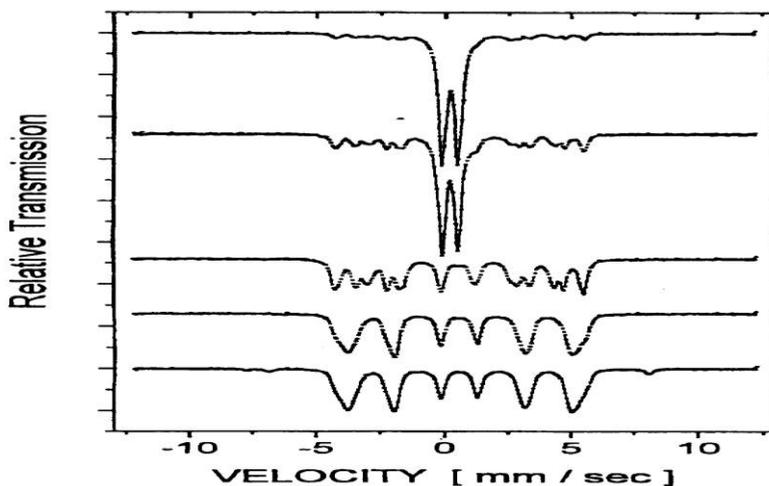


Figure 28. Mossbauer spectra of pyrite heated for 2.5, 8, 16, 43 and 97.5 hours (bottom to top) at 530°C isotherm.

6 SYNCHROTRON RADIATION (SR)

6.1 General

X-rays have been a powerful tool in research, industry and medicine. All aspects of x-ray research have been revolutionized by the use of high brightness synchrotron X-radiation.

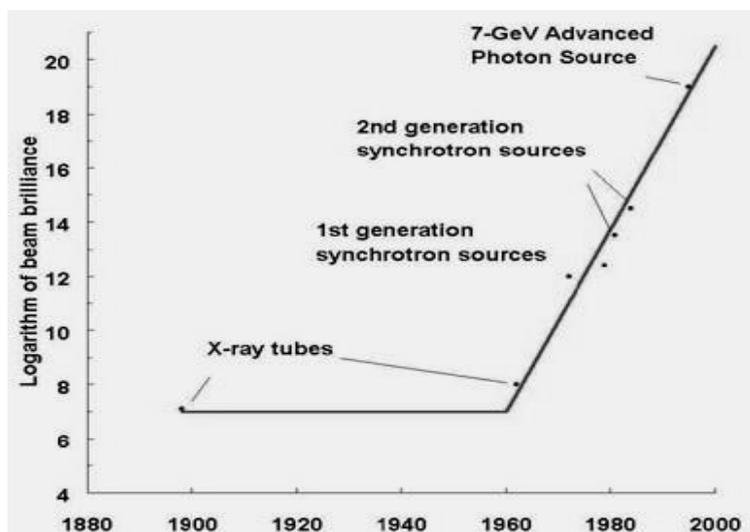


Figure 29. Year wise developments in the x-ray beam brightness.

Figure 29 above shows the rapid increase in the brightness of x-ray beams available for research, since the introduction of first synchrotron radiation facility at National Bureau of Standards Washington in 1961. First generation synchrotron sources were high-energy physics accelerators, where the synchrotron radiation was a by-product. The second generation of synchrotron radiation facilities, such as the Photon Factory in Japan, were constructed particularly to provide synchrotron x-rays for research. Recently a third generation of facilities is being completed, for example, the 7 GeV Advanced Photon Source in the USA, and are providing even higher brightness x-ray beams, about 10,000 times higher than those of the second generation.

When charged particles, in particular electrons or positrons, are forced to move in a circular orbit, photons are emitted. At relativistic velocities (when the particles are moving at close to the speed of light) these photons are emitted in a narrow cone in the forward direction, at a tangent to the orbit. In a high-energy electron or positron storage ring these photons are emitted with energies ranging from infrared to energetic (short wavelength) x-rays. This radiation is called Synchrotron Radiation. A schematic diagram of the synchrotron source is shown in Figure 30.

The synchrotron radiation has several unique properties that are being exploited in various applications. The electron storage ring produces extremely

intense, highly collimated, plane polarized pulses of white beam covering a wide range of energy upto the hard x-ray region. This higher intensity enables in finding the solution to the problems, which cannot be obtained through the use of conventional x-rays

The high brightness of the third generation source is ideally suited to microbeam and imaging applications, including x-ray microscopy, Fluorescence micro-analysis and micro-diffraction. For example, the fluorescence x-ray microprobes planned will have detection limits several orders of magnitude higher than current techniques (a few parts per billion for most elements) and a resolution of better than 0.1 microns. The environmental science, geophysics and medical physics communities will utilize these microbeam techniques. Soft x-ray microscopy offers a resolution of about 100 Angstroms and the ability to image wet biological samples. This is finding important applications in biology.

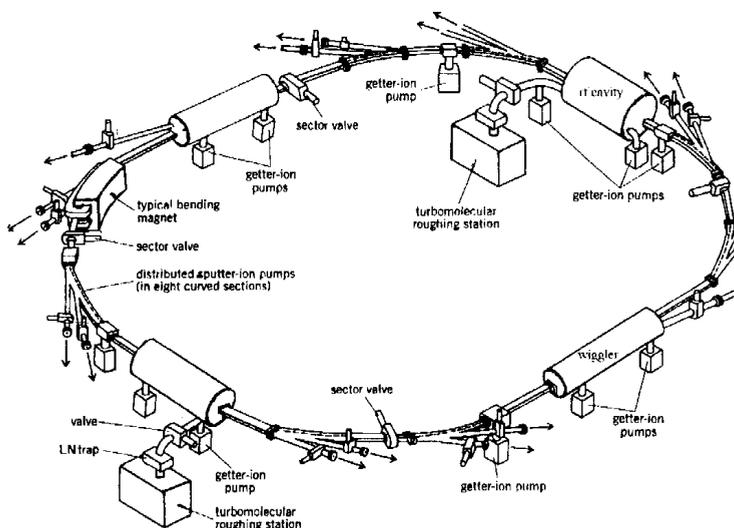


Figure 30. A typical synchrotron source with large number of beam ports.

6.2 Applications

6.2.1 Time-resolved diffraction studies

Time dependent processes can be studied using synchrotron radiation by collecting data in energy-dispersive mode. A typical example is the study of polymorphic phase transitions of sodium sulphate [33]. Sodium sulphate (Na_2SO_4) has five well-established modifications, which are designated as phases (I) to (V) and a rather complicated transition behaviour. There was a controversy in the literature concerning the presence of phase (IV) and how the various phases transform from one to the other [34-35]. Sodium sulphate sample was cooled from 500K at the rate of 15 degree per second, while the

PSD recorded consecutive diffraction patterns for every 200 ms. In this way fifteen patterns were collected in 3 seconds. The existence of the phase-IV at ambient pressure can be seen in the diffraction patterns (Figure 31). Na_2SO_4 -IV was found to be a short lived intermediate during the transition from phase -III to Phase -V.

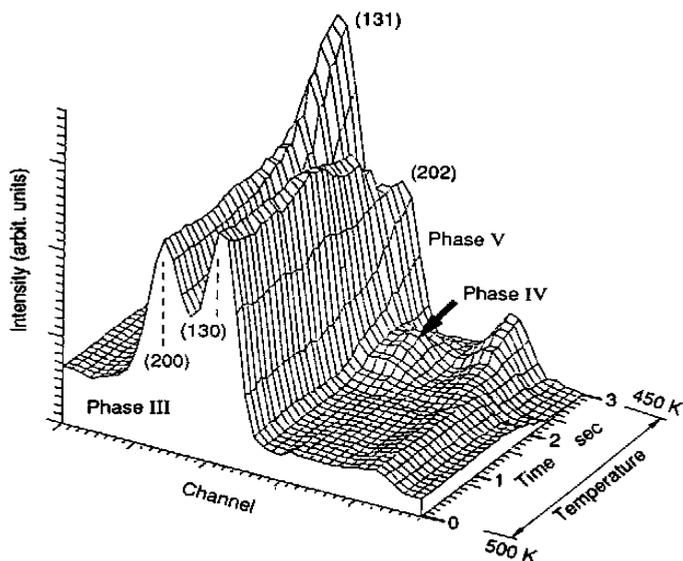


Figure 31. A sequence of Na_2SO_4 powder diffraction pattern.

6.2.2 Electron jump in solar cell materials

The jump of an electron occurring within the femtoseconds interval [36] was observed by one or two research groups in the world when they excite an electron from a dye molecule which sits on the upper surface of a nanocrystalline titanium compound which is a prime candidate for solar cell and memory devices.

The incident synchrotron light excites electron in the nitrogen so much that it jumps into the sub-layer beneath, thus causing a current flow. This electron must jump into titanium oxide sub-layer in less than 5 femtosecond otherwise it will be swallowed by another process and lost to the current. Such experiments are only possible with synchrotron light whose energy can be set to extreme accuracy. Figure 32 shows progress of such process.

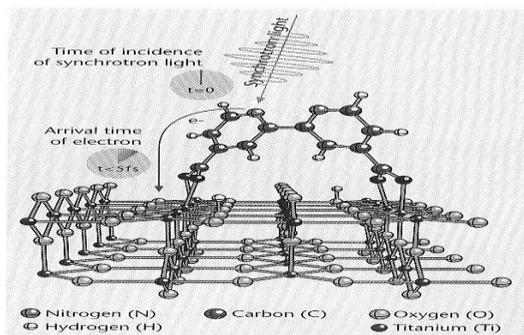


Figure 32. Progress of the electron jump in solar cell material.

6.2.3 Zero thermal expansion ceramics

ZrP_2O_7 is a ceramic material that is of interest because it has low thermal expansion over a wide temperature range, a property that is intrinsically linked to its particular crystalline structure. This is one of the most complex structures ever solved by powder diffraction, but it required the combination of five sets of data from neutron and x-ray diffraction and NMR [37]. High-resolution (synchrotron) x-ray diffraction gives information on the basic structural framework and accurate lattice parameters. Neutron diffraction is needed to give more precise information on the O positions and thermal parameters, which are of particular importance. However the refinements were not entirely satisfactory and the choice of space group was ambiguous. Three sets of NMR data were needed to unambiguously determine the space group, leading to an accurate solution and refinement of the crystal structure (Figure 33). This is an interesting example of using three techniques for complimentary approach to solve scientific problems.

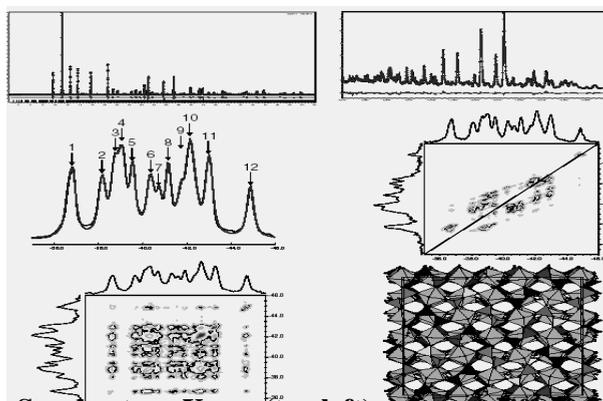


Figure 33. Synchrotron X-ray (top left), neutron diffraction (top right) and NMR spectra of ZrP_2O_7 .

7 ACKNOWLEDGEMENTS

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Development of Technologies for obtaining New Materials

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1 INTRODUCTION

At the Institute of Physics and Technology in Almaty (Kazakhstan), new technologies for obtaining advanced material have been successfully developed during the last few years. This is a short review of these technologies.

2 DEVELOPMENT OF A TECHNOLOGY OF SILICON PRODUCTION BY RECYCLING PHOSPHOROUS INDUSTRY WASTES

2.1 Process background

The most widely used silicon production processes are based on the purification of inexpensive but impure silicon, which is obtained in large quantities by carbothermal reduction of quartz, and on the production of pure silicon by the use of purified carbon and quartz in carbothermal reduction process. Another method of pure silicon production is a process of quartz sand reduction with aluminium in a slag medium based on alkaline earth metal silicates [USA patent № 4,457,903]. The slag thereby simultaneously serves as a solvent for the aluminium oxide that forms and as an extraction medium for impurities.

The electric furnace method of phosphorous production that is generally used in industry produces large quantities of slag, which predominantly consists of calcium silicate [1]. The phosphorous waste comprising the silicon dioxide, the alkaline earth metals, calcium, magnesium and other substances may be used as a raw material for silicon recovering by aluminium. This technology of silicon extraction from phosphorous industry wastes based on the aluminothermic processes has been tested experimentally in laboratory conditions.

A prominent feature of this new low-cost raw material - phosphorous industry slag - utilization technology is the extraction of intermediate silicon-contained alloy. This alloy is convenient both for further silicon cleaning and

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<http://www.sci.kz/~mukashev/Mukashev.html> (Editors).

for preparing highly reactive metal powder for silane synthesizing. [Preliminary patents of Kazakhstan: "A method of silicon obtaining" №. 4627 (1997) and "A method of silane obtaining" №. 4628 (1997)].

The technological stages of semiconductor silicon production by phosphorous industry wastes recycling are shown in Figure 1. The effectiveness of the chemical refining and silane synthesis depends on the initial input and the conditions of the aluothermic reduction process.

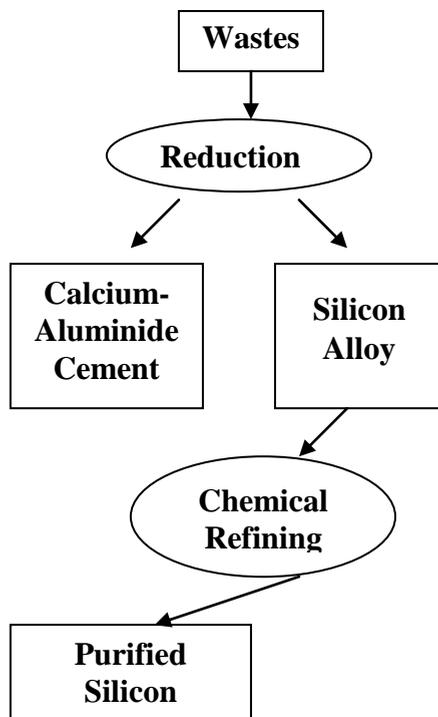


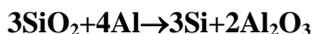
Figure 1. Main technological stages of silicon production from phosphorous wastes.

The phosphorous slag is a complex mixture with the composition shown in Table 1. Due to phosphorous production technological demands, the waste has a stable composition.

Table 1. Phosphorous industry wastes composition

№.	Component of the slag	Mass (%)
1.	SiO ₂	45-47
2.	CaO	43-45
3.	Al ₂ O ₃	3.2-3.6
4.	MgO	2.2-2.5
5.	P ₂ O ₅	0.8-1.3
6.	F ₂	2.2-3.0
7.	Fe ₂ O ₃	0.35-0.45
8.	MnO	0.1-0.5
9.	S	≈0.07

The phosphorous slag is introduced into a reaction vessel, which preferably is made of graphite and heated by induction. The presence of calcium and fluorine compounds decreases the melting temperature (down to 1200-1300°C) and reduces the viscosity of the slag. Then the commercially available granular aluminium of purity 99.86% is added to the molten slag and heated to reduce the silicon dioxide by the formation of aluminium oxide. The quantity of aluminium must be enough to provide complete reduction of the SiO₂ in the slag. Good results are obtained when the slag and aluminium are mixed in a proportion corresponding to the reaction:



The reaction is initiated at 1275°C, and subsequently the temperature rises due to exothermic nature of the reaction up to 2000°C.

Because of the exothermic nature of the reduction process, the reactor needs external heating only for slag melting and reaction initiation. This leads to considerable energy savings in comparison with regular carbothermic process.

When the reaction material has completely reacted, the produced metal and secondary slag are cast in the graphite moulds in which the cooling rate is relatively slow. The mixture of silicon and secondary slag can be easily separated, due to difference in densities, so that the slag begins to settle in the graphite mould. The silicon formed collects on the surface of the slag. Oxide impurities, which are formed as a result of reaction with atmospheric oxygen on the surface of the silicon, dissolve excellently in the surrounding slag. Therefore, it is possible to perform the process in an open system, with air being admitted.

Secondary slag is another valuable output product of the aluminothermic reduction, because this slag contains calcium-aluminate compounds suitable for production of high-quality cements.

The results of analyses of elemental and phase composition of silicon-contained alloy and secondary slag are given in Tables 2 and 3. It is seen that the silicon-contained alloy is Si-Ca-Al one with the typical composition Si (80%), Ca (8.4%) and Al (~3.5%). The composition varies depending upon reaction conditions: temperature, reaction rate, initial slag compositions. The secondary slag consists of calcium-aluminate compounds.

Table 2 Main components of the silicon-contained alloy and secondary slag. Results of chemical analyses

Alloy		Slag	
Element	Content (wt%)	Element	Content (wt%)
Si	80	Si	6.9
Ca	8.4	Ca	19
Al	3.5	Al	32.5

Table 3. Phase composition of the silicon-contained alloy and secondary slag. X-ray analyses of phases

Alloy		Slag	
Element	Content (wt%)	Element	Content (wt%)
Si	80	Ca ₂ Al ₂ SiO ₇	40-45
CaAl ₂ Si ₂	13	CaAl ₄ O ₇	40-45
CaSi ₂	7	Others	10-20

2.2 Chemical refining

As mentioned above, a metal obtained by aluminothermic method from phosphorous slag contains up to 10% Ca and that allows better purification of silicon [USA patent #4,539,194]. The ingots obtained after cooling are mechanically crushed. The size of the resulting clumps is not critical. Generally, good results are achieved with a size of few centimetres.

The silicon lumps are leached with a dilute inorganic acid such as, for example, hydrochloric acid, hydrofluoric acid, nitric acid or mixtures thereof. This leaching results in rapid cracking of the metal grains along the grain borders.

Leaching is carried out at a temperature ranging from room temperature to 80°C, generally employing acids in an aqueous solution at 2.5-10% concentration and ratios by weight between the acid solution and the silicon between 1.5 and 5.

The duration of leaching is an inverse function of the temperature and will usually range from 20 to 50 h.

After the unwanted impurities are dissolved, the solvent and dissolved fines of smaller particles of size 0.06mm are then decanted. The remaining material is screened on 1.0mm and must be thoroughly washed in distilled or ion exchanged water. As a result of such operations we have obtained the silicon powder with purity of 99.99% and higher.

Silicon powder characterization by using the mass spectrometry reveals that the concentrations of impurities are as follows: (element - Concentration):

Fe<0.2ppm; Al-40ppm; B-10ppm; P<0.5ppm; Mn<0.2ppm; Cu<0.3ppm; Cr<0.2ppm; Zr<0.2ppm; V<0.1ppm; Ti<6ppm; Ni<0.2ppm; Ca-70ppm; Mo<0.3ppm.

Other impurities levels are <0.1 ppm. The additional refining is possible by reactive gas blowing on the molten charge.

2.3 Czochralski grown crystals

Large-block polycrystalline silicon ingots with a resistance of about 0,05 - 0,1 Ohm-cm and a dislocation density of 10^3 - 10^4 cm⁻² have been grown from the

chemically refined silicon powder by using the Czochralski** method. Such material can be successfully used in photovoltaics. Preliminary experiments have shown that it is possible to decrease the concentration of boron to a level of 1 - 2 ppm by liquid extraction using calcium fluoride in the molten state. This additional refining is made possible by reactive gas blowing of the molten charge.

2.4 Silane production

A very interesting feature of the silicide alloy is the possibility of using it to synthesis high-purity monosilane by a simple chlorine free reaction using acids at temperatures from 20 to 90°C. Ibis process based upon silane chemistry is proposed as a simple low cost technology, which is an alternative to the Union Carbide process based on silicon chlorides. The rate of the silane synthesis and hence the output of silane depends upon the alloy chemical composition, which may be easily controlled by varying the parameters of the aluothermic reduction process. Experiments have shown that a yield of silane exceeding 50% can be achieved, which is significantly higher than the yield of 25 - 30% in the process of silane reduction from Mg_2Si [2].

2.5 Conclusion

A novel low cost, non-chlorine, environmentally benign technology for the production of photovoltaic grade polycrystalline silicon has been described. The process is based upon the aluothermic reduction of silica in waste products from the phosphorus industry. Preliminary experiments have shown that impurities, including boron, can be removed by chemical refining which provides opportunities for the production of large quantities of feedstock for the production of semiconductor grade silicon. However, further detailed studies of the process are necessary to optimise the processing parameters.

3 SYNTHESIS OF NANOCCLUSERS IN SILICON

Hydrogen is a very mobile and chemical active impurity in silicon that lead to a number of phenomena pertaining to the interaction of hydrogen with defects and impurities [3,4]. As a result of the interaction, hydrogen-containing complexes are formed. Complexes of hydrogen with III acceptors and V donors [3,4], metals [5], oxygen [6,7], carbon [8] and other impurity atoms and radiation defects were discovered and identified. In many cases the interaction with hydrogen leads to the passivation of electrical activity of defects. Both donor and acceptor impurities may be passivated because hydrogen can act as a donor when it is located in the bond-cantered (BC) position, as well as an

** http://www.tf.uni-kiel.de/matwis/amat/elmat_en/kap_5/advanced/t5_1_4.html
(Editors).

acceptor in the T_d interstitial state [9]. As a result of hydrogen-impurity interaction, neutral donor-acceptor pairs with no levels in the gap are formed. The passivation of defects is secured by the ability of hydrogen to saturate dangling bonds.

Moreover, the hydrogen atoms may not be incorporated in a defect directly but can control significantly all defect- and impurity-related processes. For example, hydrogen enhances the oxygen diffusion and precipitation in silicon. This enhancing can be accounted for by the formation of metastable hydrogen-oxygen centre that has low energy barrier for migration (~ 1.6 eV) in comparison with interstitial oxygen (~ 2.55 eV). Therefore, the presence of hydrogen may change the character of precipitation processes in a supersaturated solution of impurity or defect and hydrogen can induce the formation of defect nanoclusters.

Samples of silicon were prepared from high-purity, float-zone refined (FZ) silicon ingot with resistance of $\sim 3000 \Omega \times \text{cm}$, Czochralski-grown silicon samples (Cz-Si) with resistance of $\sim 1-10 \Omega \times \text{cm}$ and FZ silicon doped with 5×10^{16} aluminium/ cm^3 . Several different ways were used to introduce the hydrogen into samples. First, samples were implanted with 30 MeV protons. Using of 4 mm thick aluminium absorber led to the distribution of hydrogen within the 100 μm thick layer under the surface of samples. To introduce hydrogen more homogeneously, additional 50-200 μm thick aluminium absorbers were used. Typical hydrogen concentration was $\sim 10^{17}$ H/ cm^3 after 80 K implantation and $\sim 10^{18}$ H/ cm^3 after 300 K implantation. Secondly, thermal annealing of samples at 1250°C for 30-60 min in sealed quartz ampoule containing $\sim 10^{-3}$ ml of distilled water was applied to introduce hydrogen homogeneously up to a concentration of 10^{16} H/ cm^3 . To introduce hydrogen skin-deep, the treatment in hydrogen plasma at 100-250°C was used. Radiation defects were introduced by the irradiation with protons (or α -particles) without absorber. In this case, hydrogen implantation into the bulk of the samples was completely avoided, since the 30 MeV proton range in silicon is ~ 4.5 mm, while the thickness of the sample was 0.3-0.5 mm. Thus, only radiation defects were introduced.

The presence of hydrogen atoms in silicon changes considerably the character of impurity and defect related processes and leads to the formation of vacancy-related, interstitial-related and impurity clusters.

The vacancy-related extended Si-AA17 centre observed by EPR in hydrogen-implanted silicon is characterized by two silicon atoms with dangling bonds positioned at $\sim 12 \text{ \AA}$ interval along a $\langle 111 \rangle$ axis (Figure 2). The dangling bonds are probably formed due to lattice relaxation created by large vacancy defect (hexavacancy) disposed in the centre of the complex. IR data demonstrate that there are extended defects composed of several SiH_2 fragments; the most likely model of the defect is completely passivated hexavacancy Si_6H_{12} . DLTS results show that effective traps of interstitial atoms

are introduced by hydrogen plasma treatment at 230°C. The $\langle 111 \rangle$ oriented platelets may play the role of these interstitial traps.

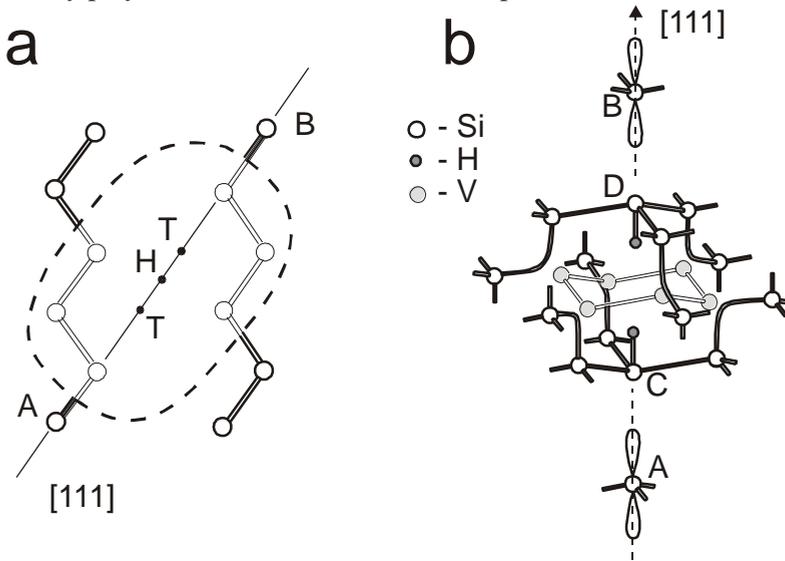


Figure 2. (a) Structure of Si-AA17 EPR centre determinate from experimental data. Two paramagnetic electrons are localized on A and B atoms. A vacancy-related defect is situated in the area delineated; (b) Tentative model of Si-AA17 centre.

When hydrogen-implanted silicon is annealed at 300-450°C, the precipitation of hydrogen and its interaction with intrinsic defects lead to the formation of interstitial-related clusters (Figure 3). Electron structures of the clusters and oxygen thermal donors are very similar, but oxygen is not required to form the interstitial clusters, whereas the role of hydrogen is determinant. Hydrogen may be incorporated at least into the clusters, which have shallow donor levels and also can be a catalyst of extended interstitial defect formation.

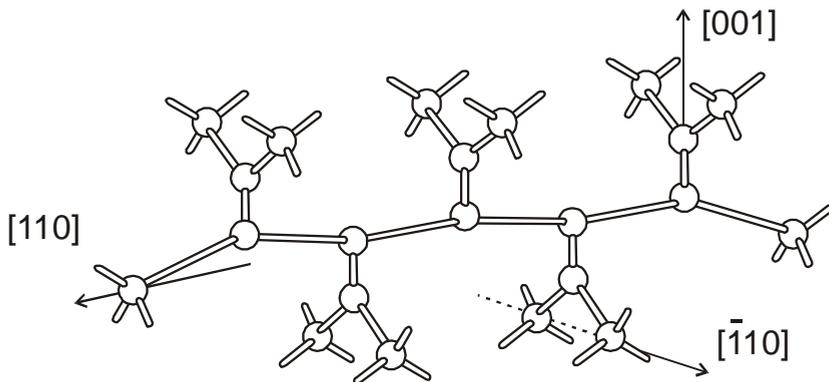


Figure 3. Possible model of the interstitial cluster in silicon.

The presence of hydrogen leads to enhanced diffusion of oxygen in silicon. Aluminium is the second impurities demonstrating hydrogen-enhanced diffusion, but in this case the presence of radiation defects is necessary, too. A distinguishing feature of the diffusion is low temperature required (<200 K). As a result of the hydrogen-enhanced diffusion of Al_i atoms, a supersaturated solution of Al in silicon is dissociated, that induces Al-Al pairs and more complex aluminium containing defect appearance.

4 DEVELOPMENT OF TIN OXIDE FILMS BY MAGNETRON SPUTTERING

Tin oxide thin films are important for many fields of optics, optoelectronics and solar energy conversion. They are also widely used for detection of oxidizing and reducing gases. One of the most promising methods for depositing tin dioxide thin films for gas semiconductor sensor microtechnology is magnetron sputtering. This provides rather high homogeneity of deposited films and the possibility to control their thickness and structure. SnO_x films have been deposited on polished and previously prepared Al_2O_3 , substrates (polycor), fused quartz and annealed in a vacuum at a temperature of $200 - 250^{\circ}C$ for least 10 min. Tin sputtering has executed with using a magnetron addition to VUP 5M unit in Ar and O_2 containing atmosphere. High purity (99.99%) tin targets have been used. The magnetron sputtering mode parameters have been the cathode voltage $U_c=175$ V, the ion beam current $I_{ion}=100$ mA and the argon — oxygen mixture pressure inside the chamber 1 — 2 Pa. The oxygen concentration has been approximately 10%. The temperature of the substrate has been $200^{\circ}C$. At such operating conditions the growth rate of the films have not exceed 0.5 A/s. After fabrication, the films have been annealed in air at 200 and $550^{\circ}C$ to stabilize their optical and electrical parameters.

Figure 4 shows a set of optical transmittance spectra for SnO_x film after its deposition and annealing at temperature of $550^{\circ}C$ for 0.5, 1 and 2 h. Optical constants for the tin oxide films were estimated by the envelope method from the transmittance data [10]. Accordingly this method the optical constants of a thin film can be determined by means of measurement of alone optical transmittance if the film has low absorption coefficient and optical thickness. The maximum and minimum transmittances appear when optical thickness is a multiple of quarter and half wavelengths, so it can be used to calculate the refractive index (n) and the film thickness (d) from envelope curves at maximum and minimum transmittances, respectively.

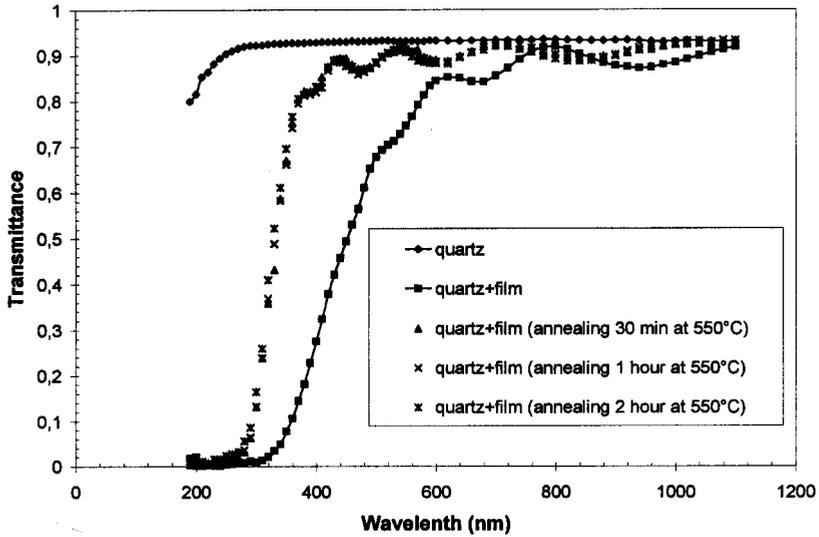


Figure 4. Transmittance spectra for quartz-slide and for a tin oxide film on a quartz substrate after deposition at once and after following annealing.

The transmittance spectra in UV region show that the transition corresponding to the fundamental absorption falls in this region of the electromagnetic spectrum. Then, the absorption coefficient was evaluated from the equation [11]

$$\ln T(\lambda) = -\alpha d$$

where α represents the absorption coefficient of the film of thickness d and, $T(\lambda)$ represents the transmittance for the wavelength λ . The obtained results are shown in Table 4.

Table 4. Optical characteristics of some of the SnO_x thin films

Sample	Thickness d (nm)	Refractive Index (n)	Absorption coefficient for $\lambda=350$ nm (cm ⁻¹)	Optical band gap E_g
<i>Substrate-glass slide</i>				
Post-deposition	445	1.81 ($\lambda=805$ nm)	6.64×10^{-4}	3.35
Post-annealing for 2h at 550°C	430	1.58 ($\lambda=800$ nm)	1.22×10^{-4}	3.85
<i>Substrate-quartz slide</i>				
Post-deposition	385	1.59 ($\lambda=805$ nm)	8.41×10^{-4}	3.35
Post-annealing for 2h at 550°C	335	1.59 ($\lambda=750$ nm)	1.26×10^{-4}	3.95

The optical band gap was determined from the expression for allowed direct transition [11]

$$\alpha = A(h\omega - E_g)^{1/2}$$

where E_g , is the energy gap and A is a constant.

The result of optical measurements did not change significantly if the annealing duration was increased. We assumed the dependence of the absorption coefficient from the annealing time at $T=550^{\circ}\text{C}$ was due to the film structure transformation and formation of polycrystalline tin oxide phase [11]. The decrease of the film thickness after the annealing indicated an increase in the film density.

Gas sensitivity of thin films was determined by ratio $\gamma=(R_0-R_r)/R_0=\Delta R/R_0$; where R_0 , R_r are film resistance in pure air and in gas mixture of air and ethanol vapours, respectively. A typical temperature dependence of a resistance for a sensor with an operating area 1 mm^2 ($1\times 1\text{mm}^2$) is shown in Figure 5. Around the clock a group of investigated samples was maintained under the operating conditions $T=200^{\circ}\text{C}$ for 1 month or longer. Their sensitivity to ethanol vapour with concentration 1 g/mm^3 ($T=200^{\circ}\text{C}$) was checked daily. The data are shown in Figure 6 also.

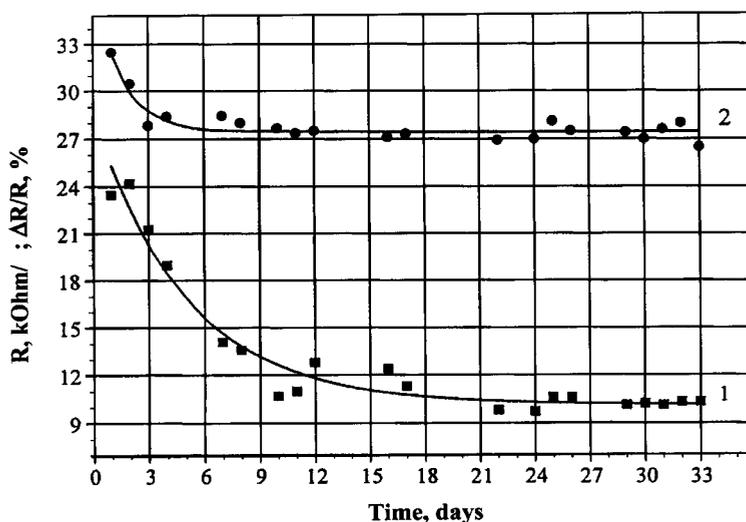


Figure 5. Resistance (1) and sensitivity to ethanol (2) for SnO_2 thin films as functions of operating time. The concentration of ethanol vapours is 1 g/mm^3 .

The aforementioned results have shown that the resistance of investigated 81гиспек stabilized after approximately 450 operating hours at 200°C . During this time the gas sensitivity decrease of the films was usually no more than (10 - 15)%. Observations, which were made during 1 year or more, have shown that after such training the sensor parameters variation was practically within the $\pm 5\%$ range. Annealing of the films at 550°C for 20 h or more decreased their resistance four to five times. The decrease of gas sensitivity was less than 20%. We conclude that both annealing conditions (200°C , 450 h and 550°C , 20 h) lead to an approximately identical structure for SnO , thin films deposited by magnetron sputtering.

5 DEVELOPMENT OF NEW PROCESSING STRATEGIES FOR TITANIUM ALUMINIDES

5.1 Ion irradiation as a method of treatment of titanium aluminides

Titanium aluminides based on γ -TiAl, which contain a small volume fraction of α_2 -Ti₃Al phase, are potential materials for high temperature aerospace application. Their low density, high temperature creep resistance and strength, high oxidation resistance make them excellent potential engine materials. The mechanical properties of these alloys are very sensitive to microstructure, which, in turn, varies considerably with change in minor alloy composition and in processing parameters [12-16]. Also, TiAl compounds have recently been considered as potential nuclear materials [17], due to their creep resistance and to their low neutron-induced radioactivity as compared to that of stainless steels. Therefore it is very important to understand the effect of alloying, heat treatment and irradiation on the stability and formation of microstructure in two-phase titanium aluminide alloys to develop processing strategies for these materials.

The samples of nominal composition Ti-48% Al-2% Nb (all compositions are given in atomic percent) used in research were prepared by electric-arc melting 99.99% Al, commercial Ti and Nb. The ingot was given a hot isostatic pressing treatment at 1300°C. Samples with a side of 8×8×1 mm were cut from ingot. The samples were homogenized at 1150°C for 160 h. They were wrapped in tantalum foil and sealed in quartz tubes. Then the samples were heat treated at 1300°C for 0.5 h and quenched in oil. The quenched samples were irradiated by 60 keV Ti⁺ ions up to dose 10¹⁷ ions/cm². The current density of ion beam was 10 mA/cm². The pulse repetition frequency was 25 Hz. The pulse length was 250 μ s. The temperature of the samples during irradiation did not exceed 150°C. Then the quenched samples and quenched irradiated ones were aged in vacuum of 10⁻⁵ Pa at 650 and 800°C for 0.5, 2 and 6 h and further cooled in a furnace.

The preliminary irradiation of the quenched Ti-48Al-2Nb alloy greatly affects dynamics of phase transformations during aging. Structural changes, and first of all it is apparently redistribution of alloy composition in near-surface region which are not limited to the radiated-damaged layer [18], considerably influence on the phase transformation behaviour and stabilize structure of quenched alloy at the initial stages of aging at 650 and 800°C. It is possible to assume, that as a result of an ion irradiation the steady defect clusters are formed in samples, which play a role similar to an alloying addition, and make changes to thermodynamics of phase transformation [19]. It is necessary to note that after quenching the structure of alloy was very inhomogeneous and during irradiation of such system, free energy of every phase is changed differently because of various ability to accumulation of point defects. As is known [19-20], even minor alterations of free energy of the present phases, result in

significant changes kinetics of the phase transformations and influence on a sequence of structural formation in two-phase ($\gamma+\alpha_2$) alloys.

On the other hand, during aging at the initial stages of the structural reformation of the quenched-irradiated samples, first of all the annealing of irradiation-induced defects may occur. In this case there is a thermodynamic driving force, which tend in reducing concentration of defects up to equilibrium value. When the temperature is raised after irradiation the accumulated vacancies migrate annihilate the interstitial clusters. In turn this recombination process can retard the decomposition of metastable phases at the initial stages of aging. As known the mobility of the point defect sharply grows at increase of temperature therefore at ageing at 800⁰C their annealing occurs faster than at 650⁰C. After their concentration decreases and approaches certain value, the decomposition of metastable phases dramatically accelerates.

The preliminary irradiation of the quenched Ti-48Al-2Nb alloy greatly affects kinetics of phase transformations during aging. The speed of the phase transformations in preliminary irradiated and non-irradiated samples is various. Structural changes of near surface region resulting from ion irradiation slow down the processes of structural recovery and stabilize structure of quenched samples at the initial stages of aging at 650 and 800⁰C and dramatically accelerates them in process of increase of aging time. The ion irradiation gives unique opportunities concerning structural control of two-phase ($\gamma+\alpha_2$) alloys and creation of near surface region in which can exist metastable layer with the changed composition and properties compared with basic volume.

5.2 Development of protective coating based on titanium aluminides

As titanium aluminides are excellent materials for high temperature application it is reasonable to develop processing strategies for protective and high temperature coating based on them [21]. The point is that the thing films can be produced under different non-equilibrium conditions and as a result many metastable states, which it is impossible to receive in bulk materials, can be formed in them [22,23]. Now in we are developing the mode of sputtering Ti-Al alloys, created Ti-48Al thing films as protective coating. Thin films have been produced by magnetron sputtering of the Ti-48Al alloy (all compositions are given in atomic percent). The Ti-48Al alloy has prepared by electric-art melting 99.999% Al and 99.999% Ti. The one was homogenized at 1150⁰C for 160 h. Pressure during sputtering was 0.8 Pa. The temperature of the substrate during sputtering was 300⁰C. The speed of sputtering was 0.11nm/c. The thickness of the received films was 6 μ m. As the substrates glass ceramics and polycore were used.

The process of the target's sputtering has been established to go on uniformly. Despite this fact the films obtained have the composition close to that of the target. The sputtering coefficient for aluminium is higher than that for titanium, that is why at the very beginning of sputtering the target's surface loses aluminium (Table 5). Soon on the target's surface there appears the

titanium-enriched domain. Some steady-state target composition is achieved, and on further sputtering the film with the same composition as the initial target's one is deposited. Therefore, by magnetron sputtering the Ti-Al alloys one can get the film, the composition of which will correspond to the target's one.

Table 5. Chemical composition of the target

State	Ti	Al
Before Sputtering	51.889	48.111
After Sputtering	55.578	44.422

The microstructure of the films obtained after sputtering depends on the substrate structure (Figure 6a and b). However, in both cases the Ti_3Al -based phase is formed in the films. According to the TiAl equilibrium diagram [24], for the given chemical compositions the stable and main phase is the Ti_3Al -based phase compound. This proves that the Ti_3Al -based phase obtained in the films after sputtering is metastable. Metastability can be maintained by the deformation fields, which always exist in the films.

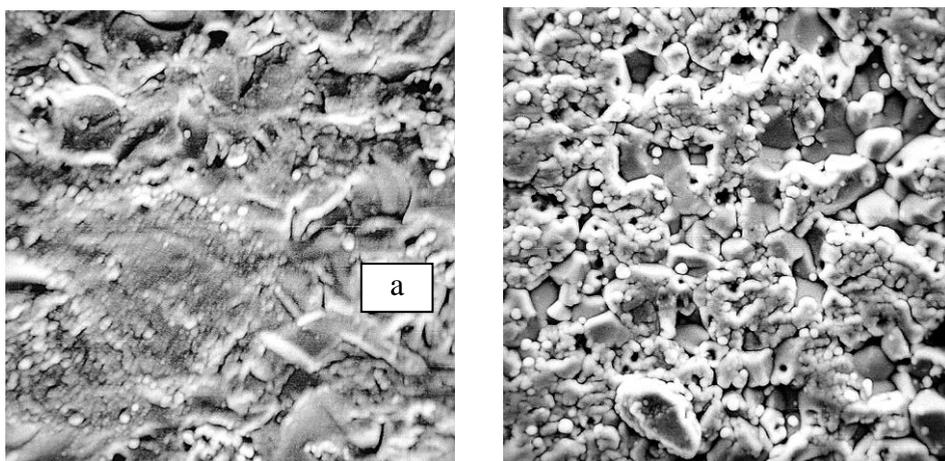


Figure 6. Microstructure of the thin films on the (a) Glassceramic and (b) Polycore substrates.

After 0.5 hour annealing the films contain more titanium and less aluminium than in the initial state (Table 6). Taking into account that the mobility of aluminium atoms is higher than that of titanium it can be assumed that aluminium atoms diffuse into substrate during annealing. As a result the average chemical composition of the films changes dramatically. With the further increase of the annealing time to 2 hours the film compositions become the same in the volume. Both on sital and polycore the films have practically

identical composition after 2-hour annealing. The film microstructure gradually becomes, more homogenous. Besides, during annealing the reorientation of the films' crystallites takes place relative to the substrate planes. The crystallites start to be oriented in the definite crystallographic direction.

Table 6. Chemical composition of the thin films

Substrate	Initial	Annealed, 0.5 h	Annealed, 2 h	Annealed, 6 h
Glassceramic	Al- 49.553	Al- 35.982	Al- 37.512	Al- 36.699
	Ti- 49.841	Ti- 62.871	Ti- 61.672	Ti- 62.733
	Substrate- 0.606	Substrate- 1.147	Substrate- 0.816	Substrate- 0.568
Polycore	Al- 44.853	Al- 39.154	Al- 38.129	Al- 45.495
	Ti- 54.774	Ti- 60.185	Ti- 61.416	Ti- 54.127
	Substrate- 0.373	Substrate- 0.661	Substrate- 0.455	Substrate- 0.378

On annealing the film structure rearrangement kinetics also depends on the substrate structure. When there is a great discrepancy in crystallographic parameters of the substrate and the film, as is the case with sital, during 0.5h annealing surface cracks are formed, which are gradually "healed" with the increase of the time of exposure. Besides, the intermediate metastable phase on the film on polycore is formed after 2 hour annealing, but metastable phase in the film on sital is formed after 6 hour annealing. With the increase of annealing time to 6 hours the composition of different parts becomes the same and approaches the average composition of the film on sital. However, the chemical composition of the film on polycore remains stable only at increasing the annealing time to 2 hours. After 6 hour annealing the film chemical composition changes dramatically. A new stage in the reconstruction of the film structure on polycore is likely to begin. That is the structure, kinetics of phase transformation and evolution of the film microstructures depend on the structure and morphology of the substrate.

6 CONCLUSION

The recent major expansion of the semiconductor industry during recent years meant that the rejected material has become scarce and more expensive. As a consequence, the price for solar-grade silicon has increased rapidly. Because of the continuing expansion of silicon based photovoltaic devices, the photovoltaic crystalline silicon industry will eventually require a dedicated supply of polysilicon feedstock. In addition the overall demand for silicon will increase at a very fast rate. Therefore developing new sources of silicon for photovoltaics and microelectronics are objectives of strategic importance. Alumothermic reduction of silica from the waste products of the phosphorous industry has been developed by the Institute of Physics and Technology, Alamy, Kazakhstan, and was looked at in brief in the paper.

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Neutron Diffraction and the Structure of New Materials

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1 INTRODUCTION

New materials are everywhere! Imagine all the tiny magnets in the electric motors of a new car, the lighter, longer-lasting batteries that power a portable telephone or computer, the selective catalysts used to create new fuels and clean up the environment. Imagine machines made from new kinds of fibres, with motors made from new kinds of ceramics – both lighter and tougher than the metals they replace. Imagine storing greenhouse gases at the bottom of the ocean, or finding vast reserves of energy in this “inner space”. But who could imagine, a few years ago, new super-conducting materials that could conduct electricity without loss, and be used in more powerful magnetic scanners to map the human body in the finest detail? Who can imagine the future without working on the materials that will make it possible?

In this lecture we will describe some of the advantages of neutron diffraction for this kind of work, compared to X-ray and electron diffraction, and give specific examples of recent applications to our understanding of the structure of new materials.

2 WHY NEUTRONS?

The properties of materials are largely determined by their structure – structure on the atomic scale, or nano-structure. The distance between atoms is only about 0.1 nm (nanometer or billionth of a meter) much smaller than the wavelength of light (400-700 nm), so clearly we cannot use light. But neutrons, along with electrons and X-rays, can provide a new kind of ‘microscope’. Neutrons are sub-atomic particles that act like waves – like X-rays, and electrons. Since the wavelength of ‘thermal’ neutrons is similar to the distance between atoms, they have the potential for providing details of structure on the atomic scale. The advantages of neutrons:

- Neutrons are electrically neutral, unlike electrons, which have a negative charge. They can therefore penetrate deeper inside materials, and are even

more penetrating than X-rays. This can be important for ‘non-destructive’ measurements of engineering components, and of materials under extreme conditions, such as inside pressure cells, furnaces and refrigerators;

- Neutrons interact with the tiny central nuclei of atoms, while X-rays are scattered by the surrounding clouds of electrons. Neutrons can then locate atoms more precisely, and scattering from point objects is strong even at high scattering angles;
- More importantly, the scattering power of atoms for neutrons does not depend on the atomic mass number, as it does for X-rays and electrons. This means that light atoms such as hydrogen and oxygen scatter neutrons as strongly as heavy atoms like lead (Figure1). We will see why hydrogen and oxygen are important for many new materials;
- Even more importantly, neutrons act like tiny magnets, and are a unique tool for determining the magnetic structure of materials; and
- Finally, the energy of thermal neutrons is similar to the energy of vibration of atoms in solids, and other types of “excitations” involving magnetism – the energies of X-rays are very much higher. Then neutrons can be used to study the dynamics of materials, and the forces between atoms.

These latter two advantages in particular earned the 1994 Nobel Prize for Bert Brockhouse and Cliff Shull, two of the pioneers of neutron diffraction.

Figure 1 compares the scattering power of electrons, X-rays and neutrons for scattering at moderate angles. X-ray scattering is proportional to the number of electrons, and electron scattering depends on the electrical potential, which also depends on the atomic number. However, neutron scattering is of similar magnitude for all of these atoms, heavy or light.

Furthermore, the scattering centres for X-rays and electrons are atomic spheres of finite dimension d , so the scattering power for X-rays of wavelength λ then falls off rapidly with scattering angle 2θ , decreasing by half when $\sin\theta = \lambda/d = 1$ i.e. when the X-ray wavelength is comparable to the size of the atoms ($\lambda \approx d$). Thermal neutrons, with similar wavelength, are scattered by the much smaller nucleus, so $\sin\theta$ can have large values without any fall-off in intensity. Large scattering angles are needed to obtain high resolution of structural details.

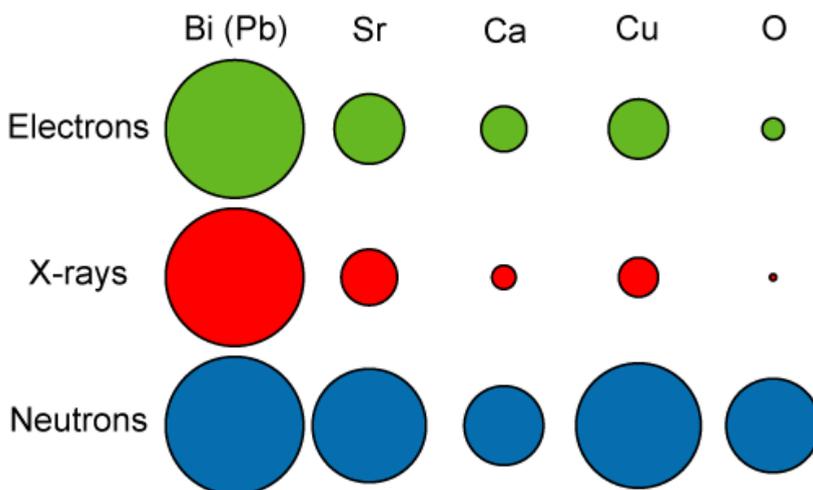


Figure 1. The scattering power for X-rays, electrons and neutrons of the different atoms in oxide superconductors. The diameters of the circles are proportional to the scattering amplitude, and the areas to the intensity, for scattering at angles 2θ such that $\sin\theta/\lambda = 1$.

3 HOW DO WE OBTAIN NEUTRONS?

Excess neutrons are produced by the fission of heavy elements, since light elements contain proportionally fewer neutrons. Nuclear fission occurs either via a chain reaction in a nuclear reactor, or in an accelerator where a heavy metal target is bombarded by energetic protons to produce neutrons by “spallation” fission. Europe possesses both the best reactor and best spallation neutron sources, respectively at the Institut Laue-Langevin (ILL) in Grenoble [1], and at the ISIS pulsed source near Oxford [2]. Although neutrons are the ideal probe for studying the structure of materials, the number of neutrons, even at ILL - the world’s highest flux source - is still only a tiny fraction of the number of electrons in the beam of an electron microscope, or the number of X-ray quanta from X-ray sources.

These fission neutrons are very energetic, and must be “moderated” or slowed down before they can be used for diffraction. The moderator may be just a tank of (heavy) water surrounding the fission source. The neutrons lose energy by colliding with the hydrogen atoms in the water, and after a few collisions end up with the same energy as these atoms i.e. “thermal energies” with neutron wavelengths of ~ 0.1 nm. Thermal neutrons are then ideal for measuring both the structure and energy of materials on the atomic scale. Less energetic, longer wavelength neutrons (~ 1 nm) can be produced by using a “cold” moderator such as liquid hydrogen, and shorter wavelength neutrons (< 0.1 nm) by using a “hot” source, such as graphite heated to 2000 degrees centigrade.

It would be expensive to build a more intense neutron source, but cost effective to make better use of the source that we already have, since many neutrons are wasted because our detectors are small. New types of detectors can increase the number of neutrons that we actually count, by a factor of 10 or more. As well, neutron optical elements, such as focusing monochromators and super-mirror neutron guides (which act like optic fibres for light), can bring more of the available neutrons to our samples. These techniques are particularly important for the study of structure with neutrons, since new materials are often only available in small quantities when first produced.

4 WHAT KIND OF EXPERIMENTS CAN WE DO?

On a reactor source, we generally use a large crystal monochromator to select a particular neutron wavelength, just as the different wavelengths of light can be separated using a prism or fine grating. The material to be studied is placed in this monochromatic neutron beam, and the scattered neutrons collected on a large 2D detector. The sample can be a liquid, a bunch of fibres, a crystal or a polycrystal. A polycrystal is the usual form of solid matter, such as a lump of metal or ceramic, and is made up of millions of individual crystals.

To understand how neutron diffraction works, imagine how light is diffracted by a regular grating or grid. Scattering from the different lines of the grid interferes to give diffraction lines and ‘spots’ with spacing inversely proportional to the spacing of the grid lines. X-ray and neutron diffraction work the same way, but the grid is now the array of atoms in the material. This interference condition is called “Bragg’s law” (Figure 2). By measuring the intensities and positions of the scattered X-ray or neutron Bragg peaks, we can deduce the atomic structure.

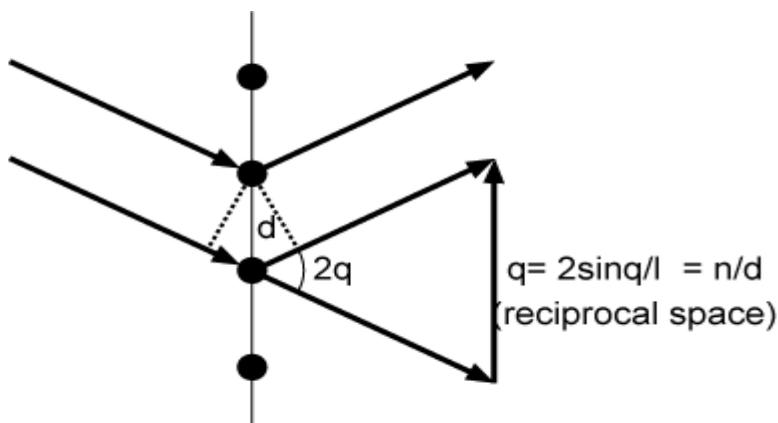


Figure 2. Bragg’s law is simply the condition for constructive interference for scattering by angle 2θ with wavelength λ from a set of planes of d -spacing d .

5 NEUTRON POWDER DIFFRACTION

Neutron diffraction experiments are then really quite simple, and available to a wide variety of users – materials scientists, chemists, physicists and biologists. The simplest is called ‘neutron powder diffraction’, first used by Shull to obtain magnetic structures, where a polycrystalline lump of material, often ground to a fine powder, is placed in the beam (Figure 3). Neutrons are scattered at specific angles, corresponding to the spacing between atomic planes, and by measuring these angles and intensities, the atomic structure of the material can be deduced.

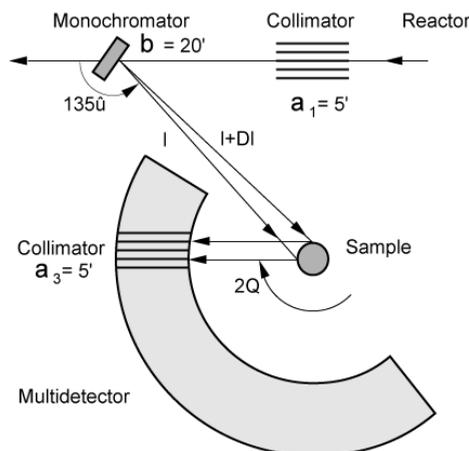


Figure 3. The high-resolution powder diffractometer D2B at ILL Grenoble [3]. A Söller collimator is used to define the incident beam direction to 5' or 30' of arc, and a (vertically focussing) monochromator crystal is used to select a particular wavelength, such as 0.16 nm. Further 5' collimators in front of the 64 ^3He detectors define the scattered beam.

If instead of a crystalline powder an amorphous or liquid sample is used, there are only broad peaks at specific angles corresponding to average interatomic distances. To obtain more data, short neutron wavelengths are used, and sometimes one type of atom is replaced by its isotope – chemically identical, but with a different nucleus and different neutron scattering power - this difference then gives information specific to that atom.

On the other hand, if a large single crystal of the material is available, it can be oriented to select the particular atomic plane of interest, which greatly simplifies the analysis of the data. Inelastic neutron scattering also uses single crystals if available, but is a little more complicated. Here the change in neutron energy is measured as well, and this gives information about the energies of vibrations and other excitations in the sample. Just as the incident energy, or

wavelength, is selected by a monochromator crystal, the scattered energy is measured with an analyser crystal in the so-called 3-axis machine invented by Brockhouse.

On a pulsed (spallation) neutron source, things are a little different. Instead of a steady stream of neutrons, intense pulses are produced with high peak intensity but low average flux. The so-called TOF method is used to separate the neutron wavelengths, instead of using monochromating or analysing crystals. Over a long flight path, the neutrons arrive at the sample spread out in time, so their energy or wavelength are obtained by measuring this “time-of-flight” (TOF). In practice, the slowest neutrons arrive just before the fastest neutrons from the next pulse. Some experiments, such as 3-axis measurements are best suited to reactor sources, and some – those for which the TOF method is an advantage – to pulsed sources. Many experiments can be performed on either type of neutron source.

6 SINGLE CRYSTAL NEUTRON DIFFRACTION

Sometimes it is possible to grow large single crystals of the material of interest (at least 1 mm^3), and it may then be best to perform neutron diffraction on these crystals, rather than on polycrystals. The advantage is that single crystals can be aligned to select each individual atomic plane (Bragg peak), so there are no overlapping peaks and data analysis is easier. The single crystal neutron diffractometer looks like its X-ray counterpart, except that it is bigger. A precise mechanism (chi-circle) is used to align the crystal in the neutron beam, and a detector is positioned to measure the diffracted beam. The crystal is then re-aligned for the next atomic plane and the measurement repeated for as many different planes as possible. A computer controls all this of course, and the machine works 24 hours per day, usually with the sample in a refrigerator, a furnace, or a pressure cell. The neutron beam may even be magnetically polarised when magnetic materials are being measured.

A very important advance has been made recently to increase the efficiency of such single crystal diffractometers. Instead of collecting Bragg peak’s one at a time, a large 2D area detector can be used to collect many peaks simultaneously, just as is commonly done with polycrystalline samples. This only works if a band of wavelengths is used, or if the crystal structure is so large that many peaks simultaneously satisfy the Bragg condition for diffraction. New 2D detectors are being made using arrays of wires to determine the positions of the different Bragg peaks, or more simply using a kind of photographic film.

Neutrons themselves cannot be “photographed”, as can light and X-rays, but a neutron scintillator coating can be used to first convert the neutrons to X-rays or gamma rays. This is the basis of amazing new single crystal diffractometers recently constructed at EMBL-ILL Grenoble – the “neutron image plate camera” [4]. Figure 4 shows such a machine, with the neutron detecting film or

image plate wrapped around a cylindrical drum surrounding the sample. The image is read out using a laser and a mechanism similar to that of a photocopying machine!

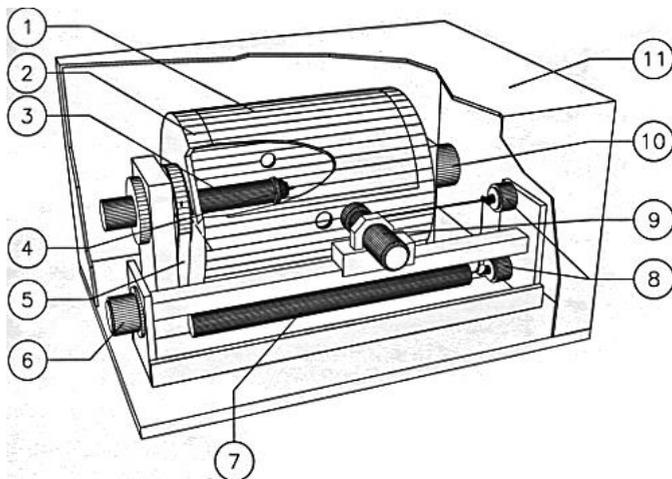


Figure 4. The first neutron image plate diffractometer [4], developed at EMBL-ILL Grenoble, showing the image plate (1) on a rotating drum (2) surrounding the crystal on its supporting rod (3). The neutron beam enters and exits through the small holes in the drum, and the remaining components allow the laser (9) to scan the surface of the image plate, and also to erase it after reading out the diffraction pattern.

Similar machines can be used on pulsed neutron sources, but here the continuous reactor source has a distinct advantage, since it is the time-averaged flux that is important, not just the peak neutron flux.

Figure 5 shows a diffraction pattern obtained on the new *Vivaldi* image plate camera at ILL Grenoble. Hundreds of diffraction peaks are obtained simultaneously, just as with photographic techniques on X-ray sources. Neutron image plates are especially powerful for hydrogenous materials, such as this vitamin B12 sample, and for magnetic materials as well as for materials that undergo magnetic or structural transitions. In this they can be compared with powder diffractometers in that they survey the whole of scattering space as a function of temperature, magnetic field etc.

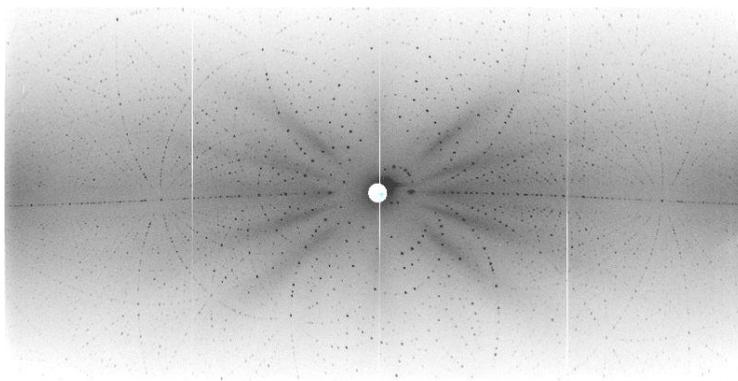


Figure 5. A neutron diffraction pattern obtained from Vitamin B12 on the latest neutron image plate diffractometer *Vivaldi* at ILL Grenoble [5]. A great many Bragg peaks are obtained simultaneously with a large band of neutron wavelengths, using almost all of the neutrons available from the continuous high flux source.

7 RIETVELD REFINEMENT FOR NEUTRON POWDER DIFFRACTION

Neutrons have a particular advantage over X-rays when used with polycrystalline or ‘powdered’ material; because of the great penetrating power of the neutron, an average is obtained over many more crystalline grains than is possible with X-rays or electrons.

Powder diffraction, like classical crystallography, requires the measurement of the scattering power of the various crystal planes, but of course, with a powder it is not possible to select these planes by orienting the crystal, as it is with single crystals. The different planes are separated only by the different “d-spacings” between them, not by their orientation. Different d-spacings produce constructive scattering at different angles ($\sin\theta/\lambda$), and the neutron diffractometer must have high angular resolution to resolve these “Bragg peaks” (Figure 6). Even so, there are many peaks, corresponding to different crystalline planes, which are still not resolved.

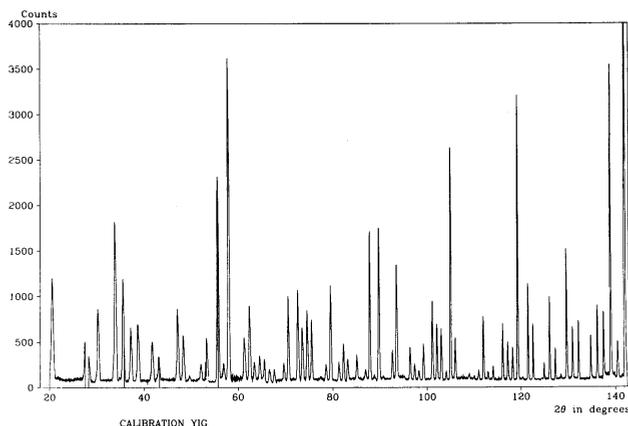


Figure 6. The results of a high resolution neutron powder scan for the 12Å unit cell of yttrium iron garnet (YIG) on the D2B machine at ILL Grenoble [3]. Notice how sharp the Bragg reflexions are throughout the entire pattern, and how strong the peaks are at high scattering angle, where X-ray patterns fall off because of the ‘form factor’.

A major advance came when Rietveld [6] showed that rather than extract the individual peaks and use them to obtain the crystal structure, it is much better to refine the crystal structure to fit the observed diffraction pattern directly. This is because the peak positions (d-spacings) are all determined by at most 6 parameters, the dimensions and angles of the primitive structure unit (unit cell). The peak intensities are then all determined by the positions of the individual atoms in the unit cell for a periodic structure.

In Rietveld refinement, only physically real parameters describing the crystal structure are refined – the atomic co-ordinates, unit cell dimensions etc. Alternatively, attempts to fit a series of overlapping peaks, without imposing such physical constraints, inevitably results in strong correlation between the individual peak heights and positions. The atomic co-ordinates obtained with neutron powder diffraction are often more reliable than those obtained with classical single crystal methods, because in practice it is very difficult to obtain good single crystals, and even when it is possible, the crystals may break up on undergoing structural transitions at lower temperature.

The powder experiment is also much easier and faster, and because of this the structure can be determined at many different temperatures, instead of the one or two temperatures usual with classical crystallography.

8 APPLICATIONS OF NEUTRON DIFFRACTION

Rietveld and his co-workers used his method mainly for the determination and refinement of magnetic structures, and this remains an important application. But the "Rietveld Method" of neutron powder diffraction is now applied to many different branches of solid-state chemistry and physics, as listed in Table 1.

Table 1. Applications of neutron powder diffraction

Suited to Powders	and Suited to Neutrons	Other applications
Structural transitions	Magnetic structures	Minerals
Solid liquids & gases	Heavy metal compounds	Polymers & biological
Zeolites	Hydrides & H₂ storage	Other structures
Intercalates	Hydrogen bonding	High pressure
Catalysts	Other bonding	Thermal expansion
Solid electrolytes	Mixed valence	Texture & stress
Other disorder/defects		Techniques
Superconductors		Synchrotron papers
Ceramics		
Other X-ray applications		

The first column lists those areas for which powders have natural advantages over single crystals. For example, materials that undergo phase transitions often break up on cooling, or at least form multi-domain crystals less suitable for conventional crystallographic study - the sample is more naturally available in powder form. In particular, solid liquids and gases are easier to prepare and handle as powders. Other materials, such as zeolites, may be only available as powders and some materials may break up on intercalation. Catalysts are usually powders, and the purification process of crystal growth may be undesirable for the study of solid electrolytes (ionic conductors and electrode materials). Other defected or disordered structures and non-stoichiometric compounds may also be changed by single crystal growth.

Oxide superconductors already formed an important category in 1984 and included materials such as partially oxidized Chevrel phases, where the transition temperature is sensitive to the stoichiometry. Finally 'ceramics' includes those other oxides, nitrides, etc., which are usually produced in powdered ceramic form - for example, as dielectrics.

The second column in the table lists powder-diffraction subjects that are particularly suited to neutron diffraction. Magnetic structures are, of course, the typical example, since neutrons see the magnetic moments on the atoms. Because the neutron scattering factor is of similar magnitude for all nuclei, heavy metal compounds such as transuranics, on the one hand, and hydrides and hydrogen bonds, on the other, usually require neutron diffraction. Metal hydrides were studied for their potential applications for hydrogen gas storage.

The study of other types of bonding, and of mixed valence compounds, may also be better done with neutron powder diffraction. This is simply because

systematic errors in X-ray powder diffraction are more important, reducing the precision with which bond lengths can be determined: for example, quite precise bond lengths are required to distinguish between Fe^{2+} and Fe^{3+} using the Zachariasen/Brown-Shannon rules. This is a technique that has since proved especially valuable for the study of the new oxide superconductors, as we shall see.

The third column of the table lists other subjects for which powders have been used with advantage, ranging from mineral structures to polymers and biological materials. High-pressure structures can sometimes best be done with powders, and of course systematic measurements, as a function of temperature, may be less time-consuming with powders.

Finally, we have a category for texture, stress and strain measurements. This is a well-established subject for X-rays, but has acquired new applications with neutron powder diffraction; the greater penetrating power of the neutron permits non-destructive testing of the interior of objects of cm^2 dimensions - welds, pressure-vessels, rolled and worked metal, pre-stressed composite superconducting wires, etc.

9 DI-ELECTRIC AND FERRO-ELECTRIC CERAMICS AND STRUCTURAL TRANSITIONS

This is an early example of the use of Rietveld refinement [7] that is of particular relevance to the study of oxide superconductors, because many of the same types of material (oxide perovskites) were studied, and many similar phenomena (small displacements of atoms) were of interest. In the classical ferro-electric BaTiO_3 the electrical dipole is created by a structural transition involving small displacements of positively charged cations in opposite directions to the displacements of the negative oxygen ions. The dipole moment requires the measurement of the magnitude of these displacements, and this is the objective of Rietveld refinement. The idea was to measure the powder diffraction pattern at a number of temperatures, and to obtain the atom co-ordinates at each temperature.

The resulting atomic co-ordinates obtained with Rietveld refinement for the similar KnbO_3 (Figure 7) are in this case much more reliable than those obtained with classical single crystal methods, because in fact it is very difficult to obtain good single crystals. When such crystals are grown at high temperature, they are in the cubic phase. When they are cooled to the orthorhombic phase, there are several possibilities for the (a,b,c) axes, and the crystal breaks up into microscopic domains corresponding to each possibility. 'Single' crystals can be obtained by applying a very strong electric field to the crystal as it is cooled from the cubic phase, but even then the resulting strains in the material affect different reflections in different ways.

The powder experiment is also much easier and faster, and because of this the structure can be determined at many different temperatures, instead of the one or two temperatures usual with classical crystallography. The proof of the success of the method in this case was the fact that the polarisation obtained by

measuring the microscopic displacements of the ions agreed well with macroscopic measurements.

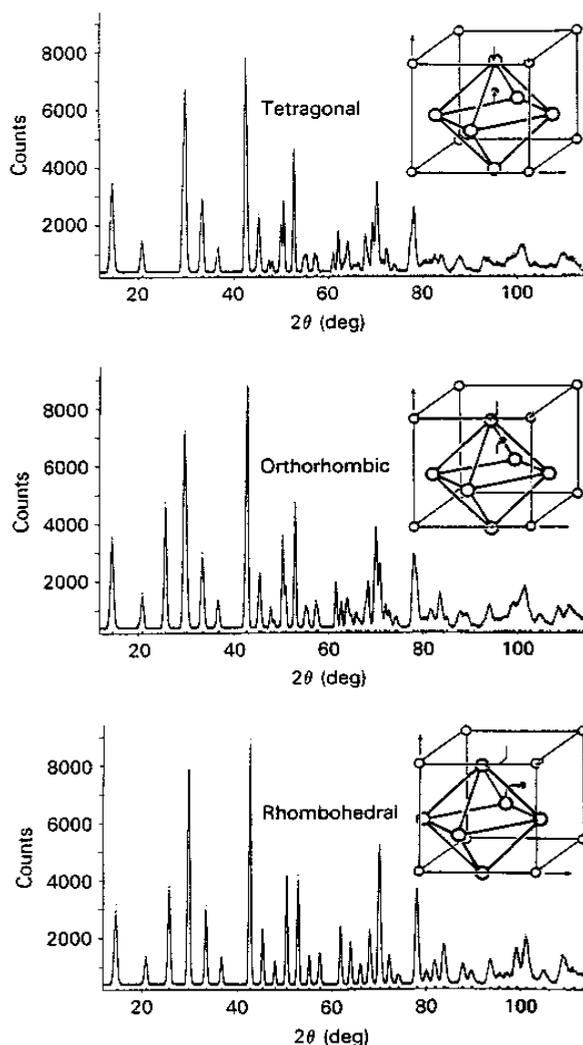


Figure 7. The diffraction patterns obtained for KNbO₃ at temperatures corresponding to the (a) tetragonal, (b) orthorhombic and (c) rhombohedral phases. Even though the atomic displacements are small, large changes are produced in the neutron diffraction patterns. These patterns [7] are the first application of the Rietveld method to such problems; modern diffractometers produce much better resolution, and the changes are even more striking.

10 NEW HARD MAGNETS AND MOLECULAR MAGNETS

Conventional permanent magnets are everywhere: in the car, the kitchen, the phone, the computer – in all kinds of electrical motors and recording devices. Neutron diffraction is of course unique for the determination of magnetic structures, and again real materials are first produced as powders. In fact the first uses of Rietveld refinement were to magnetic structures in the 1970's, and since then magnetic structure determination has always been an important application of the method.

In the early 1980's a Nd-Fe-B alloy was found to have remarkably good magnetic properties up to 585K, with an energy product of up to 360 J/m³. Even the chemical formula of this new phase, Nd₂Fe₁₄B, was not known until the crystal and magnetic structures were established [8]. The Nd and B atoms were found to occupy layers, separated by Fe-layers. The strong anisotropic magnetic properties of these materials up to room temperature and above, due to the rare earth ions, and the relatively large proportions of common iron compared to expensive rare-earth-cobalt magnets such as SmCo₅, make these hard magnet materials particularly attractive.

On the other hand, the use of soft molecular compounds to make permanent magnets is a fascinating possibility due to their potential lightness, transparency, solubility, optical properties and biocompatibility. Since the discovery of the first ferromagnetic molecular compound (T_c = 4.5 K) in 1986, great progress has been made, and it is now common to create molecular magnets for which the critical temperature is above room temperature, opening up many practical applications.

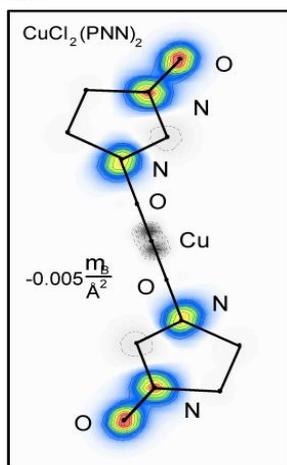


Figure 8. Spin density of the Cu complex $\text{CuCl}_2(\text{NitPh})_2$ projected along the π -direction of the Nit [9]. The density is positive on most of the two NitPh atoms and negative on the copper. The lack of magnetization on O1 shows that we are here in an extreme case where the spin distribution of the nitronyl nitroxide has been completely upset by the magnetic interaction with the copper.

In conventional insulating materials, the distribution of the magnetization is the sum of contributions due to individual magnetic atoms. The magnetic moments are well localized on the metal and a small part of the density can be transferred on the ligand. In the case of molecular compounds, the situation is completely different (Figure 8), the magnetism of a free radical, a building brick often used to synthesize molecular magnets, can be attributed to one unpaired electron described by a molecular orbital built up from the orbitals of the atoms constituting the molecule.

Polarized neutron diffraction allows us to determine the distribution of magnetization, which contains information on the electronic structure of the material. The nature of the magnetic orbitals, the interactions with neighbouring molecules in the solid, and effects such as chemical bonding, spin delocalisation or spin polarization can be revealed [9].

11 NEW HIGH TEMPERATURE SUPERCONDUCTORS

Ceramic superconductors are generally heavy metal oxides, and neutron diffraction has long been superior for the precise location of light atoms, such as hydrogen and oxygen, in the presence of heavy atoms. The advantage of neutron diffraction for locating oxygen is obvious from Figure 1, which compares the scattering powers of the different atomic constituents of high temperature superconductors for electrons, X-rays and neutrons. This is important if we are to understand the oxidation state of these materials, which controls their superconducting temperature. In practice, neutron diffraction is no more difficult to perform than X-ray diffraction, except of course that it must be done in a central laboratory rather than in the local basement.

A second reason for using neutron diffraction is that these new materials are often only available in polycrystalline or 'powder' form. While X-ray studies and electron diffraction may be superior for initial structure determination, neutron powder diffraction provides a more precise measure of important structural details. For example, precise measurements of metal-oxygen distances with neutron diffraction can be used to determine the valence state of the metal ions such as copper (Cu). This simply means that Cu^{+++} is smaller than Cu^{++} , which is smaller than Cu^+ , so the oxygens are slightly closer to the metal atom. It was this kind of measurement that resulted in the idea that superconductivity in layered copper oxides can be controlled by the oxidation/reduction of "charge reservoir" layers, a concept that led to the successful search for new materials with thallium, bismuth or mercury oxide charge reservoirs. Neutron diffraction was also important because neutrons are scattered by magnetic moments, and magnetic coupling of electrons is believed to be necessary for high- T_c superconductivity.

One of the key questions about new materials concerns their precise atomic structure and stoichiometry. For example, Figure 9 compares the structure of the original 90K superconductor, $\text{YBa}_2\text{Cu}_3\text{O}_7$ as obtained with X-rays at Bell laboratories [10], and as obtained with neutrons at ILL Grenoble [11]; these are typical of the results obtained by several laboratories using the two techniques.

Even though both the X-ray and neutron models are correct in principle, the X-ray model looks very different, and would be very misleading for chemists trying to make similar materials. It emphasizes the heavy atoms and appears to show that the material is simply an oxygen deficient perovskite, a common mineral structure containing copper oxide “octahedra” as predicted by Bednorz and Muller [12].

The inspiration for Bednorz and Müller's discovery of high temperature superconductors came in fact from their earlier work on perovskite ferroelectrics. They argued that small displacements of oxygen atoms, surrounding a 'mixed valence' cation such as copper, could provide the electron-phonon coupling thought to be necessary for superconductivity.

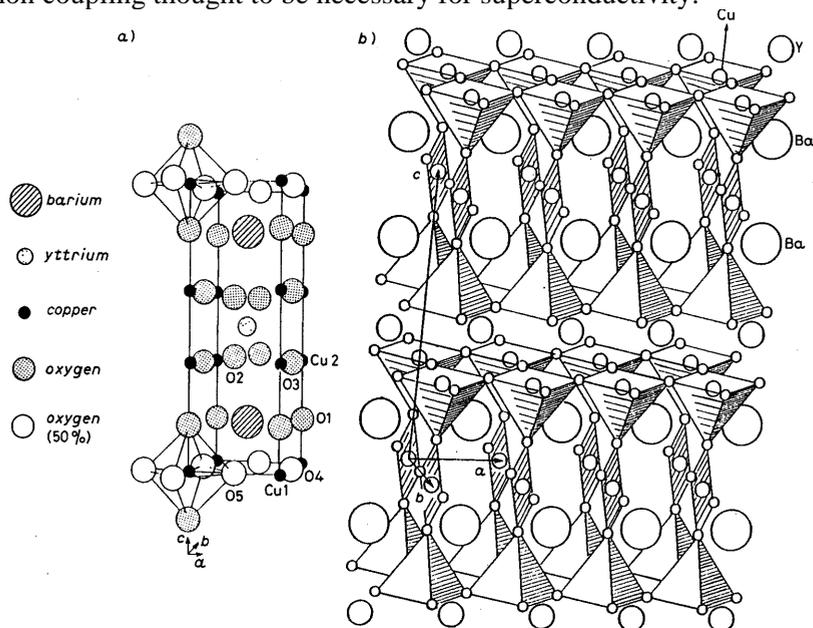


Figure 9. Structures of the 90K superconductor:
 (a) $\text{YBa}_2\text{Cu}_3\text{O}_{9-x}$ obtained by X-rays [10] and of
 (b) $\text{YBa}_2\text{Cu}_3\text{O}_7$ obtained by neutrons [11].

The neutron model, much more sensitive to oxygen, shows that there are no such octahedra in this material. This was a sensational discovery, and at first hotly contested by Bednorz and Muller, who were to be nominated for the Nobel Prize! Neutrons showed that there were two very different kinds of copper, the one in the “chains” with 4-fold square oxygen co-ordination typical of Cu^{2+} and the other in the “planes” with 5-fold co-ordination indicating perhaps a higher copper oxidation state. Neutron diffraction also showed that the oxygen is lost from the chains when the material is reduced, destroying superconductivity. The oxygen atoms were simply not well located with the first X-ray experiments, and this resulted in an incorrect understanding of the structure.

12 CHARGE RESERVOIRS AND THE SEARCH FOR NEW HIGH TC MATERIALS

Evidence for coupling between the charge on copper and the distance to oxygen, as predicted by Bednorz and Muller, had to await detailed measurements with neutrons. Since $\text{YBa}_2\text{Cu}_3\text{O}_7$ can be made non-superconducting simply by heating it to reduce the oxygen content in the charge reservoir CuO -chains, an obvious experiment was to use neutron diffraction to measure the oxygen content of these chains, and compare this with the changes in copper-oxygen distances, on passing from the superconducting phase (Figure 10a) to non-superconducting phase (Figure 10b).

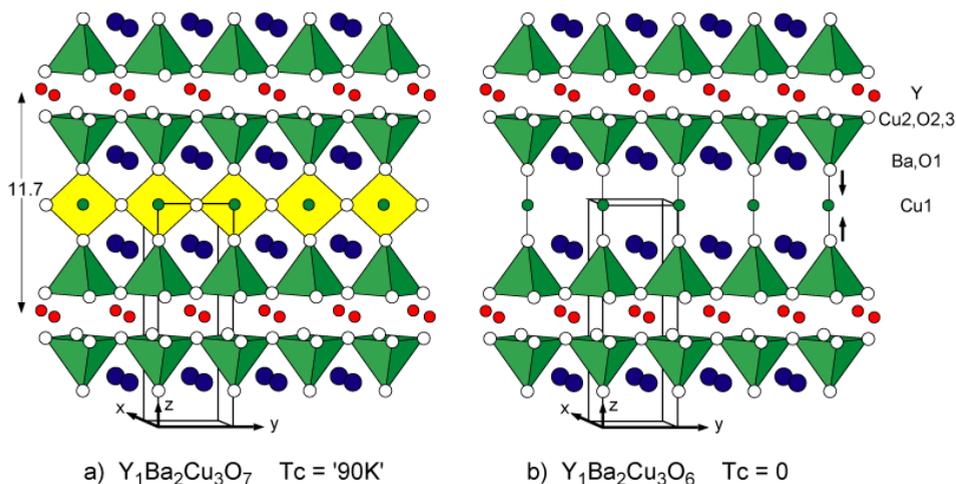


Figure 10. The difference between (a) superconducting $\text{YBa}_2\text{Cu}_3\text{O}_7$ and (b) oxygen reduced $\text{YBa}_2\text{Cu}_3\text{O}_6$. The arrows show the displacement of O1 oxygens, indicating reduction of Cu2 from Cu^{+++} to Cu^{++} in the non-conducting phase.

Cava et al. [13] found that for well ordered samples of $\text{YBa}_2\text{Cu}_3\text{O}_{7-x}$, T_c varied with x as shown in Figure 11a. Starting at 90K for $x=0$, T_c dropped first to a 60K plateau before falling to zero for $x > 0.6$. Remarkably, the Cu2-O1 distance to the apical oxygen O1 showed similar changes (Figure 11b) in contrast to the almost constant behaviour of the other copper-oxygen distances. Since the Cu2-O1 distance enters into the bond sum used to calculate the apparent valence of Cu2 in the conducting plane, it was concluded that the observed changes in T_c were directly related to the effective valence of this copper. The plateau at 60K was assumed to correspond to an intermediate super-conducting phase, with every second oxygen missing from the CuO -chains (the details of the structure of this second phase were determined later).

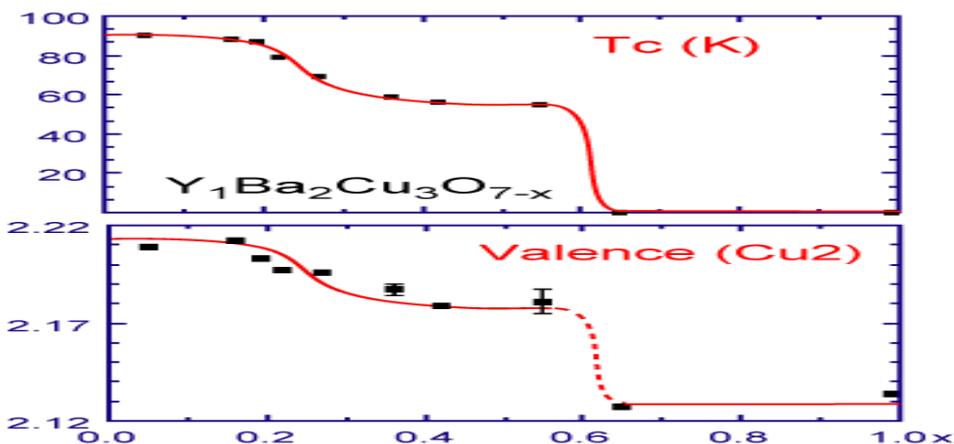


Figure 11. Variation of T_c with oxygen loss in $\text{YBa}_2\text{Cu}_3\text{O}_{7-x}$ showing two plateau regions followed by a sharp drop to the non-superconducting phase [13]. This variation is a reflection of the electron hole content of the super-conducting copper oxide planes, as obtained from the calculated “bond valence sum” for Cu^{2+} . The “charge reservoir” concept for high- T_c superconductor of this type lead to the discovery of new materials with record T_c 's.

Since the valence of copper in the conducting planes, and hence T_c , could be controlled by the structure and oxidation state of the charge reservoir, these neutron diffraction experiments lead to an intense search for new materials in which the copper oxide reservoir was replaced by other oxides. A great many different superconducting oxides were so discovered, and remarkably, materials with lead, bismuth and mercury oxide reservoirs were found to result in even higher T_c 's.

13 GIANT MAGNETO-RESISTIVE MATERIALS

In an oxide, metal atoms give up one or more electrons to the oxygen atoms, resulting in more stable electronic configurations for both types of atoms. Usually a fixed number of electrons are given up, characteristic of the “valence” of the metal. But some metals like copper or iron can give up a variable number of electrons. For example iron atoms can give up either 2 or 3 electrons, forming respectively divalent Fe^{2+} and trivalent Fe^{3+} compounds.

When metals exist with multiple valence in the same compound, they are said to be of “mixed valence”. A famous example is iron oxide, Fe_3O_4 , commonly called “magnetite” or “lodestone”. At ordinary temperatures, this is a metal-like conductor because an electron is free to move between the Fe^{2+} and Fe^{3+} atoms. When it is cooled to near the temperature of liquid air, it becomes an insulator because the free electron is “frozen” onto one of the Fe atoms, and

they separate into distinct Fe^{++} and Fe^{+++} ions. Fe^{+++} , with one less electron, is a little smaller and the oxygen atoms a little closer.

We have seen that neutron diffraction can be used to measure the metal-oxygen distances very precisely, and so reveal where these electrons are “frozen”. This is mainly possible because of the strong scattering power of oxygen relative to heavier metals, and the few systematic errors in the neutron powder diffraction technique.

Charge ordering in Fe_3O_4 is still not fully understood, but in simpler compounds, such as YNiO_3 , neutrons have beautifully illustrated the metal-insulator transition mechanism [14]. In fact they gave two independent proofs for the co-existence of two types of nickel atoms at low temperature; one was the difference between metal-oxygen distances, and the other was the difference between the “magnetic moments” on the two-nickel sites. Remember that neutrons are unique for measuring the magnetic scattering from atoms, since they are themselves tiny magnets.

There are more important materials for which these neutron techniques have been used to understand charge order, including superconductors and colossal magneto-resistive (CMR) oxides. In these latter materials, such as $\text{La}_{0.33}\text{Ca}_{0.67}\text{MnO}_3$, the charge-order transition can be made to occur near room temperature by adjusting the (La,Ca) stoichiometry [15]. Neutron diffraction has been used to study this charge order, allowing us to distinguish between different models (Figure 12) with very different physical implications. Because of charge ordering, there are very large changes in electrical resistivity with temperature and magnetic field, which have important applications in magnetic recording devices. IBM to make more efficient hard disks for computers is already using the earlier Giant Magneto-Resistive (GMR) materials.

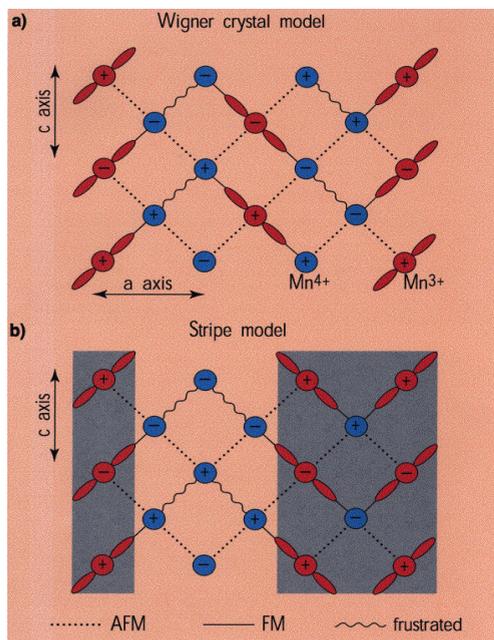


Figure 12. Alternative models for charge ordering in the CMR material $\text{La}_{0.33}\text{Ca}_{0.67}\text{MnO}_3$ [15]. The stripe model proposed from electron microscopy was ruled out by a combination of neutron and synchrotron diffraction.

14 NEW TYPES OF BATTERIES

Because neutrons are so penetrating, we can use them to study chemical reactions deep inside relatively large objects such as batteries (Figure13). And with large detectors we can collect the complete diffraction pattern in a fraction of a second, making it possible to study the electro-chemical changes in the battery in real time – during the charge-discharge process.

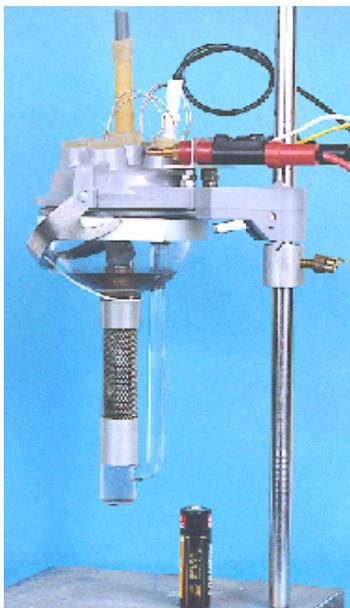


Figure 13. An electrochemical cell ready for study in the neutron beam compared to a real AA battery.

Energy storage materials have been subjects of intense research in recent years, following the rapid development of portable electronic equipment such as cellular phones and laptop computers. Two kinds of lightweight rechargeable cells are now available; Nickel-Metal Hydride (Ni-MH) and Lithium-Ion batteries. Both are charged by injecting electrons via an electrical circuit, which has the effect of intercalating light atoms (H^+ and Li^+) into the electrode. This intercalation can destroy the electrode after a number of charge-discharge cycles, and a detailed understanding of this mechanism is needed to improve the battery life. Since light atoms are again involved, neutron diffraction is the ideal tool.

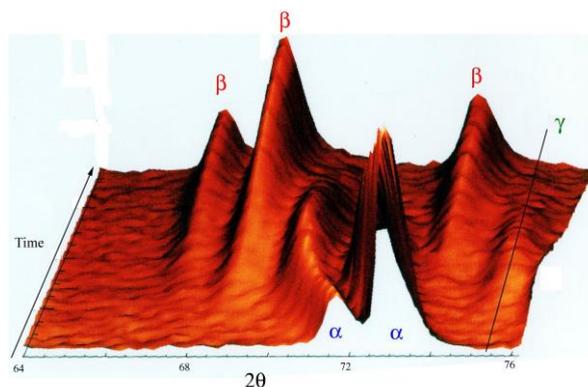


Figure 14. Neutron diffraction pattern as a function of time in seconds, showing the changes in the diffraction pattern corresponding with electro-chemical reactions in the electrical cell [16]. Understanding this chemistry should help us increase the lifetime of batteries and improve their energy storage capacities.

The neutron diffraction pattern from such a cell is shown in Figure 14, with the horizontal x-axis showing the scattering angle, the y-axis the time for charging/discharging the cell, and the vertical axis the scattered neutron intensity. The various peaks indicate changes in the structure of the electrode material. Not only can we determine these structures, but we can study the degradation of the cell as we repeat the charge/discharge cycle.

Extensive studies have been undertaken recently on the rare earth intermetallic hydrides of the LaNi_5 family, which are used as negative electrodes in Ni-MH batteries [16]. These hydrogen batteries replace highly polluting cadmium batteries, and allow more charge-discharge cycles. However, some problems remain with the use of metal hydrides. During cycling, important structural changes break up crystallites and greatly increase corrosion, thus reducing the battery cycle life. In situ neutron experiments diffractometer have helped overcome this problem by showing how the appearance of an intermediate structural phase can reduce internal stress.

Another problem is related to the high charge/discharge rates required by many applications. In situ neutron experiments could be performed during electrochemical cycling at high rates. By following the relative amounts and unit cell volumes of the metal and hydride phases, it was shown that the rate limiting factor was the kinetics of the metal-hydride transformation, rather than hydrogen diffusion.

These studies show that in situ neutron diffraction is a very powerful tool with which to study electrode materials in alkaline batteries. The next challenge will be in situ neutron studies of Li-ion battery electrodes. The aim of this work is to understand why batteries age, and the limits to their capacity, with the hope of developing lighter, more efficient and less polluting batteries that last much longer.

15 NEW TYPES OF CERAMICS

Many chemical reactions are even faster than those in batteries. If we can understand these reactions in real time we can perhaps improve the reaction yield and produce pure end products. This is the case for a fascinating new ceramic material, titanium-silicon carbide Ti_3SiC_2 that has the refractory and high temperature properties normally associated with carbide ceramics, combined with the electrical and thermal conductivity of a metal. We know that it is a layered material, with double layers of TiC interleaved with single layers of Si (Figure 15), and this laminated structure probably leads to its unusual combination of properties. This material is also quite ductile due to shearing of the layered structure that enables it to be readily worked with ordinary machine tools. Other mechanical properties include excellent thermal shock resistance, reasonable fracture toughness, a high Young's Modulus and good high temperature strength.

Unfortunately, Ti_3SiC_2 is difficult to synthesise as a pure phase, but the heat of formation is quite large, making it an excellent candidate for Self-propagating High-temperature Synthesis (SHS). SHS aims to use the heat of reaction as the primary energy source in the production of a material. Once ignited by an ignition source (laser, electron beam, furnace or electric arc) the reaction becomes self-sustaining and converts reactants to products very rapidly.

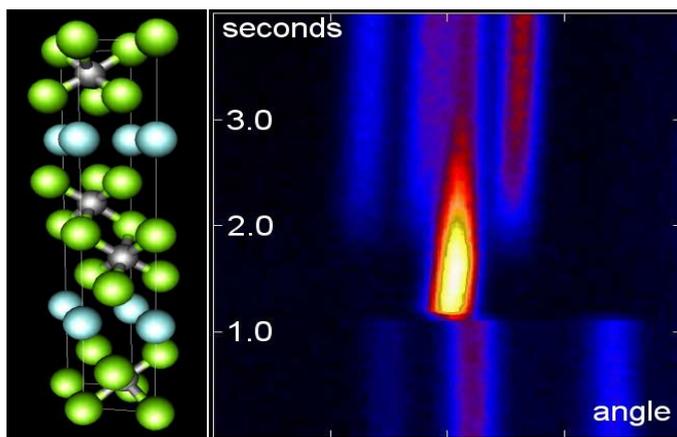


Figure 15. The structure of Ti_3SiC_2 (left) showing double layers of titanium carbide TiC (grey-green tetrahedra) sandwiched between single layers of silicon (blue). To the right we see the rapid growth and disappearance of a TiC intermediate phase during the reaction: the horizontal axis is scattering angle, the vertical axis time in seconds [17].

A recent experiment at ILL has allowed in-situ neutron powder diffraction data to be recorded at 0.9s time resolution [17]. Part of the diffraction pattern for one SHS reaction is shown in Figure 15, where it was found that pre-

ignition consists of a reaction of Ti with free C in the sample. As this reaction is exothermic, it provides local temperature increases that are the real ignition source. A single solid intermediate phase is formed in <0.9s - the SHS combustion reaction. It is believed that this intermediate phase is a solid solution of Si in TiC that is relatively stable at the combustion temperature but then becomes unstable and disappears as the temperature decreases. The final stage is the rapid nucleation and growth of the desired product phase Ti_3SiC_2 .

16 HYDROGEN STORAGE MATERIALS

The sensitivity of neutrons for light atoms such as hydrogen is naturally most important for hydrogenous materials. Hydrogen is an ideal ecological fuel. In an engine it burns to produce only water as waste, and conversely it can be recovered from water simply by using electrical energy. Unfortunately hydrogen is difficult to store, since in gaseous form it takes a lot of space, and it is very explosive.

However, new types of metal alloys can store even more hydrogen in solid form than is possible with liquified gas in a fuel tank. This hydrogen can be released simply by heating these metal “hydrogen sponges”. At present such alloys are expensive and relatively heavy. But new research at Geneva University aims to develop cheaper materials that are both light and can store large quantities of hydrogen that can be recovered by moderate heating.

The first step is to understand how hydrogen is absorbed, to localise the small hydrogen atoms in the space between the heavy metal atoms, and to imagine new more efficient structures. Neutrons are of course ideal for locating these light atoms, almost invisible to X-rays.

Two new materials discovered in Geneva, and characterised using neutron diffraction, hold the world records for the amount of hydrogen that can be stored, although neither is yet commercially cost-effective. In one of them, Mg_2FeH_6 shown in Figure 16, the density of hydrogen (150 g/litre) is more than twice that of liquid hydrogen (70 g/litre) [18]!

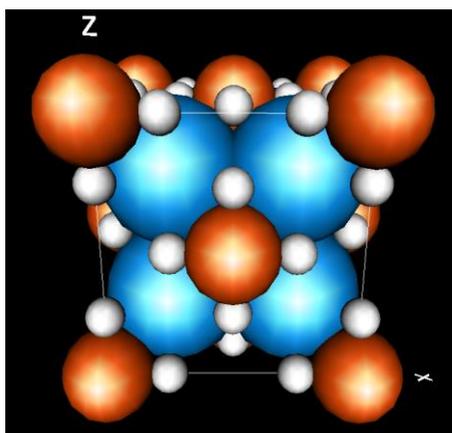


Figure 16. How 6 hydrogen atoms (H, white) occupy the interstices around the iron atoms (Fe, orange) in Mg_2FeH_6 . The density of hydrogen is then more than twice the density of liquid hydrogen [18]!

17 NEW ELECTRO-OPTICAL MATERIALS

Four decades on from the first demonstration of a lasing device, we find ourselves in the midst of an optical revolution. From high-speed optoelectronics and quantum optics, to laser light shows, and digital displays in cars and Hi-Fi's, the world has experienced this new form of light. The demand for so many different optical devices has led to a broad development and an explosion of new materials.

Non-linear optics (NLO) plays a major role, since it can enable highly desirable effects such as the doubling of the frequency of light. Known as second-harmonic generation (SHG), this frequency-doubling effect is used in lasers to change the colour of the outgoing light beam. The phenomenon can be illustrated by use of a lithium niobate LiNbO_3 crystal: when invisible infra-red laser light of a given frequency is shone through the NLO material, the SHG effect produces visible light - red, green or blue depending on the incident infra-red energy.

First observed in quartz in 1961, the materials used to generate the SHG effect have been normally inorganic - crystals of potassium dihydrogen phosphate (KDP) and lithium niobate, still being most important for industrial applications. In inorganic materials, the process relies on displacements of ions within the solid-state crystalline framework. The symmetry of the atomic structure is also crucial: SHG can only be observed in non-centro-symmetric compounds (i.e. those lacking inversion symmetry).

Structural techniques such as neutron and X-ray diffraction have played a vital role in understanding the link between atomic structure and physical properties, and this knowledge has led to the discovery of new materials that have better structural attributes for the NLO process. This has led, not only to the discovery of other inorganic materials for SHG applications, such as KTiO_3 (KTP), but also to the investigation of organic compounds. These latter studies were stimulated by the realisation that organic SHG materials involve the transfer of electronic charge across the molecule. Their optical response is therefore much faster than for inorganic materials where ionic displacements are needed.

The use of single-crystal neutron diffraction is particularly crucial where the hydrogen atoms are important for the charge-transfer process. Given that organic materials typically contain a number of hydrogen atoms, and that these necessarily exist at the extremities of molecules where the charge-transfer processes are often most important, knowledge of hydrogen atom positions and charges is often critical for understanding the SHG process.

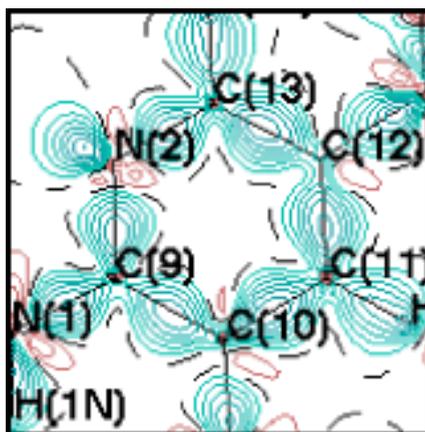


Figure 17. A contour map of the bonding electron density in an organic electro-optical material (MBADNP). Neutrons are used to locate the atom centers very precisely, especially those of the hydrogen atoms, and X-rays to then map the electron density around these centers to reveal charge transfer associated with the electro-optic effect [19].

At the ILL, the combination of X-ray and neutron diffraction data has been used to generate contour maps of electron density in several well-known organic SHG-active compounds (eg. Figure 17) in order to determine the critical regions of charge-transfer across the molecule [19]. These studies also determine the effective atomic charges and associated molecular dipole moments. They have shown that the nature of intermolecular hydrogen bonding is very important, with strong hydrogen bonding generally aiding the charge-transfer process. Some hydrogen-bonding arrangements appear to be more favourable than others.

The prospects for organic SHG materials are very good, although they have at present one major disadvantage compared with inorganic materials: that of thermal stability—organic materials have much lower melting point temperatures. In recent years however, there has been progress in overcoming this practical problem, using organometallic materials which also have a fast optical response while having good thermal stability like inorganic materials.

18 ZEOLITES AS CATALYSTS

Zeolite is derived from a Greek word meaning "boiling stone", since zeolites swell and lose water from their porous structure when heated. They have many important industrial applications due to their unique architecture, which consists of an aluminosilicate framework containing channels and cavities (Figure 18). They can be used as sieves to purify water, to separate out molecules of different sizes, to make detergents for the kitchen, to remove

radio-active elements from spent nuclear fuel, and as catalysts for many chemical reactions, especially in the petro-chemical industry [20].

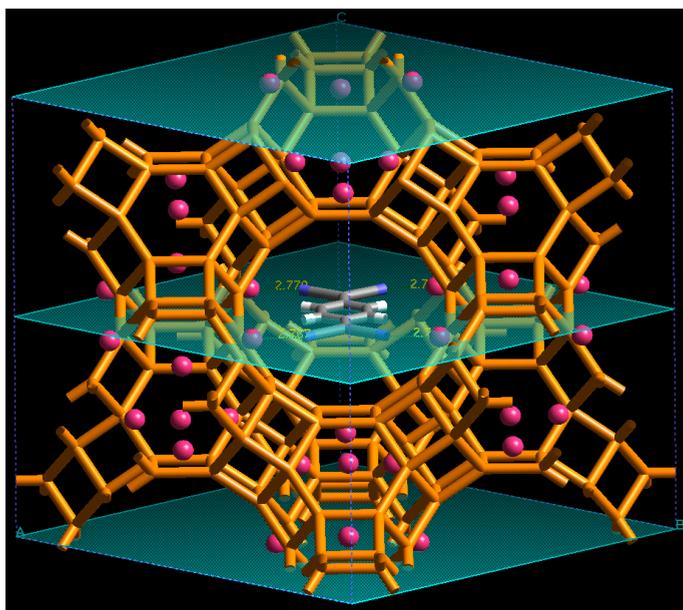


Figure 18. A small organic molecule trapped inside the pore of NaY-zeolite. Because of their porous structure, zeolites find many uses as molecular sieves and catalysts. Neutrons can help locate light atoms in such aluminosilicates, and can help distinguish between silicon and aluminium, which is more difficult with X-rays [20].

Zeolites are easily transformed to acidic or basic behaviour by adding various amounts of hydroxyl groups to the interior surfaces. In this activated form they are widely used in the petrol industry as catalysts for cracking oil, and for the production of fine chemicals. The absorptive and ion exchange capacities are the base for many washing powders.

Huge amounts of synthetic zeolites are produced every year, and a great deal of effort goes into the design of new materials with different pore systems, like the mesoporous carbide system (MCM) developed by the Mobil oil company. Neutrons are particularly suited to study both the structure and the dynamics of light cations, water or organic molecules in the voids and channels of zeolites.

19 MOLECULAR SIEVES AND ION EXCHANGERS

Toxic metals in the environment are dangerous for public health, and ways must be found to concentrate and remove them. This is a job for “ion exchangers”, which many people already use in their homes as water purifiers

or “softeners”. These minerals or synthetic resins trap the unwanted ions and replace them with harmless ions. (An ion is just an atom that has been electrically charged).

New types of mineral structures must be invented for specific ions, and we use neutron and X-ray diffraction to understand the structure of these materials, to guide their development.

For example, the ion-exchange capacity of aluminosilicate zeolites is proportional to the aluminium-silicon ratio (Al/Si), since replacing Si^{4+} with Al^{3+} allows other positively charged ions to be accommodated while still retaining charge balance. It is much easier to distinguish between aluminium and silicon using neutrons than with X-rays, since these two elements have similar atomic numbers.

In this material, the maximum Al/Si ratio that can be obtained is 1. However, the ion-exchange capacity can be further increased by replacing Si^{4+} by lithium Li^{1+} , since the lower charge on lithium will allow even more positive ions to be accommodated [21]. As well the lithium oxide polyhedra are more flexible and so can more easily accommodate other ions within their cavities. And of course lithium is a very light element, much more easily located with neutrons than with X-rays.

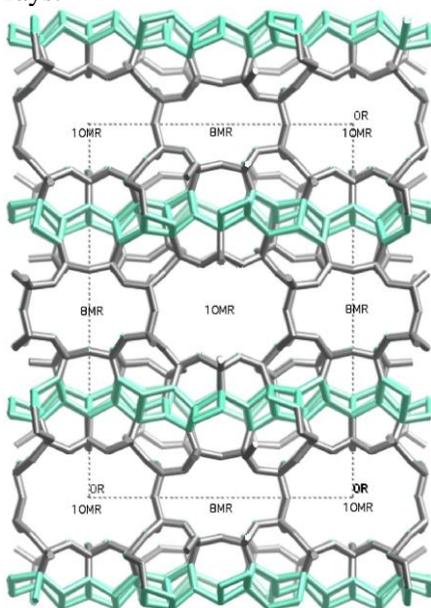


Figure 19. RUB29, a new lithium containing zeolite for removing radioactive cesium from nuclear waste [21].

Several new porous litho-silicates have been synthesized, including the complex framework structure RUB29 shown in Figure19. Here, only the Si-Si (blue) and Li-Li (grey) frameworks are shown. Notice the large channels surrounded by the flexible lithium oxide structure; these channels can accommodate large metal ions such as cesium, removing them from the

environment. This type of material is of real interest for cleaning up radioactive waste.

20 CLATHRATES

Clathrate hydrates are a little like zeolites, in that they encage small gas molecules in a framework of hydrogen-bonded water molecules. Known for almost 200 years, these gas hydrates were only recently found to exist in nature. Marine sediments were found to contain huge amounts of methane hydrate, estimated at 10,000 billion tons, a natural source of methane gas (CH_4) far exceeding other known fossil energy sources of coal, oil and gas. These clathrates will be of major economic interest once techniques for their safe extraction are established.

And one way of reducing carbon dioxide (CO_2) in the atmosphere, produced by burning such fossil fuels, may be to trap it as a CO_2 -hydrate and sink it in the ocean – a potential closed CH_4 – CO_2 carbon cycle with extraction of energy!

Clathrates are otherwise a nuisance in many gas and oil-pipelines where they cause blockages by a reaction of hydrocarbons with traces of water. Due to the wide-spread importance of these mysterious gas hydrates, many industrial nations have started research to better understand them.

Gas hydrates need high gas pressure and/or low temperatures to exist, conditions that are met on the ocean floor or in permafrost regions. Experimental work must then be done under non-ambient conditions, and because we are looking for light atoms in polycrystalline material at low temperature and high pressure, in-situ neutron powder diffraction has proved essential.

One of the main unknowns is the occupancy of the small and large cages as a function of pressure and temperature. Neutron diffraction has been used to establish this for a number of hydrates. The results allow for the first time a completely assumption-free check of the widely used statistical thermodynamic theory for gas hydrates.

Coming as a complete surprise it was found that the large cages in nitrogen hydrate were doubly occupied, violating one of the basic assumptions of the theory. Yet, in other cases (eg CO_2 hydrate) specific interactions between guest and host molecules must be introduced into the model. These findings are of major importance to chemical engineers [22].

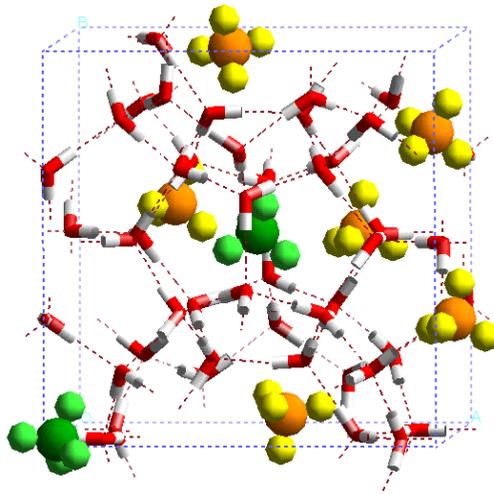


Figure 20. The clathrate “methane-hydrate” is formed when methane dissolves in water, and can be stabilized at high pressure and low temperature, for example at great depth in the ocean. Water forms a zeolite-like cage structure around the yellow and green methane molecules [22].

Another point of considerable interest is the compressibility of clathrate hydrates, needed for seismic profiling of the ocean floor. For the first time neutron diffraction has established the isothermal compressibility of a number of clathrate hydrates including methane (CH_4) hydrate (Figure 20). Finally, neutron experiments on CO_2 and CH_4 hydrate were helpful in understanding the molecular processes during clathrate formation and decomposition.

21 STRONGER AND TOUGHER ENGINEERING COMPONENTS

Every mechanical component is stressed to some extent, even when unloaded. This is due to different steps in manufacturing such as rolling and machining, heat treatment and welding. These residual stresses reside deep inside the material and influence the characteristics, performance and lifetime of the product, whether it be an automobile engine, a railway line or an aircraft wing.

To produce more reliable hi-tech products, and especially for applications where safety is a priority, it is important to know the distribution and the size of stresses in materials. Tensile stresses can favour crack development whilst compressive stresses can inhibit crack formation. For instance, hardening surfaces, by shot peening or other surface treatments, introduces beneficial compressive stresses.

The neutron strain imaging technique is a unique tool for the determination of residual stresses deep inside matter. It is non-destructive and allows mapping of stresses with a spatial resolution of typically 1 mm^3 or even finer. The high penetrating power of neutrons enables measurements through several centimetres of steel, aluminium etc. The principle is quite simple: compressive

stress shortens the lattice spacing (atomic distances) of crystallites inside the material, while tensile stress enlarges them. Neutron diffraction can be used to measure these atomic distances to a precision of 1 part in 10,000 and so it allows the determination of stress deep inside real engineering components [23].

A neutron strain scanner is an instrument for the determination of internal stress, especially for industrial applications. Of course it cannot be a routine testing method, but it can be used to learn how to develop stronger engineering components, and how best to weld, rivet or glue them together.

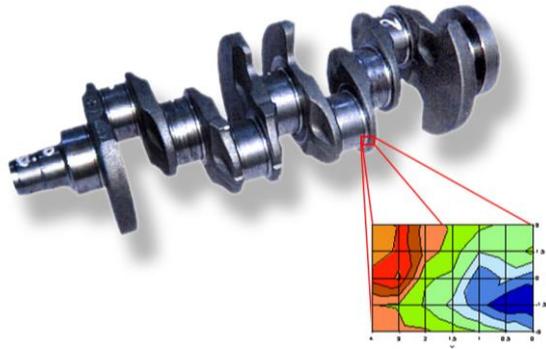


Figure 21. A typical sample for neutron strain scanning. Because neutrons are more penetrating than even X-rays, they see deep inside large objects, and can map the strain by measuring small changes in the spacing of planes of atoms [23].

Strengthening the crankshafts for automobile engines is one application. The problem is that a crankshaft can oscillate while it is rotating, and this has to be minimised to lengthen its lifetime. One way of doing this is deep rolling. During this process three wheels are turned around the work-piece while force is applied in the radial direction such that compressive residual stresses are introduced into the material to strengthen it.

The force and the length of treatment must be chosen to produce the required stress, and engineers perform finite element calculations to try to optimise these parameters. But these calculations, and the efficiency of the deep rolling procedure itself, must be checked by measuring the induced stress. That is where neutron strain scanning comes in. Figure 21 shows the result of such a measurement ± 1.5 mm around the deep rolled region and down to a depth of 4 mm below the surface. Compressive stresses are marked in blue colour, and it was found that in this case deep rolling had modified the stress field down to a depth of about 2 mm.

Due to the great potential of this technique, new strain scanners with improved characteristics for an extended range of applications are being built at

most neutron sources. They will enable measurements on specimens from 1 cm up to 2 metres in length, and weighing more than 500 kg.

22 CONCLUSION

We have seen that neutron diffraction can contribute to the understanding of many types of new materials, offering a different perspective to that obtained with the more common techniques of X-ray diffraction and electron microscopy. In practice, all of these complementary techniques are often needed. Neutrons are of particular interest for magnetic materials, or when light atoms must be studied in the presence of heavy atoms, and this is the case for many new oxides and hydrides. The disadvantage of neutrons is that the experiment can only be done at a very limited number of neutron sources – nuclear reactors or accelerators. Even then there are few neutrons so that samples must be relatively large – mg quantities. Neutrons are then often used for “definitive” experiments after all other methods have first been applied.

ACKNOWLEDGEMENTS

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Use of Small Accelerators in Materials Science

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1 ABSTRACT

High and medium energy charged particle accelerators are finding increasing applications in nuclear sciences. Small accelerators, on the other hand, are commonly used in medicine, environmental monitoring and materials science. In this article a brief review is given of applications in materials science, especially in surface analysis, wear measurement, fast neutron production for materials development, and radiation damage simulation studies. The interdisciplinary nature of work is emphasized.

2 INTRODUCTION

An accelerator is a combination of devices to produce energetic ions. In general it consists of three components:

- (i) Ion source;
- (ii) Accelerating system; and
- (iii) Beam extraction unit.

The technology related to each component is extremely advanced and there is a large variety in accelerators available today.

In principle, any charged particle could be accelerated. In practice, however, the emphasis lies on light mass particles that are more useful for practical applications. The commonly accelerated particles include e^- , e^+ , H^+ , H^- , $^2H^+$, $^3He^{++}$ and $^4He^{++}$. Heavier ions are also occasionally accelerated. They are mostly employed in fundamental nuclear studies (e.g. discovery of new elements), but some applications in materials research and cancer therapy also exist.

The energy range covered by the accelerators extends over a very broad span, from about 10 keV to several GeV. The scope of this review is limited to

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the use of small accelerators, with maximum energies of about 20 MeV. The small machines in this category include cascade voltage multiplier, betatron, van de Graaff, pelletron, cyclotron, etc. Each accelerator has its own special characteristics and, depending on the design parameters, can accelerate one or more particles. The beam quality and beam intensity, however, vary considerably from one machine to the other. The choice of a particular accelerator therefore depends upon its intended use.

Whereas high-energy accelerators involving very sophisticated technology are now being actively considered as future substitutes of nuclear reactors, both for supplying high neutron fluxes and for energy amplification, the use of small accelerators is of interdisciplinary nature and relates more to the present day practical applications. Many of the low-energy accelerators were designed and constructed for studies on nuclear reactions and nuclear structure. Although several of them are still being utilized for that purpose, the recent trend is more in the direction of medical applications, environmental monitoring and materials science.

The medical applications involve, on the one hand, production of short-lived radionuclides, especially positron emitters, for tomographic studies and, on the other, radiation therapy of tumours and sterilization of surgical instruments via irradiations with γ -rays, produced in the interactions of high energy electrons (from accelerators) with various metals. Some small accelerators are designed for work on environmental radioactivity monitoring. Several of the long-lived radionuclides, like carbon-14 (half-life = 5730 years) and iodine-129 (half-life = $1.57 \cdot 10^7$ years) can be determined rather precisely via accelerator mass spectrometry (AMS), a technique that combines a small accelerator and mass spectrometry. Of considerable interest are small accelerators also in materials science, and the present review is devoted to a description of some of the applications in that area.

As is well known, the field of materials science is very broad and almost any study dealing with some physico-chemical property of a substance could be placed under this heading. A detailed discussion of all the aspects is beyond the scope of this review. In this article four areas are considered in detail. They include surface analysis, wear measurement, fast neutron production for materials development, and radiation damage simulation. Small accelerators are ideally suited for those studies.

3 SURFACE ANALYSIS

For surface analysis two accelerator-based and somewhat related techniques, namely Rutherford Back Scattering (RBS) and Elastic Recoil Detection (ERD) are commonly used [cf. 1, 2]. The RBS involves characterization of the charged particle (mostly an α -particle) back scattered from a target nucleus. The angle and energy of the back-scattering particle are of paramount importance and a relevant spectral study leads to identification and quantification of the target

elements. Using well-established computer methods of analysis [cf. 3] it is possible to extract information on the overall composition, layer thickness and elemental concentration. The RBS technique is rather fast and, in a well-established laboratory, information about the depth distribution and elemental composition of most sample components and impurities can be obtained within about a 15 min experimental run. The technique is, however, only suitable for detection of medium and heavy mass elements. In the case of very light nuclei, the target nucleus experiences considerable recoil energy. The backscattering effect is therefore very low and the RBS technique is not suitable.

The second technique mentioned above, viz. ERD, is more suited to the study of light elements and involves the characterization of recoiling ^1H and ^2D nuclei ejected out of the sample [cf. 2]. By detecting the energy of the recoiling nuclei the depth-profile perpendicular to the surface of the target is measured. For several reasons, ERD is an ideal technique to study polymer systems, as far as the depth resolution is concerned. For a better understanding of surface and interface issues, however, a combination of several other techniques may be necessary.

Besides RBS and ERD, based on back scattering and recoil phenomena, respectively, a third technique, known as Particle Induced X-Ray Emission (PIXE), is also used for analysis of elements near the surface of the material. It involves the characterization of X-rays emitted in the interaction of charged particle beam (mostly proton) with a nucleus [cf. 1]. In general K X-rays are used for analytical purposes, and PIXE is an analytical technique of high sensitivity, especially in the medium mass region. In the case of energetic X-rays, analysis of not only surface layers but also of deeper lying layers could be performed.

The very light particle positron (e^+) also finds some analytical application. It is provided either by a radioactive source like sodium-22 (half-life = 2.7 years) or by a small accelerator. The probability of positronium formation (life time $\approx 10^{-7}$ s) depends on the chemical environment. A reconstruction of the transport process of the positron prior to its annihilation thus leads to useful information on the material properties, especially in the case of organic substances.

4 WEAR MEASUREMENTS

If the energy of the charged particle beam is sufficiently high, interaction with a target element will lead to activation, i.e. formation of a radioactive product. Since the incident beam rapidly loses energy in the material, the activation is restricted to the region near the surface and is therefore termed as *thin layer activation*. A very important industrial application of this technique is the study of wear of machine components such as gear wheels and motor parts [cf. 4, 5].

The material under investigation is at first irradiated at the available accelerator. The depth profile of the radioactive product depends on the primary energy of the particle and the excitation function of the reaction involved. Two commonly used activation products are beryllium-7 (half-life = 53 d) and cobalt-56 (half-life = 77 d). These are formed via $\text{B-10}(p,\alpha)\text{Be-7}$ and Fe-

$^{56}(p,n)Co-56$ processes on B and Fe containing materials, respectively. The next step after activation is the monitoring of the activity loss under simulated wear and tear conditions. The rate of activity loss reflects the rate of wear.

The principle of wear measurement is illustrated in Figure 1 [4,5]. A gear is removed from a machinery and a tooth is activated with a beam of 13.8 MeV protons from an accelerator. The cobalt-56 formed via the (p,n) reaction on Fe is distributed up to a depth of 190 μm . The activated gear is then reassembled in the machine, and one of two procedures is followed. The first involves removing the material debris with the circulating lubricating oil, collecting them on a filter, and measuring the activity. The second approach consists of bringing the detector near the activated component and monitoring the loss in the radioactivity. Since in both cases monitoring is continuous, the effect of various factors (e.g. temperature, additives to the oil, etc.) on wear rate can be investigated.

5 FAST NEUTRON PRODUCTION FOR MATERIALS DEVELOPMENT

For development of future nuclear energy systems, there is considerable need of production of fast neutrons to be able to study their effects on the properties of potentially useful structural materials.

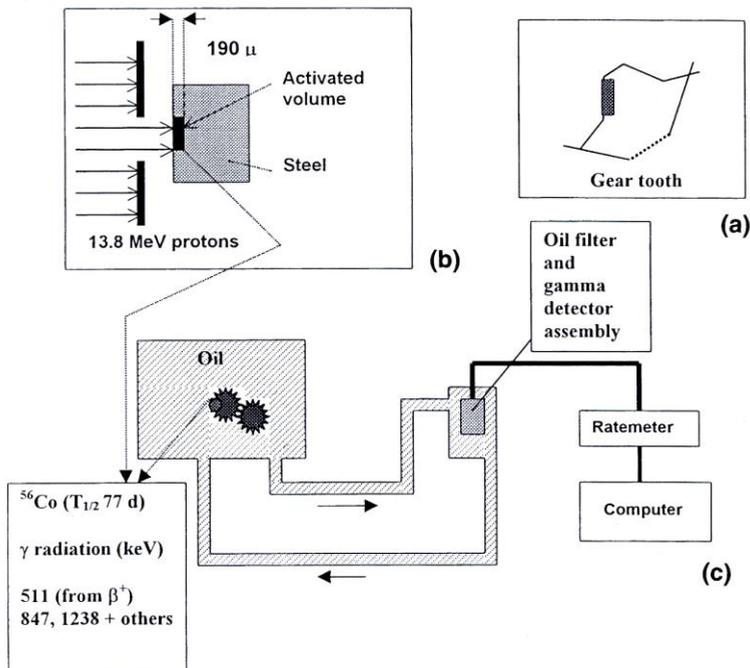


Figure 1. Study of wear rate using thin layer activation. (a) Gear tooth. (b) Irradiation of gear tooth with 13.8 MeV protons. (c) Measurement of rate of accumulation of wear debris on filter (after Refs. [4,5]).

Small accelerators play here an important role. For production of monoenergetic neutrons, use is made of the interactions of accelerated charged particles with some selected target elements like deuterium, tritium and lithium [cf. 6, 7]. The energy of the neutron depends on its angle of emission and the incident particle energy. High-energy continuous neutron spectra are commonly produced via interactions of high-energy protons with heavy elements. At small accelerators continuous neutron spectra are produced via the deuteron break-up process.

The use of monoenergetic neutrons is primarily in the determination of basic reaction cross section data relevant to the development of low activation and radiation resistant materials for fusion reactor technology. In this regard, excitation functions of all neutrons induced reactions that lead to long-lived activation products are needed. Furthermore, information is required on (n, xp) and $(n, x\alpha)$ reactions to be able to estimate hydrogen and helium gas production in structural materials.

As an example of measurement of long-lived activation products, reference is made to recent results on the $\text{Cu-63}(n, p)\text{Ni-63}$ reaction [8]. The product has a half-life of 100 years and emits only soft beta particles. It is thus difficult to identify. Measurement was done radiochemically using a small DT-neutron generator and a low energy cyclotron. These data are of great general interest since copper will be used as magnetic coil in fusion reactor technology.

It is known that radiation damage in structural materials is caused by displacement of atoms as well as by gas accumulation. Whilst the displacement effect occurring in present day fission reactors is fairly well understood, the effect of gas accumulation is rather obscure. In a fusion reactor the effect of gas production is expected to be very pronounced and hence the data need for (n, xp) and $(n, x\alpha)$ reactions is imminent. The elements investigated in recent years utilizing fast neutrons from small accelerators include Ni, Mo, V, etc. [cf. 9].

As regards continuous neutron spectra, the application is mostly in validation of differential data via integral studies. Small accelerators are thus quite important for material development programme for future fast reactor technology.

6 RADIATION DAMAGE SIMULATIONS

The damage caused by radiation to materials originates from two sources:

- (a) *Displacement of atoms.* In reactor technology, displacement damage in structural materials is caused predominantly by elastic and inelastic scattering of neutrons.
- (b) *Nuclear transmutation.* At higher neutron energies, foreign elements and hydrogen and helium gases are formed (see above). They may change the mechanical properties of the materials concerned.

Simulation experiments involving irradiations with charged particles from suitable accelerators can lead to a fundamental understanding of some radiation damage phenomena. Some results on the hydrogen induced embrittlement of martensitic steel (Fe, 8 % Cr, 2 % W) are given in Figure 2 [10]. The material was implanted with 7 MeV protons for various lengths of time. The hydrogen concentrations achieved were 0.05 and 0.11 %. The stress was measured as a function of strain. It is clearly seen that with increasing H concentration the tensile strength decreases. In other words, the material becomes harder with the increasing hydrogen concentration but the embrittlement also increases. Similar studies have been performed on materials implanted with He. Subsequent microstructure studies by transmission electron microscopy (TEM) showed that helium accumulates mainly at grain boundaries. Further investigations in this direction are continuing in many laboratories equipped with small accelerators.

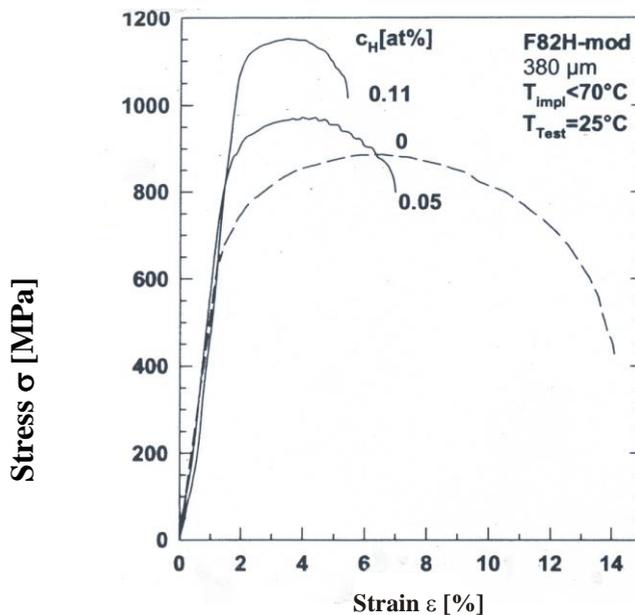


Figure 2. Hydrogen induced embrittlement of martensitic steel (after Ref. [10]).

7 CONCLUSION

Small accelerators are versatile tools and find application in many fields. Regarding materials science, they are mainly used for surface analysis, wear measurement, fast neutron production for materials development, and radiation damage simulation studies. In all types of studies, the interdisciplinary nature of work needs to be emphasized.

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Materials for the Future: A View of Academia

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1 ABSTRACT

Materials are a pivotal factor in the development of new technologies and their applications in all branches of engineering. The demanding environments of the new and existing applications require continuing development of materials with improved mechanical, physical and chemical properties. While research efforts concentrate on the study of new systems to come up with new materials, the push to improve performance of conventional materials continues unabated to keep up with technological advancement.

This review paper first discusses the evolution of traditional engineering materials by pointing out the advancement in steel and lightweight alloys with high strength and stiffness as required for automotive and aerospace structures. It is sought, furthermore, to summarize the recent enhancements in the synthesis, structural characterization, and properties, together with the potential application fields of various materials including ceramics, polymers and composites. Lastly, the striking advancements in the bulk amorphous and nanocrystalline metallic materials, the metal-hydride systems for the storage of hydrogen, and the bulk ceramic superconductors, are presented, giving also a special emphasis on their potential for the future applications in the magnet and energy technologies.

2 MATERIALS AS ENABLERS OF NEW TECHNOLOGIES

The development of many technologies that are important to society has been closely associated with the availability of materials that can fulfil a number of functional requirements. The performance of a material usually expressed in terms of mechanical, physical and chemical properties is the link between the internal structure of the material and the environment of the technology. Thus, a

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thorough understanding of the relationship between the structure and performance of a material is often the forerunner to the stepwise development of a technology.

The ever-increasing needs of society together with the exhaustibility of natural resources have been the major motivation behind technological advancement. A case in point is the energy bottleneck experienced in our era. The shortage of energy has resulted in the intensification of R&D efforts directed toward the goal to develop the renewable energy systems that proceed concurrently with energy saving measures. Access to appropriate materials can only enable the technologies needed to achieve these goals. For instance, significant quantities of energy are involved in transportation. Reduction of the weight of transportation vehicles as well as increasing engine temperature will enhance fuel efficiency. Thus, new high-strength, low-density materials have to be developed as well as materials with improved high-temperature resistance. Additional examples exist in the realm of nuclear energy, the utilization of which is hampered by the delayed solutions to material problems from fuel, to containment structures to facilitate the safe disposal of radioactive waste. Moreover, the large-scale application of solar energy will depend on the new substitutes for the presently used complex and expensive solar cell materials [1].

Like any kind of product, materials also go through a cycle from introduction, into a relatively stable period, and finally into decline (Figure 1). The word 'decline' is used here in the sense that the performance limits of the material are exceeded with increasing functional requirements. In such cases, the material should be replaced with a new one, in order to insure the viability of technology (Figure 2). It would be misleading to value the role and significance of technological development of materials in terms of its share in the final product cost. The silicon technology is a striking example that illustrates this particular point. Compared to investments made in various branches of information technologies, the material input remains at a level as low as 0.003 percent [2].

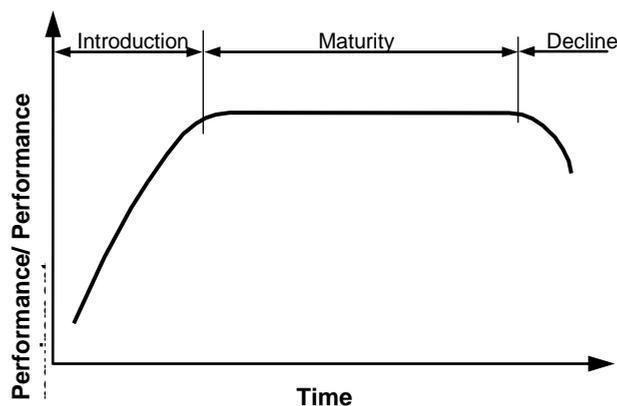


Figure 1. Modified material life cycle.

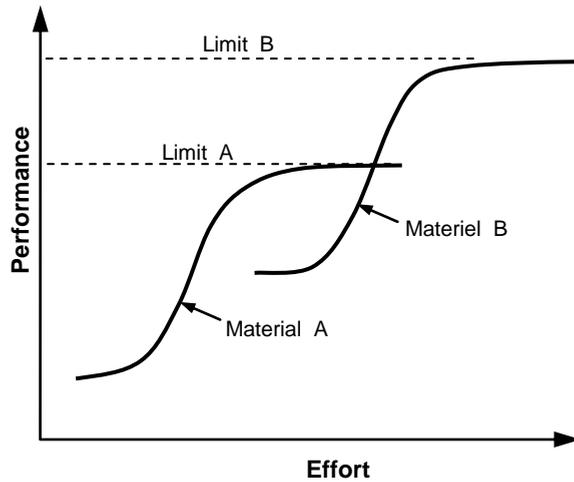


Figure 2. Replacement of material “A” with material “B” to keep up with the increasing performance requirement.

Materials that are of pivotal importance for various technologies and branches of industry are listed in Table 1.

Table 1. Materials that are of pivotal importance to various technologies and different branches of industry

MATERIAL	FIELD OF APPLICATION
Steels	Machine industry Automotive industry
Stainless steels	Chemical industry Food industry
Copper	Electrical industry
Aluminium alloys	Aerospace industry
Super alloys (nickel based)	Gas turbines
Titanium and its alloys	Supersonic flight
Hard metals	Manufacturing industry
Plastics	Packing industry Automotive industry
Fibre reinforced composites	Aerospace industry Automotive industry
Unidirectional solidified alloys and eutectic composites	High-temperature jet engine Applications
Single crystals	Turbine blades
Ceramics	Ceramic engine Space shuttles Dental implants Refractories

Table 1. (continued)

Polymers	Aerospace industry Automotive industry Electronic industry Fuel cell technology
Inorganic coating	Electrochemistry (High performance anodes) Solar energy
Silicon	Microelectronics
Glass fibre optic	Telecommunication
Gallium arsenide	Optoelectronics
Magnetic Materials	Storage of electronic information Microelectronics Electrical industry
Bulk amorphous/nanocrystalline alloys	Machinery/structural industry Electrical/electronic industry Clean energy technologies
Shape memory alloys	Electrical industry Aerospace/space shuttle industries Military/defence industries
Bulk ceramic superconductors	Energy technology Magnet technology Computer technology Medical diagnostic tool industry

3 FROM TRADITIONAL MATERIALS TO NEW MATERIALS

Based primarily on their chemistry and atomic structure, materials have been classified as metals, ceramics and polymers. Composites, semiconductors and biomaterials are the other families of materials of great technological importance. Metals are crystalline and non-directional. They are ductile and can tolerate large amount of plastic deformation. Due to the high mobility of electrons, the metals can conduct heat and electricity. In ceramics however, atoms are coupled with each other by covalent and ionic bonding. Unlike metals, the interatomic bonds in these materials are known to be directional. They are brittle and do not conduct heat and electricity, but have excellent resistance to harsh environments. The polymers are generally organic compounds that are based on carbon and other nonmetallic elements. Their large molecular structure consists of a long chain composed of entities called 'mer' units. The polymers are counted as an important group of light-weight engineering materials. They are weak but extremely flexible. High isolation capacity and excellent resistance to corrosion are additional useful properties of polymers that are of great interest to engineers.

The above grouping of materials, based also on differentiation of their performance characteristics, has been now severely violated by the continuing advancement in materials technologies. For instance, metals are obtained without a crystalline structure, when the cooling from the molten phase is carried out at rates higher than 10^6 K [3]. The so-called ‘metallic glasses’ produced by rapid solidification technique exhibit very special electrical properties that crystalline materials do not have. Unlike conventional metals, the metallic glasses perform very well in corrosive environments. Ceramics, known for their high brittleness, can now be produced with an appreciable level of toughness. Moreover, a new class of polymers is claimed to possess conductivity comparable to that of some metals. The conclusion we can draw from these limited examples is the fact that the rapidly growing diversification of materials with a wide variety of properties add numerous new alternatives to the existing materials.

Materials that are utilized in high-technology devices and products are sometimes called “Advanced Materials.” They can either be traditional materials the properties of which have been enhanced, or newly developed high-performance materials [1]. The engineering adaptation of newly developed materials is mostly a slow process. Experience has shown that the innovative work to generate a field of application needs intensive efforts on many fronts [5]. A new material with a well-defined application could be quailed as an “Engineering Material.”

The evolution and increasing pace over time of engineering materials is illustrated in Figure 3. The dominance of metallic materials in engineering applications started with cast iron technology and continued up to 1960 with the development of steels, light alloys and special alloys. Although the demand for cast iron and steel has decreased continuously, it should be envisaged that the push to develop metallic materials with improved performance would go on. The polymer and composite industries, on the other hand, are growing rapidly. In addition, ceramics and glasses and their composites are expected to expand rapidly to offer solutions to high temperature applications [4].

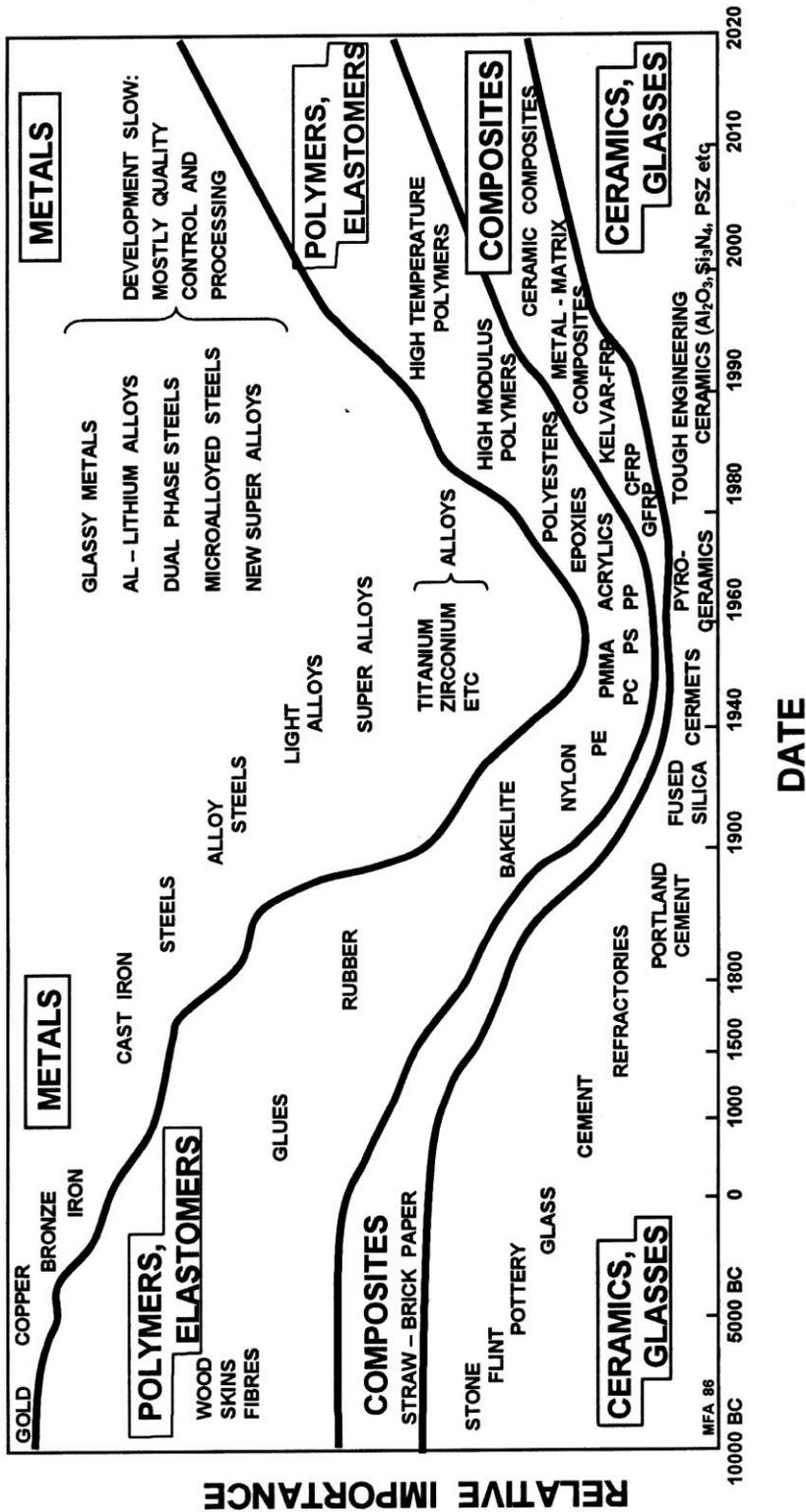


Figure 3. The evolution of engineering materials [4].

While researches and development efforts concentrate on the study of new systems to come up with new materials, the efforts to improve conventional materials continue unabated. Evidently, the threat of being replaced with a new material is the major motivation behind the rapid enhancement on the side of traditional materials [6]. The advancement in high-strength steels or lightweight aluminium alloys is a typical example of this development. Nitrogen, which was considered until recently as an impurity in steels, is utilized now as an alloying element to cause improved resistance to the pitting type of corrosion in stainless steels. In order to shed light on this important fact, the next section will deal briefly with the evolution of the two types of traditional materials, namely high-strength steels and lightweight aluminium alloys.

4 ADVANCEMENT OF TRADITIONAL MATERIALS

4.1 Steels

Among the multitude of metallic materials, steels represent by far the richest family with widespread uses in many branches of engineering. A significant part of more than 2500 types of steel available nowadays has entered the market in the last two decades. Although a treatment of all new types of steel can not be aimed at in the confines of this paper, it may be enlightening to emphasize that this oldest representative of engineering materials is still open to enhancements, in order to compete with other materials.

Lightweight construction has been the major driving force behind the development of special steels for automobile and other transportation vehicles. Steel producers have come up with a variety of high-strength steels to meet the need of automobile makers for materials with higher strength combined with improved formability. Figure 4 illustrates schematically the grain structure and strength of new multi-phase steels that derive their excellent mechanical properties from different strengthening mechanisms [7]. As a case in point, we will concentrate briefly on the dual-phase steel being currently applied by major automobile manufacturers.

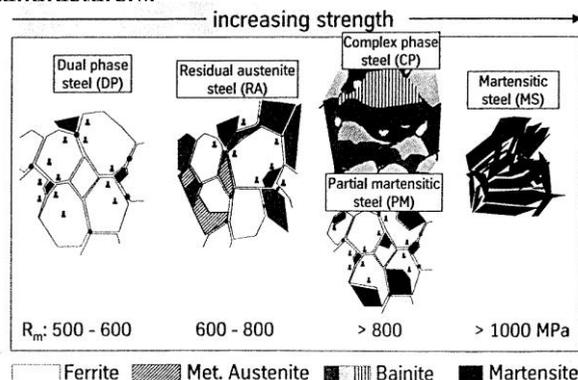


Figure 4. Enhancement of strength by different mechanisms of hardening in high strength multi-phase steels [7].

Unlike low-alloyed steels that generate their strength from precipitation hardening, dual-phase steels owe their excellent performance to a combination of two phases, called ferrite and martensite. The source of high strength is martensite embedded in soft ferrite. The ferrite surrounding the hard phase permits the easy shaping of steel. With their superior formability, dual phase steels have proved better performance in deep draw and stretch forming stamping operations. Their strength is enhanced through rapid work-hardening during the cold shaping followed by the bake-hardening. These treatments can increase the yield strength by about 80 percent over the unstretched material in sheet form. The improved strength of dual phase steels resulted in considerable decrease in sheet thickness by as much as 20 percent. As the sheet gauge became less, protection against corrosion becomes more important. Metallic coatings combined with organic ones are applied to compensate for the above disadvantage invited by the weight-reducing efforts. Another striking feature of dual-phase steels is their high strain-rate sensitivity, which makes the steel to adsorb more energy during impact loading. This means improved crash-safety achieved with less amount of steel [7,8].

In summary, the fast advancement in the science and technology of steel making has delayed the large-scale penetration to automotive industry of other lightweight materials as high-performance plastics or their composites.

4.2 Aluminium alloys

For automotive and aerospace structures, stiffness is the major requirement to secure structural efficiency. The modulus of elasticity, being a measure of stiffness, is generally proportional to the density of the metal. This situation represents one of the limiting factors of weight reduction in structures of transportation vehicles. Thus, it would be useful if this kind of structure could be manufactured using a lightweight alloy with improved modulus of elasticity. In addition, it would be advantageous if such an alloy would possess a strength increase combined with a reduction in density.

Lithium is the only element that has been known to increase both strength and modulus of elasticity when alloyed to aluminium. Since it is the lightest metal, its presence in solid solutions results in a marked decrease of density. For each one weight percent addition of lithium, the density of aluminium alloy is reduced by about 3 percent combined with an increase of rigidity by almost 6 percent. Thus, the aluminium-lithium system appears very promising with its potential to yield low-density alloys with improved strength and stiffness [9].

The effect of lithium added to aluminium is summarized in Table 2. As seen from this data, the specific modulus (modulus of elasticity/density), being a measure of enhancement, increased by 24 percent when the lithium content was increased to 5.5 atomic percent. For the same amount of lithium the increase of modulus of elasticity is 18 percent combined with a density reduction of 4.4 percent.

Nowadays, the R&D efforts on aluminium-lithium alloys are directed towards different goals dictated mainly by the demand of the aerospace industry. The first aim is to develop a medium-strength, damage tolerant alloy as a substitute for conventional aluminium-copper alloys. The second aim is to have high-strength alloys that would replace the 7000 series aluminium-zinc-magnesium alloys. Comparisons of these alternatives with the conventional aluminium alloys are given in Figure 5.

Beside high-strength and stiffness, ductility and toughness are additional requirements for automotive and aerospace structures. Unfortunately, the science of metallurgy has not yet succeeded in improving strength and ductility simultaneously. Thus, any improvement of strength is mostly at the expense of toughness. In case of aluminium-lithium alloys, it appears to be beneficial to have some magnesium in the alloy to insure an adequate level of ductility and toughness.

Table 2. Effects of lithium alloyed to aluminium [9]

Lithium at. %	Lithium wt. %	Modulus of elasticity E, GPa	$\Delta E, \%$	Density $\rho, \text{G/cm}^3$	$\Delta \rho, \%$	E/ ρ	$\Delta E/\rho, \%$
0	0	66	--	2.71	--	24.3	--
1.9	0.496	72	+9	2.67	- 1.5	26.9	+10.7
4.2	1.110	76	+15	2.62	- 3.3	29.0	+19.3
5.5	1.475	78	+18	2.59	- 4.4	30.1	+23.9

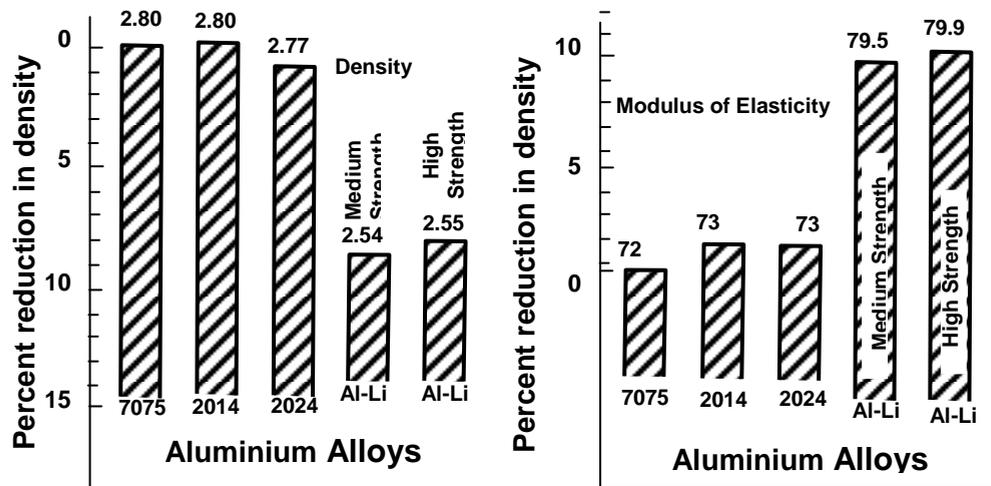


Figure 5. The density and the modulus of elasticity of medium-strength/ damage tolerant and high- strength aluminium-lithium alloys compared to conventional 2000 and 7000 series aluminium alloys.

The superplastic alloys that can tolerate shaping up to 1000 percent are of special interest to the aerospace industry. An aerospace structure that consists of many parts can be manufactured at a reduced number of components when the material behaves in superplastic manner. Superplastic shaping is claimed to yield considerable amount of material savings in the design of complex structures. Thus, the superplasticity remains one of the major directions in the future development of aluminium-lithium alloys. The enhancement of the superplastic forming ability is obtained by the addition of grain-refining elements such as chromium or manganese with an ignorable effect on the strength properties of alloys [9].

5 CERAMICS

Ceramics are compounds between metallic and nonmetallic elements that are most frequently oxides, nitrides and carbides. This existence of this class of inorganic materials we owe to the strong tendency of elements in the first two rows of the periodic table to form the strongest and stiffest solids. Many useful properties of ceramics are derived from the strong interatomic bonds of covalent and ionic nature established between the atoms of these elements. The strong directionality of this type of interatomic binding does not permit the formation of the close-packed structures. These fundamental features and the fact that the ceramics are formed with the lightweight elements explain the low density of these materials. Another useful property of ceramics is their high melting temperature, which can be attributed to very strong binding energies that keep atoms together [10].

With their high strength combined with high stiffness, low density, low coefficient of thermal expansion, low coefficient of friction, and high corrosion and oxidation resistance, ceramics offer interesting alternatives in a variety of engineering applications. However, brittleness has been their major drawback in their utilization as structural materials. Thus, one major direction in their development has been to generate some ways to overcome this disadvantage either by proper design of ceramic parts or by introducing some specific additives to the material. However, the very narrow range of solid solubility dictated by strong directionality of interatomic bonds imposes a severe limitation on this type of alloying. The so-called ‘ceramic alloying,’ therefore, will remain as an additional problem that has to be solved [10].

The big variety of ceramic materials classified as (a) silica ceramics (porcelain etc.); (b) oxide ceramics (aluminium oxide, ferrites etc.); and (c) non-oxide ceramics (carbon, silicon carbide, silicon nitride, boron nitride etc.) offers to a rich choice, especially in cases where the operational environment is severely harsh. However, the large-scale use of ceramics, as structural materials will require overcoming the following drawbacks [11]:

- The toughness and the resistance to thermal shock are inadequate for some applications;

- The control of process variables is not sufficiently precise to allow the production of ceramics with properties according to the well-established standards; and
- The measuring and controlling techniques usually applied to metallic materials are limited in their sensitivity and performance when used for ceramics. Evidently, new techniques have to be developed to insure the product quality and reliability in service.

In spite of the above drawbacks, ceramics may be successfully used in situations, where some of their useful properties can keep pace with the performance requirements. An example worth mentioning is the well-known project on the ceramic engine [3]. With an engine whose critical components are made from ceramic materials, it is aimed to overcome some limitations that are faced with conventional engines. Due to the low friction and wear, there will be no need for lubrication, meaning that a ceramic engine would be operated at higher temperatures compared to a conventional one. Owing to low heat of conduction, the heat losses will be minimized causing also less need for cooling. These enhancements will help increase the efficiency, since such engine will operate under nearly adiabatic condition. The exhaust gases that will leave the engine at higher temperature will be sent to the turbo chargers for further enhancement of efficiency. Silicon nitrides (Si_3N_4), silicon carbides (SiC), zirconium oxide (ZrO_2) stabilized partially with the yttrium oxide (Y_2O_3), and the magnesium oxide, are the potential materials that would be utilized in design ceramic engine. The partially stabilized zirconium oxide is characterized by its cubic structure combined with a tetragonal phase formed in the non-stabilized material. Owing to the crack blocking effect of this phase, the fracture toughness could be raised to a level almost twice the value achieved with silicon nitrides and carbides. Another advantage of the partially stabilized zirconia is its low thermal conductivity being especially suited to components as cylinder liner, piston and cylinder heads. The realization of the automotive type gas turbines that operates at temperatures up to $1360\text{ }^\circ\text{C}$ is a project for the distant future. Since this type of application will strongly rely on high-temperature resistance, the decay of strength with temperature should be another important design parameter. From the limited data available to date, it is evident that the material selection for high temperature applications has to be based on the optimisation between strength and sustainability with increasing temperature.

6 POLYMERS

There are many different types of polymeric materials with wide spectrum of applications that are familiar to us. These include plastics, elastomer or rubbers, fibres, coating, adhesives, foams and films. The polymer technology advanced largely through the discovery of new and improved catalyst system that enables optimisation of production and tailorable product properties. The improvements

in processing techniques and equipment include better moulding, extruding and other processes employing a wide variety of additives and reinforcements. With their great potential for improving the performance properties, polymeric materials will continue to replace other engineering materials in diverse fields from transportation vehicles to manufacture of medical devices. An example of this is the tremendous increase in demand for plastics in automobiles from 3 kg to 100 kg in the last two decades. Besides this, the polymers with improved performance will continue to enable the emerging technologies. A notable example is the fuel cell technology enhanced by the use polybenzimidazole (PBI), which provides excellent membrane property [12].

Another great advantage of this group of materials is the blend ability of two or more polymers allowing tailorable performance. Clay nanocomposites is another example of new compounding type of polymers. A 3 percent addition of fine clays uniformly distributed in the polymer matrix can increase the mechanical strength as high as 20 to 30 percent [12].

Research and development to improve polymer performance will continue to meet the need of new technologies. The future efforts in this area will aim to develop:

- (1) Shapeable polymer matrix composites as alternatives to metallic materials in autos and other transportation vehicles;
- (2) High-strength polymers that can be used also at elevated temperatures;
- (3) Conducting polymers as a new class of electronics materials and those with optical transparency; and
- (4) Polymers with special surface chemistry that can be used in different branches of biotechnology.

The most interesting advancement in the field of polymeric materials is the conducting polymer. Research in this field was initiated with the discovery, that polyacetylene, $(CH)_x$, could be doped with electron acceptors and electron donors to conductivity level ($\sim 1000 \Omega^{-1} \text{ cm}^{-1}$) approaching that of some metals. With the p- and n- type conductivity generated by this treatment, the age of the so-called 'Conducting Polymers' began.[13].

7 COMPOSITES

The well-known representative of composites is the glass-reinforced plastic (GRP), which spread quickly in the last three decades to meet needs for the weight saving materials. The push to improve the performance of polymer matrix composites continued by replacing the glass with carbon fibres. The further step of enhancement was the use of Aramid fibres with the high modulus of elasticity.

While the R&D efforts to improve the performance and in service reliability of polymer matrix composites continue unabated, attention has been

concentrated on new compounding areas. As indicated in Figure 6, the metals and the ceramics can be used as matrix material.

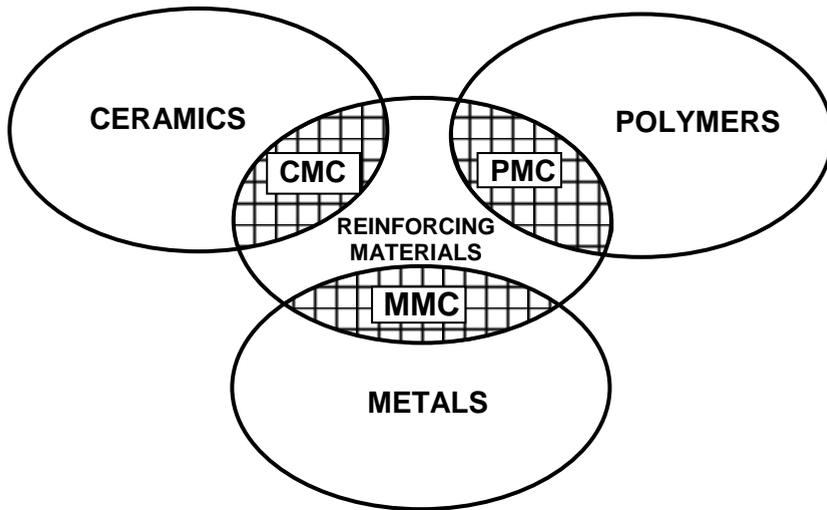
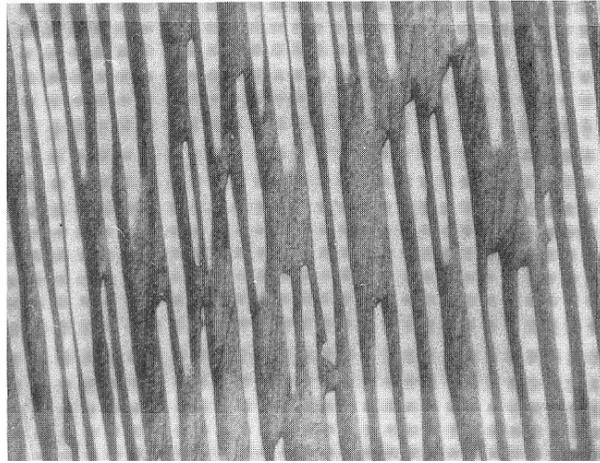


Figure 6. Composites are the products obtained by combining materials with different strength properties. MMC: Metal matrix composites, PMC: Polymer matrix composites and CMC: Ceramic matrix composites.

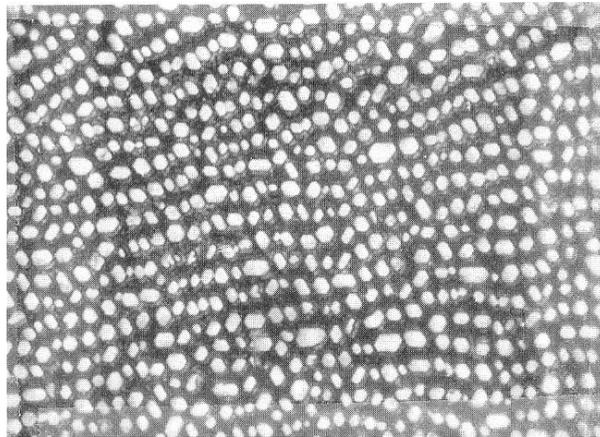
The fundamental concept underlying the metal matrix composites (MMC) is to strengthen the ductile metals or their alloys by reinforcing high-strength, high rigidity fibres. In addition to aluminium and aluminium alloys (6061, 2024 etc), magnesium, titanium, nickel, cobalt, copper and lead would be the potential metals that can be utilized as matrix material. Boron (with tungsten core), silicon carbide (with carbon core), silica, some alloys of tungsten and high-strength steels are the possible alternatives for fibre materials. In addition, the bundles manufactured from carbon, aluminium or nickel coated carbon, silicon carbide and alumina can be used as reinforcement in metal matrix composites.

Another type of the metal matrix composites is the eutectics produced by the unidirectional solidification technique. The unidirectional eutectics are considered as potential structural materials for high-temperature applications, because they have slow deformation rates and excellent microstructural stability. For high-temperature jet engine applications the unidirectional eutectics have many advantages over fibre reinforced composites produced by physical mixing of components. These advantages are the uniform distribution of fibres in the matrix, high-interfacial strength between metal matrix and each fibre, a relatively high microstructural stability at elevated temperatures and the continuous process of manufacturing since handling of fibres is eliminated. In eutectic composites, the volume fraction of fibres is not variable and fixed by the eutectic composites in the relevant phase diagram. The micrographs in

Figure 7 show the microstructure of a unidirectional solidified eutectic composite ($\text{Ti-Ti}_5\text{Ge}_3$) in longitudinal and transverse section [14].



(a)



(b)

Figure 7. Microstructure of the unidirectional solidified Ti-Ge eutectic composite: (a) longitudinal and (b) transverse sections.

Unlike the fabricated metal matrix composites characterized by a low interfacial strength between matrix and fibres, the unidirectional eutectic composites behave in a brittle manner. The low degree of misfit between matrix and fibres being the source of strong interface does not permit the blockage of cracks that may be initiated in matrix. Thus, high brittleness is the major drawback of these composites, which remain to be overcome to facilitate their utilization in high-temperature engine composites.

The increasing demand for high-temperature materials has stimulated great interest in ceramic matrix composites. As mentioned previously, ceramics are brittle, but their crack susceptibility would be diminished through the reinforcement of strong fibres. The most critical parameters that would govern the performance of this material system will be the concentration of reinforcement and the interfacial strength. The design of the ceramic matrix composites is the result of optimisation between these parameters to allow the matrix to crack first. A high interfacial strength is not desired since it would cause the simultaneous cracking of matrix and fibre. The different failure mechanisms of ceramic matrix composites compared to the metal matrix composites are illustrated in Figure 8 [15]. The potential materials for ceramic matrices include silicon carbide, silicon nitride, aluminium oxide, the partially stabilized zirconium, borosilicate glass, silica glass and LAC glass ceramics.

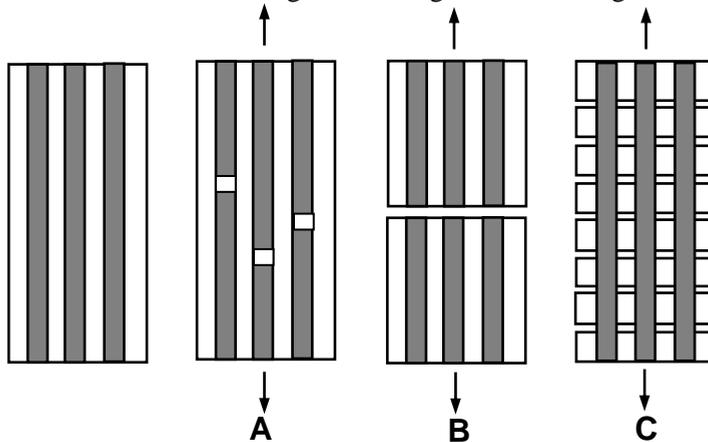


Figure 8. Failure types for fibre reinforced composites: (a) in MMC the fibres fail first to keep pace with the ductile matrix, (b) the simultaneous failure of matrix and fibre in a strongly bonded CMC, (c) the desired mode of failure in CMS's for which the weaker interfacial bond facilitates the matrix to crack first [15].

8 RECENT ADVANCEMENTS IN SOME OF NEW MATERIAL SYSTEMS

8.1 Bulk amorphous/nanocrystalline metallic materials

Amorphous metallic materials are metals and/or metal alloys with no long-range order in distribution of atoms within materials, resulting in the non-existence of defects such as grain boundaries or dislocations. These types of materials are also called glassy or non-crystalline alloys. Due to their structure, amorphous alloys show interesting properties, e.g. high strength and good ductility, superior corrosion resistance and excellent magnetic properties. Materials with each of the major bonding types, i.e. ionic, covalent, metallic, Van der Waals

and hydrogen, can be produced in the amorphous form. However, metallic amorphous materials are comparatively new in this group of materials. In 1959, Duwez and co-workers found that amorphous alloys could also be produced by the rapid cooling of a metallic alloy melt to ambient temperature by using quench techniques capable of achieving cooling rates of the order of 10^6 K/s [16]. Over the thirty years that followed, these early studies, the techniques of vapour and melt quenching have been extensively developed and elaborated for the purpose of producing a great number of amorphous alloy phases. Plasma sputtering, chemical vapour deposition and electron beam evaporation are a few of methods that are in use for the production of amorphous alloy films from the vapour phase, while melt spinning, liquid atomisation and splat cooling are examples of implementations of the liquid quench approach. Although a wide variety of amorphous alloys have been produced by using these techniques, the resulting sample thickness was limited to less than about 50 μm .

Requirement of very high cooling rates for these methods tends to limit the shape and size of the amorphous samples so that they cannot exhibit various types of desired physico-mechanical properties, which, in turn, restrict their widespread engineering applications. Amorphous sheets, ribbons and powders produced by rapid solidification techniques can be used to make a bulky shape by applying consolidation methods, however their properties are not desired ones and besides, manufacturing processes are complicated and uneconomical. Therefore, amorphous alloys produced by rapid solidification methods have not yet found widespread applications as engineering materials in many cases.

Since 1988, scientists have achieved great improvements in the glass forming ability (GFA) of the materials and have succeeded in producing new bulk amorphous multicomponent metallic alloy systems with much lower critical cooling rates and much higher sample thickness [17,18]. Figures 9 and 10 show the relationship between the critical cooling rate (R_c), maximum sample thickness (t_{max}), reduced glass transition temperature (T_g/T_m) and $\Delta T_x = T_x - T_g$ for bulk amorphous alloys reported up to date (T_g , T_m and T_x are glass transition, melting and crystallization temperatures, respectively) [17]. It is evident from these figures that, for Pd-Cu-Ni-P alloy the lowest critical cooling rate (R_c) is about 0.10 K/s and the maximum sample thickness (t_{max}) reaches values as large as 80 mm. There is a clear tendency for GFA to increase with increasing reduced glass transition temperature (T_g/T_m) and ΔT_x .

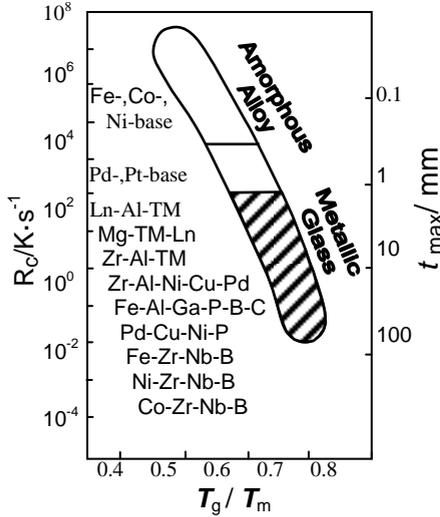


Figure 9. Relation among the critical cooling rate for glass formation, R_c , maximum sample thickness, t_{\max} , and reduced glass transition temperature, T_g/T_m , for typical bulk amorphous alloys [17].

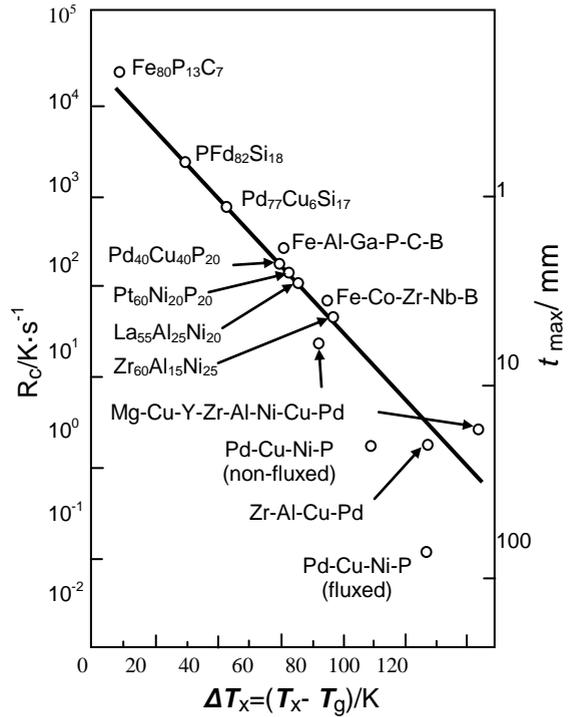


Figure 10. Relation among R_c , t_{\max} and $\Delta T_x = T_x - T_g$, for typical bulk amorphous alloys [17].

Table 3 summarises typical bulk amorphous alloy systems reported up to date and the calendar years when details of each alloy system were published [17,19,20]. Bulk amorphous alloy systems are divided into nonferrous and ferrous types. It is evident from Table 3 that bulk amorphous alloys can be produced by various solidification methods in the important engineering alloy systems of Fe-, Co-, Ni-, Mg-, Ti- and Zr-bases. The maximum sample diameter of the bulk amorphous alloys tends to increase in the order of $\text{Pd-Cu} > \text{Zr} > \text{Ln} = \text{Mg} > \text{Fe} > \text{Ni} > \text{Co} = \text{Ti}$ systems and the largest value reaches about 80 mm in diameter for Pd-Cu-Ni-P alloy as it can be seen from Figures 9 and 10.

Table 3. New multicomponent alloy systems with large glass forming ability reported up to date, calendar years when their first papers and patent were presented and the maximum sample thickness for glass formation [17,19,20]

I. Nonferrous Metal Base	Years	t_{max}/mm
Mg-Ln-M (Ln=lanthanide metal, M=Ni, Cu or Zn)	1988	
Ln-Al-TM (TM=VI-VIII transition metal)	1989	10
Ln-Ga- TM	1989	
Zr-Ar-TM	1990	30
Zr-Ti-TM-Be	1993	25
Pd-Cu-Ni-P	1996	72
Pd-Cu-B-Si	1997	
II. Ferrous Group Metal Base	Years	t_{max}/mm
Fe-(Al,Ga)-(P ,C,B,Si,Ge)	1995	3
Fe-(Nb,Mo)-(Al,Ga)-(P ,B,Si)	1995	
Co-(Al,Ga)-(P ,B,Si)	1996	
Fe-(Zr,Hf,Nb)-B	1997	
Co-(Zr,Hf,Nb)-B	1997	
Ni-(Zr,Hf,Nb)-B	1997	
Fe-(Co,Ni)-(Zr,Hf,Nb)-B	1997	6

t_{max} ; Maximum sample thickness.

Bulk amorphous alloys are an exiting new class of disordered materials because of their high strength, low friction, soft magnetism, resistance to wear and corrosion, almost zero thermal expansion coefficient and ability to be easily formed into desired shapes. Amorphous alloys show a unique combination of specific metallic and glassy properties. Some mechanical properties of bulk amorphous alloys are indicated in comparison to crystalline alloys in Figure 11 [18]. It is seen from Figure 11 that the features of mechanical properties of bulk amorphous alloys differ significantly from those of crystalline alloys. These distinct differences in the fundamental mechanical properties are very important for the future applications of bulk amorphous alloys.

Whether it can be called a revolution or simply a continuous evolution, it is clear that development of new materials and their understanding on a smaller and smaller length scale is at the root of progress in many areas of materials science [21]. This is particularly true in the development of new magnetic materials for a variety of important applications [22,23]. In recent years, the focus has moved from the microcrystalline to the nanocrystalline regime. The term “nanocrystalline alloy” is used to describe those alloys that have a majority of grain diameters in the typical range from ~1 to 50 nm. These materials will include alloys produced by rapid solidification, deposition techniques and solid-

state reactions where the initial material may be in the amorphous state and subsequently crystallized.

Over decades, amorphous and nanocrystalline materials have been investigated for applications in magnetic devices requiring either magnetically hard or soft materials, in particular, for various soft magnetic applications such as transformers, inductive devices, etc. Bulk amorphous and nanocrystalline magnetic materials, in terms of combined magnetic induction and permeability are now competitive with Si-Fe and Fe-Co bulk alloys. Relationship between permeability and saturation magnetization for Co-based amorphous alloys, Fe-based amorphous and nanocrystalline alloys are summarized in Figure 12 [22-24]. These bulk amorphous and nanocrystalline alloys have evolved over the past decades with soft magnetic properties, which now exceed those of the bulk metallic alloys based on Fe, Co and Fe-Co, as it is seen from Figure 12. Over the last few decades the most significant advancements in permanent hard magnetic materials has come in the area of rare earth permanent magnets.

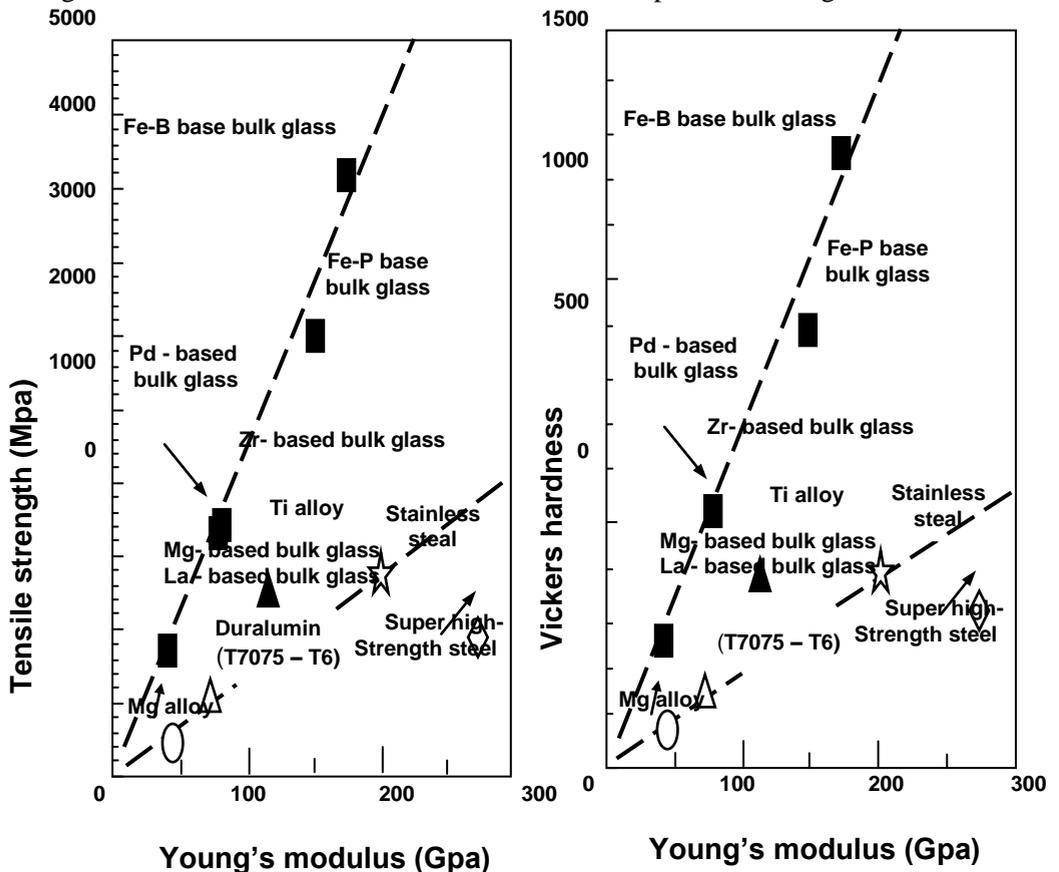


Figure 11. Interrelation of Young's modulus and tensile fracture strength or Vickers hardness for typical bulk amorphous alloys. The data of crystalline alloys are also shown for comparison [18].

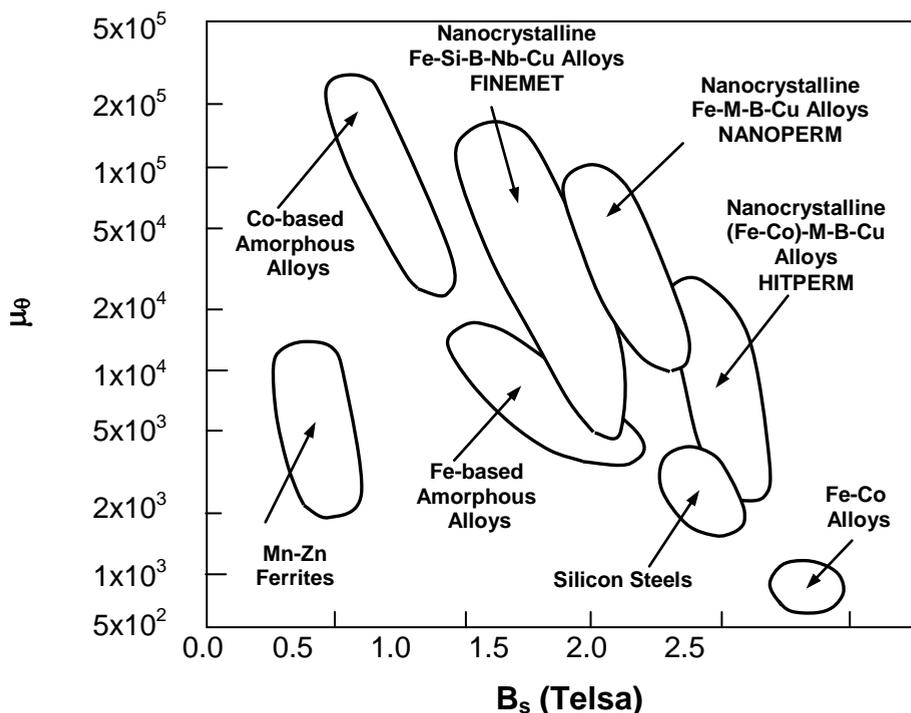


Figure 12. Relationship between permeability, μ_e (at 1 kHz) and saturation flux density, B_s , for soft magnetic materials [22-24].

These have a magnetic transition metal as the majority component, and a rare earth metal as the minority component, such as Sm-Co based and Fe-Nd-B alloys [22,23], Ln-Fe and Ln-Co (Ln = Nd or Pr) [25] based systems. For Sm-Co based alloys, optimum hard magnetic properties, notably coercivities are achieved in magnets in which the primary magnetic phase has a 50-100 nm grain size approaching the monodomain size.

Table 4 summarizes the fundamental properties and possible applications of bulk amorphous and nanocrystalline alloys [17,19,20], particularly including applications in machinery/structural materials, magnetic materials, acoustic materials, optical machinery materials, sporting goods materials and electrode materials. Unique mechanical properties, high corrosion resistance, good workability, good soft and hard magnetic properties and useful chemical properties are some of the useful characteristics of these materials. These important and unique characteristics of bulk amorphous and nanocrystalline alloys have already been commercialised in the fields of electrode and sports goods materials. Their use in machinery, structural, die, cutting tool, writing appliance and soft magnetic materials is under testing in several companies. Considering the recent significant extension of application fields, it is believed

that the importance of bulk amorphous and nanocrystalline alloys as basic science and engineering materials will increase in the near future.

Table 4. Fundamental properties and application fields of bulk amorphous and nanocrystalline materials [17,19,20].

Fundamental characteristics	Application field
High strength	Machinery structural materials
High hardness	Optical precision materials
High fracture toughness	Die materials
High impact fracture energy	Tool materials
High fatigue strength	Cutting materials
High elastic energy	Electrode materials
High corrosion resistance	Corrosion resistant materials
High wear resistance	Hydrogen storage materials
High viscous flowability	Ornamental materials
High reflection ratio	Composite materials
Good soft magnetism	Writing appliance materials
High frequency permeability	Sporting good materials
High magnetostriction	Bonding materials
Efficient electrode(chlorine gas)	Soft magnetic materials
High hydrogen storage	High magnetostrictive materials

8.2 The metal hydrides for the storage of Hydrogen

The environmental problems caused by the intensive use of fossil fuels, as well as their limited availability, are demanding a more rational and efficient utilization of our primary energy resources. When the latest desirability attached to any nonconventional energy option namely the environmental invariability (the non-polluting aspects) is coupled with the well-known factor, i.e. the depletive trend of the fossil fuels, it becomes evident that hydrogen is the potential candidate on the renewable energy problem [26]. Produced from water and on utilisation burnt back to water, hydrogen represents on the one hand the complete renewable cycle and on the other, it corresponds to almost zero pollution energy carrier. Hydrogen is a complete substitute for the important fossil fuel oil (petroleum) and can be used in a fuel cell to produce electricity. One of the most attractive features of hydrogen as a fuel is that its primary raw material is water.

Hydrogen can be produced in a variety of ways [27-29]. Regardless of the technique employed for hydrogen production, an inescapable aspect associated with the use of hydrogen as an energy carrier is its storage. Unlike fossil fuels like coal or petroleum, hydrogen has to be effectively stored before its employment in energy systems. One of the unique properties of hydrogen is that it combines with certain metals and alloys easily and in large amounts, forming hydrides in exothermic chemical reactions. When hydrides are supplied with

heat, hydrogen is released. The temperature and pressure characteristics vary for different metals and alloys. Advantage is being taken of these properties for many electrochemical and thermochemical applications (Figure 13) [30]. Smaller size hydrogen hydride batteries (e.g., for lap top computers) and larger batteries for electric cars have already been commercialised. There are demonstration projects for hydrogen-hydride air conditioning, refrigeration and heat pumps. As such utilities do not need chlorofluorocarbons, they will not damage the ozone layer. Conversion to hydrogen-hydride air conditioning and refrigeration systems will put a definite stop to ozone layer depletion.

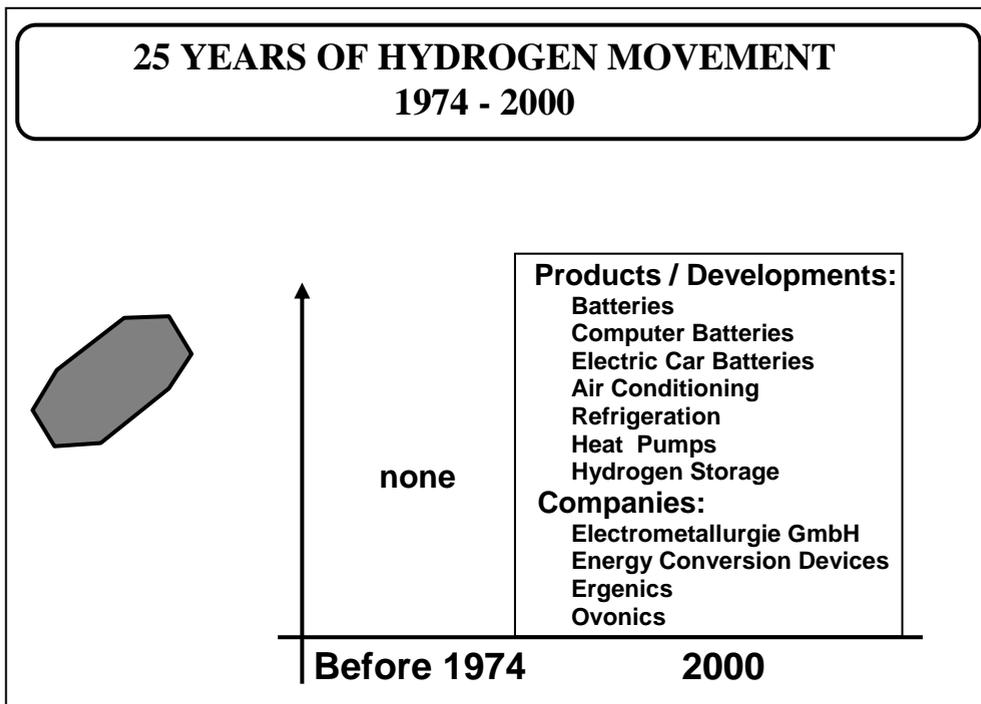


Figure 13. Hydrogen-Hydride applications [30].

The fundamental aspect to the understanding and use of rechargeable metal hydrides is the simple reversible reaction of a solid metal **M** with gaseous **H₂** to form a solid metal hydride **MH_x**. There are a number of metallic systems (intermetallic compounds) that react directly and reversibly with hydrogen to form hydride and do so at room temperature and nearly atmospheric pressure. These hydrides are called rechargeable metal hydrides. In effect, the metallic system becomes a solid sponge for hydrogen that can be repeatedly charged and discharged as well. One can draw a physical analogy with a water sponge and chemical analogy with a rechargeable electric battery. It is clear that rechargeable metal hydrides offer a number of advantages over its two

counterpart modes namely the compressed gas and cryogenic liquid storage systems. Some salient features about this are outlined below [26]:

- (1) Hydrides have an extremely high volume packing density for hydrogen. The volumetric density of H in typical hydrides is many times that of high-pressure gas and even significantly greater than that of liquid hydrogen (Table 5). This results from the fact that H-atoms are chemically bound compactly within the metal crystal lattice;
- (2) Storage of hydride mode requires low pressure. This aspect holds special importance concerning the safety factor; and
- (3) Hydride storage is more energy efficient as compared to liquid hydrogen.

The negative points related to hydride storage are the cost and the weight factors.

Table 5. Comparison of Hydrogen Storage Media [26]

Medium	Hydrogen Content Wt. %	Hydrogen Storage Capacity, g/ml of Vol.	Energy density Heat of Combustion (higher)	
			Cal/g	Cal/ml of Vol.
MgH ₂	7.0	0.101	2373	3423
Mg ₂ NiH ₄	3.16	0.081	1071	2745
VH ₂	2.07	---	701	---
FeTiH _{1.95}	1.75	0.096	593	3245
TiFe _{0.7} Mn _{0.2} H _{1.9}	1.72	0.09	583	3050
LaNi ₅ H _{7.0}	1.37	0.089	464	3051
RENi ₅ H _{6.5} (MmNi ₅ H ₆)	1.35	0.09	458	3050
Liquid H ₂	100	0.07	33900	2373
Gaseous H ₂ (100 Atm. Press.)	100	0.007	33900	244
N - Octane	---	---	11400	8020

Metal hydride compounds may be divided into three general classes: ionic, metallic and covalent [26]. This division is based on the predominant character of the hydrogen bond. For application purposes covalent hydrides can be left out since they cannot be formed by the direct reaction of hydrogen with the metal except under very special conditions. The ionic hydrides with the exception of magnesium hydride are too stable for the use in practical hydrogen systems. It is the metallic hydrides, which are most often employed in practical hydrogen storage systems. It has been shown that many alloys or intermetallics, prepared in the crystalline, amorphous or nanocrystalline form by using different production methods, react directly and reversibly with hydrogen to form hydride phases, which are often distinctly different to the binary alloy hydrides of the individual alloy constituents [27-29].

To serve as an effective hydrogen storage medium, a metal hydride must satisfy several criteria [26-29]. The most important criterion, of course, is that it must be easily formed and dissociated. From this point of view, the choice of useful metal hydrides automatically falls on the hydrides that will decompose at low temperatures (≤ 300 °C). Such hydrides are formed prominently from intermetallic phases of Mg_2Ni , $FeTi$ and RNi_5 . For the application of metal hydrides in utility devices, the consideration of the heat of decomposition of the hydrides is an important factor. To make metal hydrides self sustained energy wise, the heat of decomposition must be supplied from the waste heat of the converter with which it is coupled. From this point of view the operating temperature, the waste heat output of the energy converter and the pressure-temperature characteristics of the metal hydrides which are pertinent for their use in energy devices such as internal combustion engines, fuel cells etc., relate to their cost, safety, suitable reaction rate, reversibility, weight and physico-chemical stability. In the common usages, hydrogen can serve all the energy needs of a household. Figure 14 brings out the variety of uses to which hydrogen can be employed for a closed cycle household usage [26].

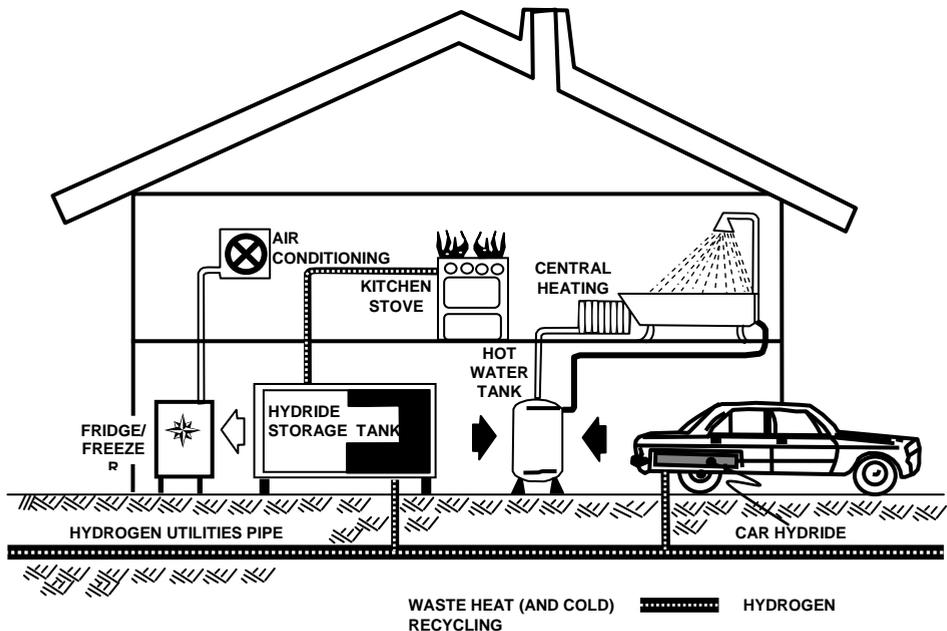


Figure 14. A closed cycle hydrogen home (waste heat is recycled by charging hydride tanks) [26].

The more general usage of hydrogen can be categorised as in the following [26-30]:

- (1) Automotive;
- (2) Electricity load levelling- Electricity storage;

- (3) Thermal storage- heating or cooling;
- (4) Waste heat storage;
- (5) Electricity generation;
- (6) Hydride compressors;
- (7) Pumping (e.g. water lift pump);
- (8) Hydrogen purification; and
- (9) Deuterium separation.

Therefore, it is apparent that the storage of hydrogen in the form of reversible solid hydrides is feasible and appears best (safe and may be even economic). Nevertheless, the limitation in this field is the rather poor storage efficiency. Because of this, there are on-going research activities for production of new more effective hydride materials, such as surface modification of well-known storage materials of LaNi_5 (MmNi_5), FeTi and Mg_2Ni , the synthesis of new transition metal complexes, composite materials and carbon variants (fullerens /tubules/fibres) with best storage properties [26-30].

8.3 Bulk Ceramic Superconductors

In late 1986 and early 1987, a major scientific breakthrough occurred in materials science. A new class of materials was discovered that displayed superconductivity at unusually high temperatures [31]. It is well known that superconductors are metals capable of conducting electricity with no losses of any kind. The possibility of cooling with liquid nitrogen instead of liquid helium made the application of superconductivity in energy technology much more probable and economically feasible. These superconductors constitute different classes of compounds than the old ones, raising the intriguing possibility of an entirely new mechanism of superconductivity. After the first observation of the phenomenon in 1911 in mercury at 4.2 K transition temperature, 19 years passed before reaching 9.2 K with niobium metal [32,33]. It took another 24 years to reach 18.1 K transition temperature with niobium-tin [32,33] and 19 additional years to go up 5 more degrees to attain 23.2 K with niobium-germanium [32,33]. In only 10 years since 1986, the transition temperature was raised progressively from 23 K to 35, 52, 95, 110, 125 and 133, Table 6 [34]. Applying a pressure of 30 GPa raised the transition temperature of the mercury superconductor to 147 K. There appears to be no end in sight and perhaps some day there will be a room temperature superconductor. A great source of motivation for the material development is commercialisation in useful systems built out of high temperature superconductors (HTSC). There are two major fields of applications for bulk and conductor material made from ceramic superconductors, namely magnet technology and energy technology.

Table 6. Progress in raising the superconducting transition temperature, T_c , since the discovery of Cuprates in 1986 [34].

Material	T_c (K)	Year
$Ba_xLa_{5-x}Cu_5O_9$	30-35	1986
$(La_{0.9}Ba_{0.1})_2Cu_4O_{4-x}$ (at 1 GPa pressure)	52	1986
$YBa_2Cu_3O_{7-x}$	95	1987
$Bi_2Sr_2Ca_2Cu_3O_{10}$	110	1988
$Ti_2Ba_2Ca_2Cu_3O_{10}$	125	1988
$Ti_2Ba_2Ca_2Cu_3O_{10}$ (at 7 GPa pressure)	131	1993
$HgBa_2Ca_2Cu_3O_{8+x}$	133	1993
$HgBa_2Ca_2Cu_3O_{10}$ (at 30 GPa pressure)	147	1994

Magnet technology is the traditional field of superconductivity and the first commercial applications of conventional superconductors were in the field of magnets for laboratories and particle accelerators. With the HTSCs, a further possible application is magnets that can be operated without a cryogenic liquid, using a closed-cycle refrigerator [33]. Still, the competition between conventional and HTSCs is very hard. The only opportunity for HTSC magnets will be in fields where the conventional superconductors definitely are at their limit. These areas of application are very-high field magnets and particle accelerators [35,36].

The idea of loss-less current transport in superconductors has encouraged much development work in the field of energy technology. Energy transmission cables made from HTSCs could meet the increasing energy demand of big cities using the old underground lines of the conventional copper cables. It was estimated that three times the electric power could be provided within the same underground cable tunnels by replacing the copper transmission cables by HTSC conductors [37,38]. Other AC systems in the power grid suitable for operation with superconductors are transformers, motors and generators [39]. Magnetic levitation (MAGLEV) offers a further possibility for the application of superconductivity. Magnetically levitated trains are being built in Germany [40] and Japan [41]. Superconductivity can also be used in energy storage devices where there are two possibilities, namely energy storage in a magnetic field and storage as mechanical energy in a flywheel [42].

All these systems have a few things in common [33]. For their fabrication, a long length of conductor or a large amount of good-quality bulk material is needed. Fabrication processes have to be found which provide reliable standard-quality material with reproducible mechanical and superconducting properties, sufficiently high critical current densities and affordable costs. This is not an easy requirement to meet. On the way, a lot of work has to be done in

understanding the specific properties of these materials and preparation processes have to be developed [33].

9 CONCLUSION

- (1) Materials have had the greatest impact on the development of many technologies that affect the quality of life in our complex society. The emerging technologies closely associated with solutions of the most severe problems in our era including energy and the environmental issues will require more sophisticated and specialized materials.
- (2) Viability of any technology will largely depend on the accessibility of materials with improved properties to fulfil the ever-increasing performance requirement. Thus, any delay in on-time replacement of an improper material causes a break off in the development of technologies.
- (3) The rapidly growing diversification of materials with a wide variety of properties adds new alternatives putting an end to the dominance of a group of materials for a certain of application. For instance, the high temperature superconductors or conducting polymers will replace the conventional metal conductors.
- (4) While the R&D efforts concentrate on the study of new systems to come up with new materials, the push to improve performance of traditional materials continues unabated. The notable examples of this development are the weight saving high-strength steels and light aluminium alloys.
- (5) New materials can be utilized in cases where their performance can keep up with the environment of an emerging technology. A case in point is the ceramic engine enabled by the excellent high- temperature resistance of ceramic materials.
- (6) Improvements in additives and processing techniques will continue to revolutionize the polymer technology. With their blends and composites, the polymers will allow tailorable performance characteristics.
- (7) The most effective way to enhance the performance of materials is to compound two or more solids. Polymers, metals and ceramics reinforced with high-strength fibres or particles result in composites with a tremendously wide range of properties.
- (8) The discovery and recent progress of exciting new bulk amorphous and nanocrystalline alloys, produced in rod, sheet and ring forms by using various casting processes, with unique and advanced physico-mechanical properties which cannot be obtained for conventional amorphous and crystalline materials, is promising for the future development of these nonequilibrium materials as basic engineering materials.
- (9) The production and storage of renewable and clean energy, such as hydrogen energy, has been one of the great scientific, technological and economic problems in the energy fields. During last quarter of the 20th century, hydrogen has made significant progress and inroads in several

directions in the energy fields, due to its unmatched superior properties and characteristics as an energy carrier.

- (10) Metal-hydrides based on intermetallics, disordered multicomponent alloys, carbon nanostructures and composite materials, provide a safe, low-pressure and high-volumetric density option for hydrogen storage, especially suited for smaller-scales and domestic use. The integration of photovoltaic electricity, water electrolysis and metal-hydride hydrogen storage will be critical for the introduction of hydrogen applications for general use, particularly in developing nations.
- (11) The recent discovery of new ceramic materials that possess superconductivity with inordinately high critical transition temperatures (above liquid nitrogen temperature of 77 K) has opened a new world of opportunities in the fields of energy and magnet technologies. However, technical barriers remain to be solved because these brittle ceramic superconductors must be processed into wire or similar structures without breaking.

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New Materials Applications in Medicine: A Snapshot

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1 ABSTRACT

Since time immemorial, materials have been used for the treatment of the health problems of mankind. Such materials included herbs, organic and inorganic materials (minerals, silver, gold, etc.) and products of alchemy, though their chemistry was not so well known as today.

This brief overview will deal with the use of modern materials or new materials in the field of medical applications, particularly in recent decades. This also will reveal the important aspect of the “interdisciplinary science” and the need for its further focus. Extensive use of new materials with stainless base, carbon base, ceramic base and titanium, observing the conditions of biocompatibility has been made in recent surgery and substitution of human parts, such as hip joints, knee caps, artificial heart (with titanium and polymeric materials), contact lenses in ophthalmology, artificial semiconductor eye, artificial pancreas and liver function aid materials etc. The functioning of an artificial heart for a couple of months for a terminal patient at a hospital in Louisville, Kentucky, USA, is an exotic example of this current year (2002).

New dental materials, ceramic screws, pastes, cements and alloys matching physical and thermal properties of teeth for better treatment are extensively in use.

Investigation of materials in medical science - particularly in structure determination of biological materials has led to several applications in gene therapy and genetic engineering. Recent examples are on the exotic use of nano-materials as drug-engines for *in-situ* treatment of tumours. In current research the use of Synchrotron Radiation (SR), a source of intense x-rays, obtained from Nuclear Accelerators, is providing an extensive information on biological

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materials in medical uses and related uses for angiography, mammography, osteoporosis etc. particularly improving the imaging techniques in health care. The health related materials investigations at nano-scale are thus a great promise in the field of medicine.

This brief description focuses on the importance of interdisciplinary science emphasising the use of the knowledge of physics, chemistry, and biology in modern medicine and medical studies in a complimentary approach. Some recent examples in the area of protein folding and other examples of protein handling are given.

2 INTRODUCTION

With the evolution of mankind, materials have evolved and so have their applications. With the passage of time, man discovered new materials, improved the production processes and discovered exotic applications to improve their life standards. Like man, materials have evolved through history from the Stone Age, to the Bronze, Iron, right the way through to the nuclear age and the current age of New Materials and Nanomaterials.

With reference to the use of materials in medicine, man has used these materials in the form of herbs, minerals, laboratory produced chemicals and pharmaceuticals for treatment of various ailments. Radio-pharmaceuticals are continually being used for diagnostic as well as for therapeutic purposes. Recent innovations in biomaterials are leading to the development of exotic bio-sensors and molecular engines for targeted drug delivery to specific tissues or organs.

In recent years, advanced materials with very special properties of strength, corrosion, flexibility, and biocompatibility have been prepared (Ball, 1999). In particular biomaterials are being used as replacement of body parts; artificial heart, hip joints, knees, etc. (Nordenberg, 2003; and Callaghan 2003), and for diagnostic and treatment of various diseases. With the introduction of nanomaterials and nanotechnologies, it is possible to produce materials with enhanced properties as compared to conventional counterparts. This has accelerated the pace of developing newer and newer applications (Drexler, 1997; McKeown 1997; NNI 2000).

Already, the use of new materials is extensive in medicine and rapid introduction of new applications is coming up. Therefore, only a brief description will be suitable in this “Snap Shot.” These applications mainly involve “Biomaterials” (Speidel and Uggowitz, 1998).

3 MATERIALS IN MEDICINE: BIOMATERIALS

3.1 General

Use of the new-materials in medicine has mainly the requirement of biocompatibility so that the materials used do not have damaging effects on the body.

“Biomaterials” (e.g. metals, alloys, polymers, carbons or composites) are defined as materials that interface with biological systems and are used to treat, augment or replace tissue, organ, or function of the body. These materials are generally no different in structure and properties to materials used in chemical, aerospace, or nuclear industries and are adaptations of these materials. Some of these materials in use for medical and dental purposes are given in the (Tables 1 and 2).

Table 1. Materials used in medical and dental applications based on biofunctionality

GROUP	PERFORMANCE
Pure Metals (Platinum, Gold, Titanium)	Aesthetics (in dentistry) Anti-bacterial activity, structural – orthopaedics, Structural – dental casing/hermetic sealed
Alloys (Ti – 6% Al-4% V, Co-alloys, Fe-alloys stainless steel)	Structural – orthopaedics, articulating surfaces Structural – dental, heart valves
Inert ceramics	Articulating surfaces, structural – dental
Bioactive ceramics and glass/ceramics <ul style="list-style-type: none"> • (Aluminium oxide Al₂O₃) • Calcium Compounds, Carbonates, and Phosphates. 	Structural – orthopaedics, Tissue regeneration Joint replacement bones and teeth
Carbons Carbon Fibres (reinforced polymers)	Control of blood flow
Thermoplastics	Control of blood and other fluid flow, articulating surfaces, minor structural, light transmission, drug delivery, membranes, tissue regeneration
Elastomers	Space filling, control of blood and other fluid flow, heart valves
Composites	Structural – dental, structural – orthopaedic, tissue regeneration
Biologically – derived materials	Tissue regeneration, control of blood flow, space filling

Table 2. Recent production of some biomaterials

Material	Producer	Claimed Properties	Applications	Status
Polyolefin film	Exxon	Highly porous, good barriers	Wound dressing	Customer testing
Polyurethane/silicon, composites	Corvita	Resists degradation in body	Organ implants	Customer testing
Amide elastomers	Elf Atochem	High flexural modulus, hydrophilic	Surgical drape, wound dressing, catheters	Customer testing
Thermoplastic polyurethane	PolyMedica Industries	Resists degradation in body	Organ implants	Customer testing
Shape Memory Polymers (SMP)	Mitsubishi	Temperature changes shape	Catheters	In use
Collagen Polymer Tube	Prof. H. H. Chen Medical College, Tainan, Taiwan.	Nerve Regeneration	Nerve Repair	Experiments on animals

3.2 Biocompatible Materials

Some examples of use of biocompatible materials; particularly in surgery are:

3.2.1 Artificial Heart: Jarvik- 7

Over seven hundred thousand persons die in the USA every year from heart failure making it the number one cause of death in that country. Although thousands need donor hearts for transplants in the US alone, about 2000 donor hearts per year are available for transplants. The need for artificial hearts has been felt over several decades and various attempts have been made in the past and in the recent years to replace the failing human heart with an artificial one.

The first artificial heart transplanted in a human was Jarvik-7 designed by Dr Robert K. Jarvik in 1970s. A team led by William Devries of the University of Utah implanted Jarvik-7 into the first patient, Barney Clark in 1982. He survived for 112 days with this Total Artificial Heart (TAH). (<http://sln.fi.edu/biosci/healthy/fake.html>). Another patient of Devries's named William Schroeder, implanted with Jarvik-7, survived for 620 days, and died in August 1986 (<http://www.journalisum.uts.edu.au>).

The Jarvik-7 Artificial Heart (Fuller and Rosen, 1986) has greatly benefited from advances in polymer development. The cutaway shows the left ventricle during systole. An inflow of air has expanded the diaphragm, forcing blood out

of the overlying cavity and into the aorta. The polyurethane Biomer, which is inert, flexible, and durable, is a major component of the housing and the diaphragm. Liquid Biomer is also poured into the cavity to form a smooth, uninterrupted blood-contacting surface. Other polyurethanes form the base and the openings at the top. Dacron, a polyester, gives rigidity to the housing. Of the non-polymers, graphite lubricates the diaphragm and gives shape to the valve disks; pyrolytic carbon makes the disks strong and glassy with titanium as the durable, non-corrosive frame for them. The essential design and parts, and the type of the materials are given in (Figure 1) and (Tables 3 and 4). The later model, Jarvik-2000 was implanted in a patient from Israel (<http://www.journalism.uts.edu.au>).

Table 3. Components of the Jarvik-7: Complete artificial heart

Ventricle housing, diagram, general adhesive, coating on base	Segmented poly (etherurethane-urea) (PEUU) (Biomer)
Quick connect fittings (between housing, arterial cuff and arterial graft)	Polycarbonate (with PEUU Coating)
Vascular graft anatomic connection (Weaves)	Poly (ethylene terephthalate)
Reinforcing mesh for housing	Dacron
Heart valves, discs, rings and struts	(Medtronic-Hall or Bjork-Shiley) Carbon (Pyrolite-coated) Titanium
Right and left ventricle connectors	Polypropylene or nylon (Velcro)
Base (for air chamber)	Aluminium
Tubes (to air supply)	Poly (vinyl chloride plasticized and wire reinforced)
Lubricant between diaphragm bladders	Graphite

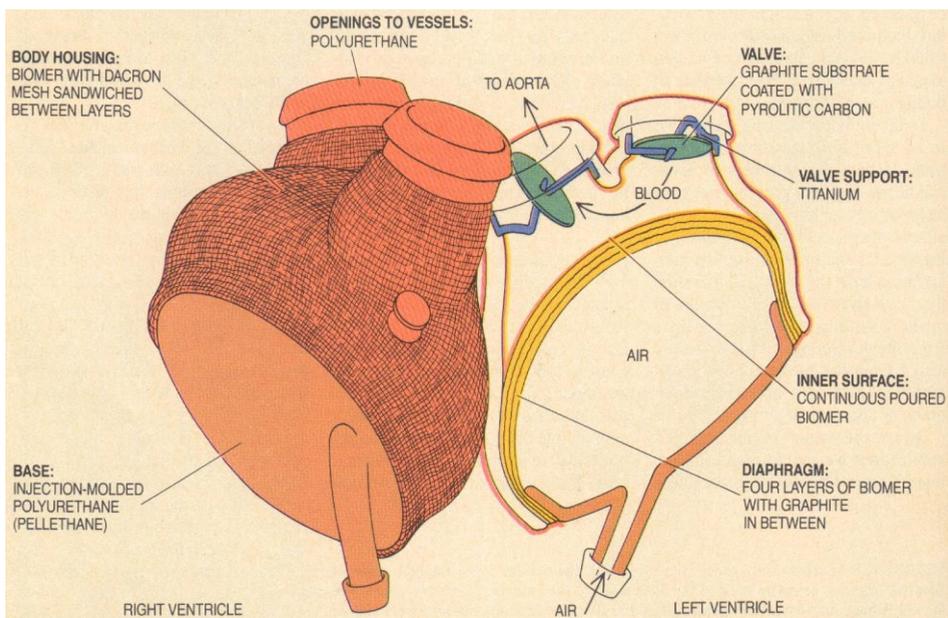


Figure 1. Jarvik-7 artificial heart.

Table 4. Polymeric biomaterials

Properties	Examples	Uses
Soft (rubbery) Low water sorption	Silicone rubber, polyurethanes, poly (vinyl chloride)	Tubes, diaphragms, coatings, implant, catheters, pacemakers, adhesives, and blood bags.
High water sorption	Poly (hydroxyethyl methacrylate)	Contact lenses, burn dressings, coatings.
Amorphous (hard)	Poly (methyl methacrylate)	Contact lenses, intraocular lenses, dental and orthopaedic cements.
Semicrystalline Low water sorption	Poly (ethylene terephthalate), Polypropylene, poly (tetrafluoro-ethylene) Nylons, poly (glycolic acid) Polyethylene, poly (perfluoro-ethylene-propylene), cellulose acetate	Sutures, vascular grafts, sewing, anchors, tissue ingrowth materials Sutures (biodegradable) Intrauterine devices, bone joints, catheters, hollow-fibre dialysers, contact lenses.
Moderate water sorption	Cellulose	Dialysis membranes

3.2.2 AbioCor models of artificial heart

In recent times, a more widely used model of the total artificial heart was designed by the company M/S ABIOMED Inc. This TAH model called AbioCor can currently benefit over 100,000 people as claimed by this Company (<http://www.hearpioneers.com>).

A very famous AbioCor successful implant was done recently by a team at the University of Louisville, Kentucky, USA led by L. A. Gray Jr and R. D. Dowling on a patient, Robert Tools, on July 2 2001 (<http://www.abcnews.go.com>). The device is powered by an external battery without piercing the skin for any leads. The power is transmitted to the device through a coil inside the body. The transmission of power to the device from outside without leads is a great advancement in the technology of artificial heart programme of AbioCor.

One of the major difficulties with Jarvik-7 was the problem of blood clotting which has been solved by making the walls of TAH microscopically smooth. With the advent of nanotechnology, it may be possible to achieve smoothness level at the nanoscale, thereby reducing the chances of blood clotting still further.

Presently AbioCor Artificial Heart implants cost about \$160,000, which is mostly used design. As of March 2003, ten such total artificial hearts had been implanted and two recipients remained alive (Website: ECRI Press Release: March 28, 2003).

3.2.3 Pace-maker leads

To help the weaker heart “pace-makers” are frequently being used for stimulation of nerves. The successful ‘leads’ inside the body for the electrodes used in the pace-makers are made from CF lead wires.

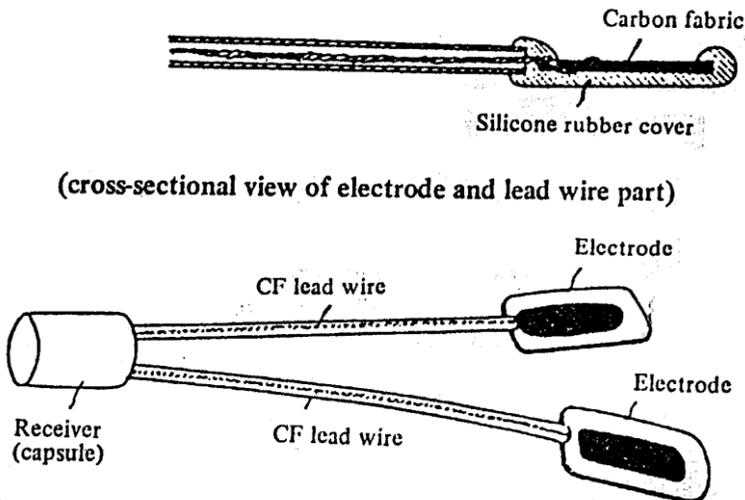


Figure 2. Electrodes embedded within the body.

The advantages of CF leads are mainly that they have: (i) No foreign body reaction; (ii) Good electrical conductivity; (iii) Flexible (un-breakable); and (iv) No degeneration of body tissues for long use.

3.2.4 Hip- joints

Hip and knee joints of normal active person are loaded and un-loaded, by flexing and extending them, between 1-3 million times per year. They may need to be replaced in some cases. In addition, hip joints in old age, particularly of women, often get broken when fall occurs due to some accident. In recent years total hip – joint replacements using biomaterials have been successfully made extensively. Nickel-Cobalt-Chromium alloys have been found very effective (Donachie, 1998). The hip-joints replacements may have life as long as thirty years which is indeed more useful for old age implants (Nordenberg, 2003).

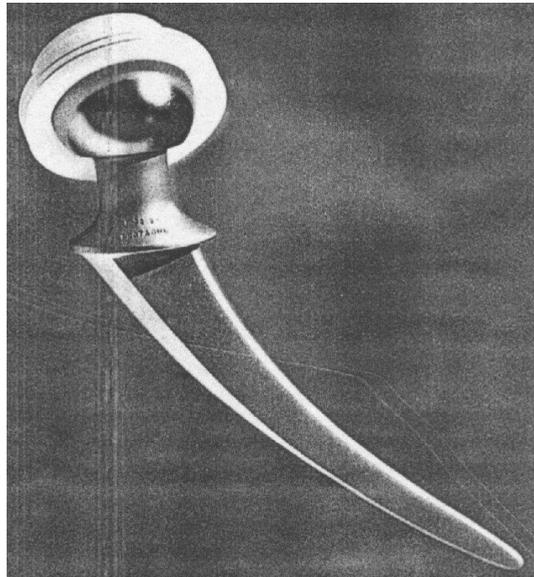


Figure 3. Stainless steel cobalt-chromium.

Such biomaterial alloys have specific mechanical and corrosion - resistant properties useful for such surgical applications. They are also of choice for angioplasty stints, pace-maker leads and cases and surgical clips and staples. For structural applications in the body, the most common metals are stainless steel, cobalt chromium alloys and titanium and its alloys. Tantalum is used for cranial plates and surgical staples. New developments in Total Hip Joint replacements have come up with metal with plastic cup and some successful attempts have been made with ceramic bearings.

(<http://www.other.cz/etypes.htm> dated 25 August 2003).

3.2.5 Bioartificial Liver

Bioartificial liver developed at the University of Minnesota in collaboration with Regenerex, a tissue engineering company in Minneapolis, consists of many thin hollow fibres arranged in parallel within a cylindrical cartridge.

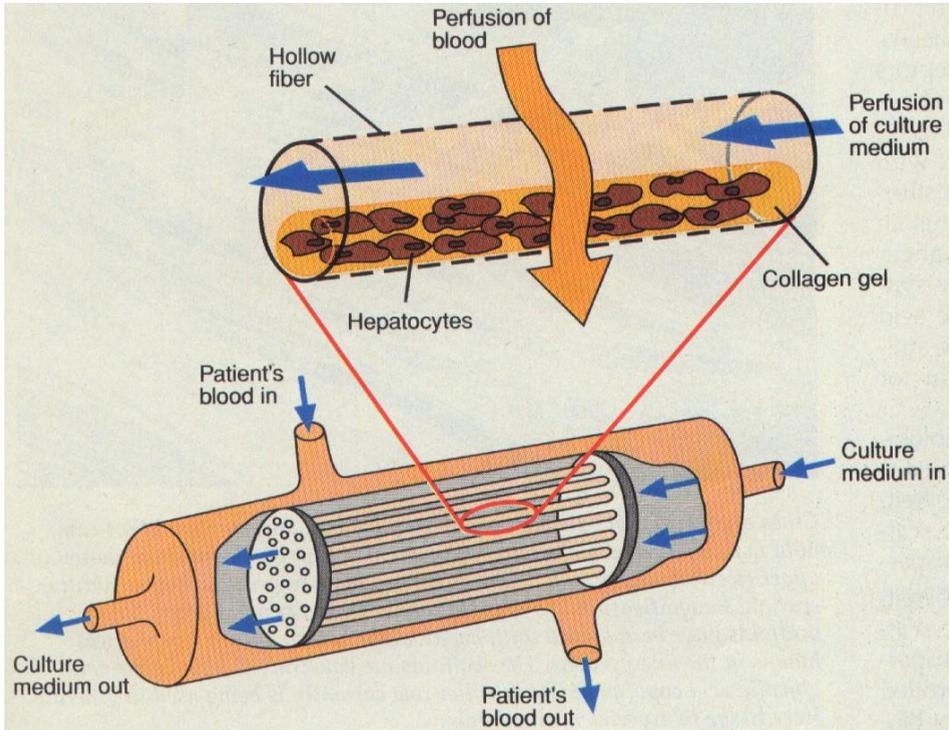


Figure 4. Bioartificial liver (Ref. Hubbell and Langer, 1995).

Each hollow fibre (inset) contains pig liver cells (hepatocytes) embedded in a collagen gel over which culture medium flows. The cartridge is encased in a larger container that has inlet and outlet ports for the patient's blood, which perfuse around the fibres, allowing the hepatocytes to remove toxins from it. The culture medium delivers nutrients to the hepatocytes to help keep them functioning. Each cartridge contains 13,500 fibres, and each fibre contains more than 200,000 hepatocytes.

3.2.6 Artificial pancreas

Experiments are in progress for the use of artificial pancreas in humans to address to the problem of diabetes, this common disease the world over. Artificial pancreas reduces blood sugar levels to normal levels in dogs with experimentally induced insulin-dependent diabetes. A coiled, tubular, hollow-fibre ultra-filtration membrane (green) housed in an acrylic disk (grey) is connected to Teflon grafts (blue) that are sewn to abdominal blood vessels as a

shunt between an artery and a vein. Insulin-producing cells injected through ports in the housing into the cavity (red) between the coil and the housing supply insulin to blood flowing through the coil. The membrane, which has a molecular weight cut-off of about 50,000 Daltons, is permeable to insulin, nutrients, and cell wastes but impermeable to immunoglobulins and other components of the host's immune system. Such a device may one day be used to treat insulin-dependent diabetes in humans (Figure 5).

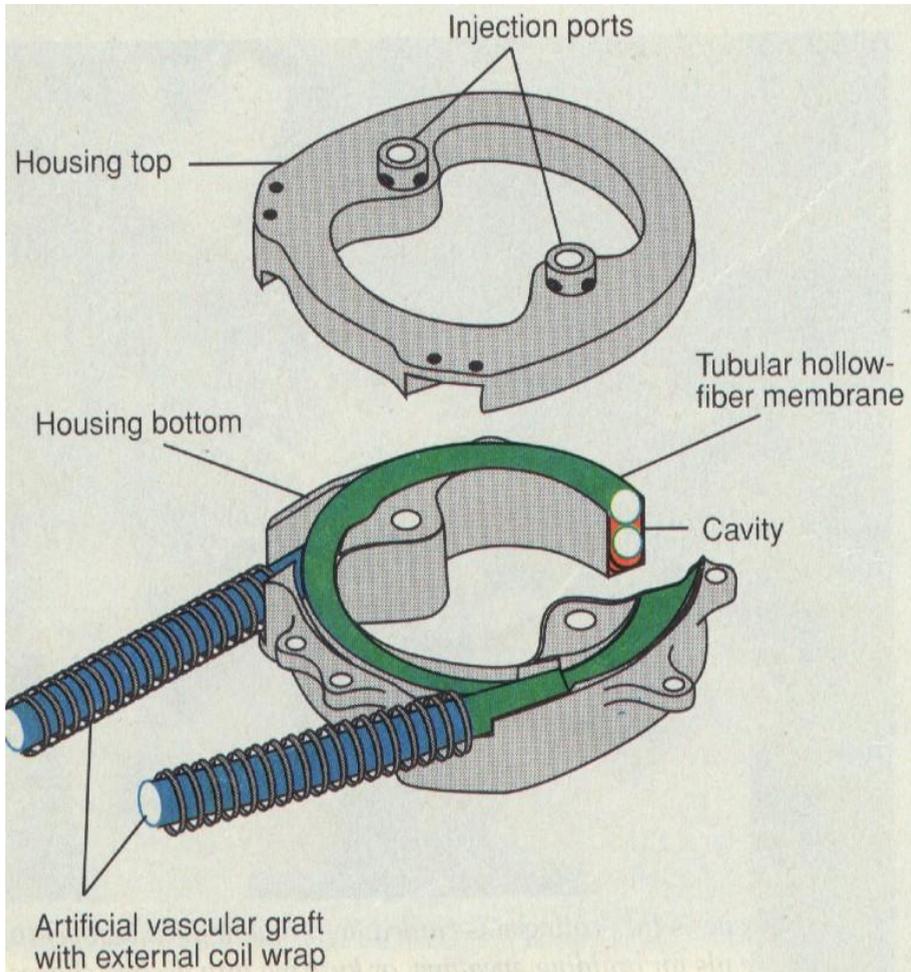


Figure 5. Artificial pancreas device (Hubbell and Langer, 1995).

3.2.7 Artificial eye

The cases of blindness where the damaged retina could be replaced by an electronic eye are under investigation. The eye functions based on the optical and electronic principles of physics, with the optical parts effectively working as sensors of the light scattered from the objects before the artificial device. The

electrical pulses generated are transferred to the brain to form the image of the object. The coupling of the electronic signals to the “*optic nerve*” is not yet successfully solved. But, the line of action will lead one day to a successful artificial eye to treat blindness. The design is shown in (Figure 6).

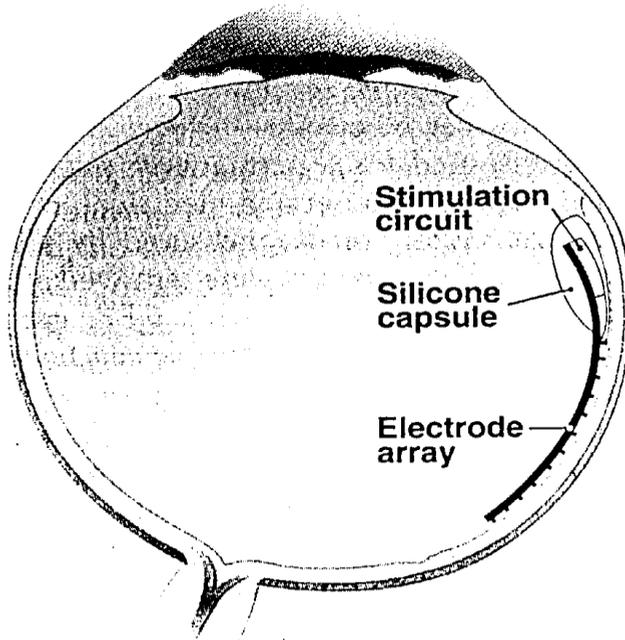


Figure 6. This microchip assembly could substitute for a damaged retina.

3.3 Degradation

The biocompatibility in all the materials used is an essential requirement for their use in the above-mentioned applications. However, while some parts in such applications have to be stable for life-long periods of existence, the others have to degrade with time and need to be absorbed in the body without harmful effects. Some materials degrade fast while others degrade with time. In surgical procedures, the sutures used for stitches need not be removed and degrade with time when the operated parts are healed up, and (the sutures) get absorbed into the body. These are particularly useful in the operations of inner parts of the body.

Materials degradation can be classified as under:

Table 5. Materials degradation

Degradation	Materials
Fast	Co-based compounds aliphatic polymers.
Medium	Polyamides, polyurethanes
Slow	Polyesters
Stable	Alumina, Zirconia

4 NUCLEAR MATERIALS AND MEDICINE

Radioisotopes are extensively used for diagnostic and therapeutic applications. Recent diagnostic methods through Positron-Electron Tomography (PET) and Single Photon Emission Computed Tomography (SPECT) are particularly useful in locating defects of the brain. The reader could refer to literature on Nuclear Medicine for further studies.

(http://www.snm.org/nuclear/whats_nm.html).

5 NANOMATERIALS AND MEDICINE

5.1 General

The advent of nanotechnology has revolutionized the applications of new materials in medicine. The present fervour and fever in the area of “nanotechnology” is affecting the pace of exotic and unique applications of materials in all spheres of use, be it defence, health, environment or domestic products.

The handling of materials at the “nano-meter” ($1\text{nm} = 10^{-9}\text{m}$) scale, i.e. of atoms and molecules in the laboratories and factories is producing products of small sizes and tremendously improved properties such as materials of ultra high strength, specific insulating or conducting heat properties, improved magnetic and electrical sensing properties. Moreover, the small size products such as molecular motors and molecular engines and molecular targeted drug systems in the area of medicine are enormous. The nanotechnology of biomaterials will make *self-regulating* pharmaceutical dispensers compatible with biosystems so that they will not be rejected by the human body and will be longer lasting in the environment of the human body. Carbon nano-wires and tubes have found many uses in medicine also. Some of the “nano-biotechnology,” applications are briefly mentioned below.

5.2 Bioanalysis

The use of nano-particles (dots, bars, rods) as “labels” for biomolecules for separation and screening, as well as nano-pore and nano scale fluidic assay systems and self-assembling arrays of nano-particles, provide more sensitive and highly specific detection and analysis capabilities. They provide a promise for significantly improved signal generation and detection in high throughput, multiplexed biological assays.

For example, if successful, this research will greatly reduce the time, effort, and expense of DNA sample preparation and analysis. The PCR tests will be available in much shorter times.

5.3 Diagnostics

The core advances in the biosensor field will occur using novel improved surface engineering and patterning techniques and systems integration. Biosensors are being developed using nano-wires, nano particle arrays, and nano-fluidic systems. They will provide unprecedented sensitivity of detection. The ability to detect proteins down to a few molecules, the diagnostics will come down to the fundamental level of a “single cell.” The detection of “cancer” at single cell levels can make the treatment of cancer extremely useful. For molecular detection, for a patient monitoring and diagnosis, the assay may require only a single breath. The molecular detection system often requires the method of attachment of molecules to the sensor surface. The methods of coupling bio molecules to sensors include; (i) Physical adsorption; (ii) Covalent bonding; (iii) Membrane entrapment; and (iv) Porous encapsulation.

The detection can be performed optically, electro chemically, thermally or through various other techniques. Some specific and unique applications in diagnostics in pollution and nuclear techniques are being made available using Nuclear Accelerators and Synchrotron Radiations [SR] in the range of nano-technology for medical diagnostics.

5.4 Therapeutics

This area has taken the quickest advances in nanotechnology of materials. Some of earliest applications have appeared in sunscreens and cosmetics. Methods have been developed for “in vivo” drug delivery via nano-particles (such as nano-crystals, nano-spheres, nano-capsules).

By the nature of nano-sizes, these delivery systems traverse membrane boundaries and can readily be adsorbed into the blood stream avoiding the use of injections. The drug delivery market is estimated to be about \$20 billion in the year 2002, and is ever growing because of new discoveries.

Targeted nano-therapeutics suggests the promise of “tissue-specific delivery” with a strong localized dose requiring a lower overall concentration of the drug causing a lower patient toxicity and lower side effects. This would lead to accelerated therapeutics for protein and macro molecules drugs, infectious diseases and cancer.

The nano-particle inhalation technology provides a patient friendly alternative to injection and may permit lower dose strategy with “protein drugs” like insulin.

The ability of crossing blood-brain barrier may evolve new methods of diagnosing and treating neuro degenerative diseases. The new “nano-biotechnology” may promise new treatments for cholesterol removal and nano-structured silicon to treat osteoporosis. There are thus unlimited promises in hiding.

5.5 Material Devices

Nano particles may have lower-dose for tissue specific targeting and retention much better than current procedures. This may have strong impact on markets of MRI and X-Ray contrast agents. These diagnostic products are estimated to be of the order of 400 million dollars and 3 billion dollars, respectively, per year.

Further down the road are potentials of reconstructive bone surgery and it has been demonstrated that nano-particles can assist in the preparation of “new bone matrix material.” Protheses can be designed to enhance integration of artificial structures and living tissue. Devices like “retinal implants” can take the advantage of nano-scale solar technology where nanoporous electrodes provide a high-density interface with nerves of the retina. (Ref: <http://membersites.namezero.com/ltmazzola.earthlink.net>).

6 NEW MATERIALS AND FUTURE MEDICINE

The development of new materials with special biocompatibility merits particularly with emerging nanotechnology. The replacement of better body parts and implants and unapproached treatments of artificial tissue and nerve grafting have great promise. The future looks bright but thought needs to go into handling the “safety and human health security risks,” in working with nano-size materials, be it human or environment hazards.

The area of nano-pharmaceuticals is to play a great part in health related industry. The development of biomedical and bioengineering research is gaining a lot of attention the world over. Nanotechnology being excessively multidisciplinary in nature, cooperative research programmes are being evolved in USA, Europe, Japan and other places, both at the level of individual universities and research institutes as well as national and international level (For example see <http://www.nsf.gov/home/crssprgm/nano/nni.htm>).

To mention one of the several such examples, one may look at the research programme of the Institute for Bioengineering and Nanoscience in Advanced Medicine (IBNAM); Northwestern University’s Interdisciplinary Research Institute, established in 2000. The institute bridges the frontiers in Medicine, Engineering, and Science. It is a partnership of the Northwestern University Feinberg School of Medicine, McCormick School of Engineering and Applied Sciences and Weinberg College of Arts and Sciences.

About 76 professionals with 64 PhDs and 37 full professors and 12 departments of separate disciplines are cooperating in this effort. Twenty-six research groups on specific projects listed below have been formed in this research programme. Some of the specific projects to be under taken are as under:

- (1) Acoustic Emission Characterization of Vascular Trauma and Catheter Development;
- (2) Biomechanics of Cells within a 3-D Environment;

- (3) Cell-based Screening using Microfabricated Cantilevers for Detection;
- (4) Design of Smart Microparticles and Nanoparticles;
- (5) Design, Synthesis, and Biomedical Applications of Conformationally Pre-organized Peptide Nucleic Acids;
- (6) Development of Silicon Nano-Particle as Fluorescent Tag and Photo-Sensitizer;
- (7) Drug Delivery by Solid Phase Cyclodextrin Hosts;
- (8) Growing a Neural Network in Culture and using it to Design Treatments for Dystonia;
- (9) Helical, Amphipathic Peptoids as Biostable Mimics of Antibiotic Peptides;
- (10) High-Density Biomedical Nanosensors;
- (11) Investigation of Meniscus Cell Processes in Aligned Fibrous Gels for Meniscal Regeneration;
- (12) In Vitro Maturation of Primary Ovarian Follicles;
- (13) Mechanisms of Gene Delivery under Conditions of Mechanical Stretch;
- (14) Microtube Assemblies for Artificial Lungs;
- (15) Minimally Invasive Surface-enhanced Raman Scattering Nanobiosensors for Intraocular and Subcutaneous Multianalyte Detection;
- (16) A Nanoelectrode for Neurophysiology and Neuroprosthetics;
- (17) Novel Rigorous Electromagnetic Field Modelling of Bioelectric Signals within the Human Body;
- (18) Polymeric Micelles with Covalent Anticancer Cores;
- (19) Probing Nano- and Micro-organization of Living Tissues for Early Cancer Detection using UV-visible Light;
- (20) Protein-imprinted Carbohydrate Recognition Patterns on Lipid Surfaces;
- (21) Stem Cell Bioengineering;
- (22) Study of Gene Expression in Early Embryo Development by Single-Cell RNA Microarray Technology;
- (23) Synthesis, Assay, and Mechanism of Cyclic Peptide Antitumor Agents;
- (24) Time-of-Flight Mass Spectrometry of Biological Molecules using Atom-probe Microscopies;
- (25) Tissue Engineering of Human Bladder Urothelium; and
- (26) The use of a Modified Poly (L-lactic Acid) Scaffold to Support Growth and Function of Surrogate Pancreatic Beta Cells.

In the above projects, the extent of biomaterials and research at the molecular level involving nanotechnology is amply clear.

7 CONCLUSION

The future use of new materials is greatly focused on the replacement of body parts by artificial implants that may last for several decades. A representative future prediction on this aspect is given in Figure 7. The era of nanotechnology emerging in 21st century has great promise for improved artificial body parts.

The two important items are therefore:

- (a) Replacement of body parts; and
- (b) Improvement in this entire field through “Nanobiotechnology.”

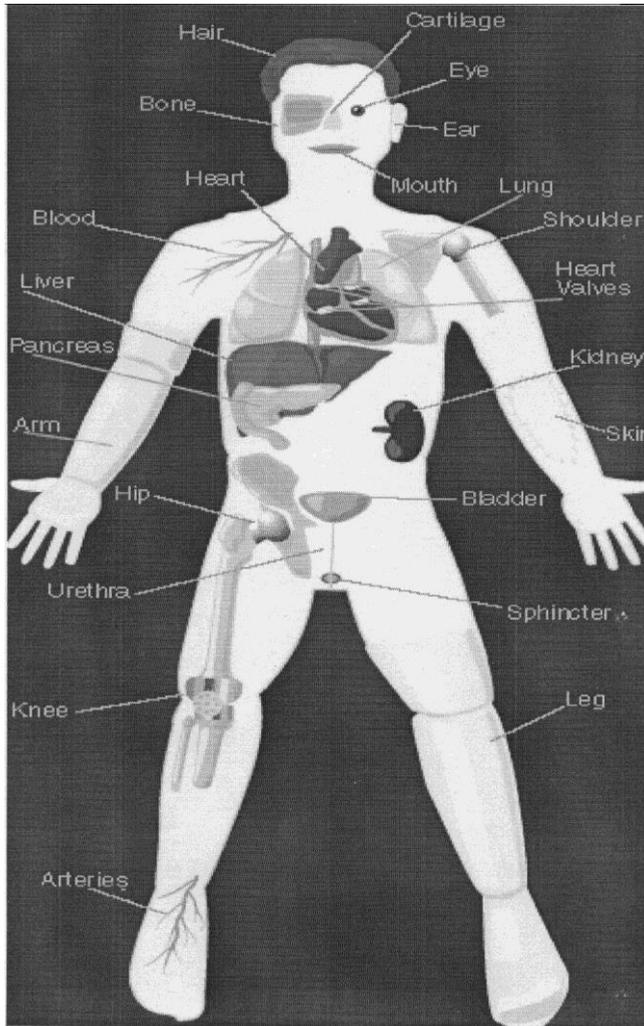


Figure 7. Parts of the human body.

ACKNOWLEDGMENTS

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Sustainability Assessment of Material Resources

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1 ABSTRACT

Throughout history, our civilisation has been constrained by economic, social and ecological pressures that have influenced its development. Since the beginning of the industrial revolution, the need was recognised for the harmonised development of different commodities leading to a better life. In this respect, economic and social development has been based on the natural capital available at the respective level of technology development.

It should be noticed that throughout the history of human society, the changes in patterns of social structures have been linked to the cyclic development of the human structure. Near the end of the industrial revolution, it became evident that complex indicators such as population, economics, material resources, social structure and religious devotion have reached the state that requires our special attention.

Energy, water and environment are essential commodities that are needed for human life on our planet. The Club of Rome was among the first to draw the world scale attention to the potential limits in availability of the natural capital on our planet.

Multi-criteria assessment has become a powerful tool for the decision-making procedure in selecting appropriate route for the future strategic planning of the use of natural resources. In this respect, materials science and technology development strategy has to be based on the multi-criteria evaluation of different options. It is of great importance in this evaluation to take into consideration appropriately defined indicators in justification of individual routes of development and their rating under different constrains.

In this paper, the potential application of multi-criteria evaluation methods for the assessment of potential route for the science and technology development of copper, silicon, aluminium and iron technologies will be demonstrated.

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2 HOW LIMITED ARE THE RESOURCES?

2.1 The backdrop

Energy, water and the environment are essential commodities that are needed for human life on our planet. In the development of our civilisation these three commodities have served as the fundamental resources for economic, social and cultural developments. In the early days of human history, it was believed that there are abundant resources of these commodities. With the industrial revolution, the use of these resources became the essential driving force for economic and social development. With the increase of population and respective rise in the standard of living, natural resources have become scarce in some specific regions. With further increase in demand, it has become evident that the scarcity of natural resources may lead to a global problem, and affect human life on our planet. The Club of Rome was among the first to draw the world scale attention to the potential limits in availability of the natural capital on our planet. The energy crises in 1972 and 1978 have focussed the attention of our community to investigate the limits in energy resources. This was a moment when our society through the different institutions launched programs that aimed to investigate global scarcity of natural resources on our planet. It became obvious that the modern society has to adapt a new philosophy in its development, which has to be based on limited natural resources.

2.2 Energy

2.2.1 General

Energy resources have always played an important role in the development of human society [1]. Since the industrial revolution, energy has been a driving force for the modern civilization development. Technological development and consumption of energy, along with the increase in the world population, are interdependent. The Industrial Revolution, and the change from reciprocal engines to the great horsepower of steam engines in the late nineteenth century, which brought about a revolution in dynamics – marked a drastic increase both in consumption and the population of the world [2].

The history of life on Earth is based on the history of photosynthesis and energy availability [3]. The history of such a planet lies in the capture of the solar energy and its conversion by photosynthesis in plants and phytoplankton as organic molecules of high energy content. The plants convert this energy into other organic compounds and work by biochemical processes. Photosynthesis counteracts entropy increase and degradation since it tends to put disordered material in order. By capturing the solar energy and decreasing the planetary entropy, photosynthesis paves the way for biological evolution.

Boltzman [4], one of the fathers of modern physical chemistry, wrote, in 1886, that the struggle for life is not a struggle for basic elements or energy, but a struggle for the availability of negative entropy in energy transfer from the hot

Sun to the cold Earth. In fact, life on Earth requires a continuous flux of negative entropy as the result of the solar energy captured by photosynthesis. The Sun is an enormous machine that produces energy by nuclear fusion and offers planet Earth the possibility of receiving large quantities of negative entropy. Every year the Sun sends 5.6×10^{24} joules of energy to the Earth and produces 2×10^{11} tons of organic material by photosynthesis. This is equivalent to 3×10^{21} joules/ year. Through the billions of years since the creation of the Earth, this process has led to the accumulation of enormous energy in the form of different hydrocarbons. Most of the fossil fuels belong to the type of material where molecular binding is due to Van der Waals potential between every two molecules of the same material.

Table 1. Assessed energy resources [5]

GLOBAL FOSSIL ENERGY RESOURCES, RESERVES AND OCCURRENCES, IN EJ						
	Consumption		Reserves Identified	Conventional Resources At Probability 50%	Resource Base	Additional Occurrence
	1860-1990	1990				
Oil						
Conventional	3343	128	6000	2500	8500	>10000
Unconventional	-	-	7100			>15000
Gas						
Conventional	1703	71	4800	4400	9200	>10000
Unconventional	-	-			26900	>22000
Hydrates	-	-				>80000
Coal	5203	91	25200		>125500	>130000
Total	10249	290	50000	>6900	>18200	>987000
Nuclear	212	19	1800	>2300	>14200	>1000000

Source: Nakicenovic *et al.*, 1993

Energy and matter constitute the Earth's natural capital that is essential for human activities such as industry, amenities and services. Our natural capital as the inhabitants of the planet Earth may be classified as:

- Solar capital (provides 99% of the energy used on Earth); and
- Earth capital (life support resources and processes including human resources).

These, and other, natural resources and processes comprise what has become known as 'natural capital' and it is this natural capital that many suggest is being rapidly degraded at this time. Many also suggest that contemporary economic theory does not appreciate the significance of natural capital in techno-economic production.

2.2.2 Energy resources

All natural resources are, in theory, renewable but over widely different time scales. If the time period for renewal is small, they are said to be renewable. If the renewal takes place over somewhat longer periods of time that falls within

the time frame of our lives, they are said to be potentially renewable. Since renewal of certain natural resources is only possible due to geological processes, which take place on a long time scale that for all practical purposes, we should regard them as non-renewable. Our use of natural material resources is associated with no loss of matter as such.

2.2.3 Energy consumption

The abundant energy resources at the early days of the industrial development of the modern society have led the development strategy of our civilization to be based on the anticipated thinking that energy resources are unlimited and that there are no limitations that might affect human welfare development. It has been recognized that the pattern of the energy resource use has been strongly dependent on technology development. In this respect, it is instructive to observe [6,7] the change in the consumption of different resources throughout the history of energy consumption. Worldwide use of primary energy sources since 1850 is shown in Figure 1 [6].

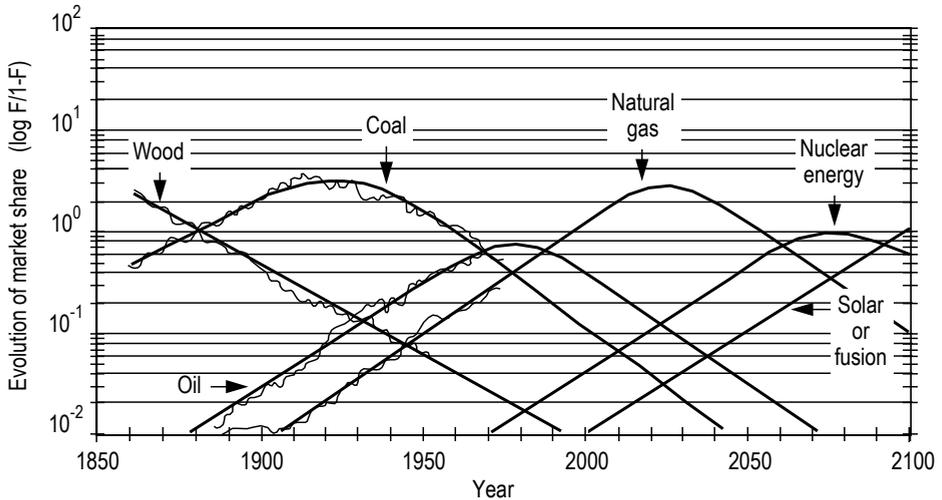


Figure 1. Worldwide use of primary energy sources since 1850.

Consumption trends of specific energy resources are related to the technology development and to the availability of the respective energy resources. Obviously, this pattern of energy source use is related to the total level of energy resources consumption and reflects the existing social structure [8,9,10]. The world energy consumption is shown in Figure 2 [1].

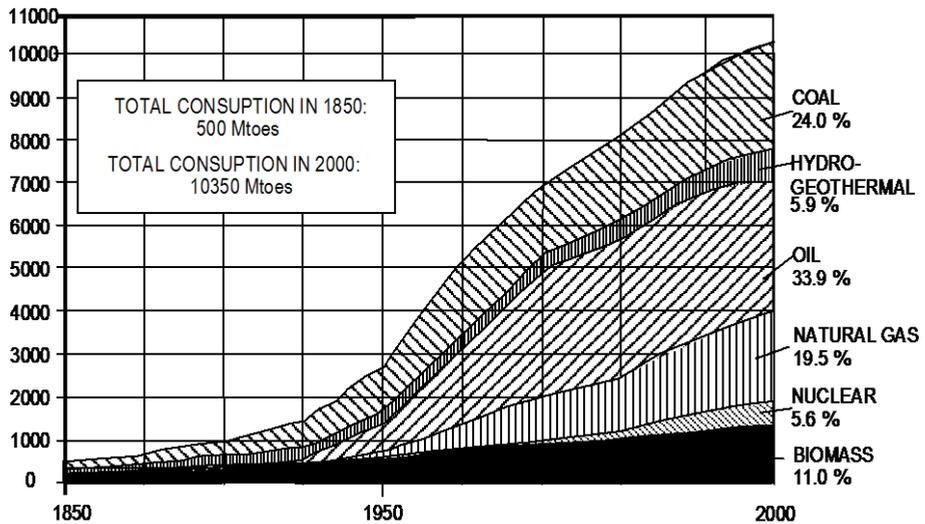


Figure 2. World energy consumption since 1850.

Looking at the pattern of consumption of energy sources at present, it can be noticed that oil is a major contender, supplying about 40% of energy. Next, coal provides around 30%, natural gas 20%, and nuclear energy 6.5%. This means that the current fossil fuel supply is 90% of the present energy use. In the last several decades, our civilization has witnessed changes, which are questioning our long-term prospects.

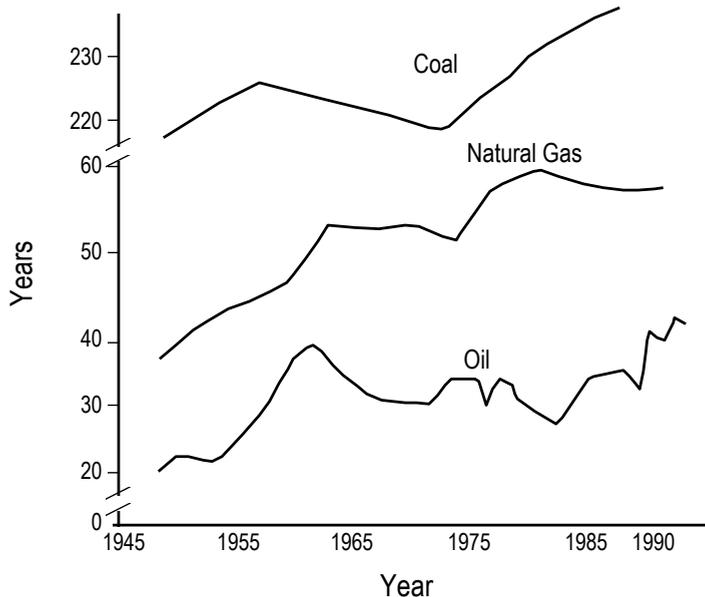


Figure 3. The ratio of discovered resources to the yearly consumption of fossil fuels.

Fossil fuel is a non-recyclable exhaustible natural resource that will one day be no more available. In this respect, it is of common interest to learn how long fossil fuel resources will be available, as they are the main source of energy for our civilization. This question has attracted the attention of a number of distinguished authorities, trying to forecast the energy future of our planet. The Report of the Club of Rome “Limits to Growth,” published in 1972 [12], was among the first ones, which pointed to the finite nature of fossil fuels. After the first and second energy crisis, the international community became aware of the possible physical exhaustion of fossil fuels. The amount of fuel available is dependent on the cost involved. For oil, it was estimated that proven reserves have, over past twenty years, levelled off at 2.2 trillion barrels, produced at under \$20 per barrel. Over the last 150 years, we used up one-third of that amount, or about 700 billion barrels, which leaves only 1.5 trillion barrels. If compared with the present consumption, it means that oil is available only for the next 40 years. Figure 3 shows the ratio of the discovered resources to the yearly consumption of fossil fuels [11].

From this figure, it can be noticed that coal is available for the next 250 years and gas for the next 50 years. In addition, it is evident that as much as the fuel consumption is increasing, new technologies aimed at the discovery of new resources are becoming available, leading to a slow increase of the time for the exhausting of the available energy sources.

2.2.4 Energy consumption forecast

It is known that the energy consumption is dependent on two main parameters namely; the amount of energy consumed per capita and the growth of population. It has been proven that there is a strong correlation between gross domestic product and the per capita energy consumption.

There are a number of scenarios that are used for the forecast of the world economic development. The future energy consumption could be calculated, as shown in Figure 4 [14].

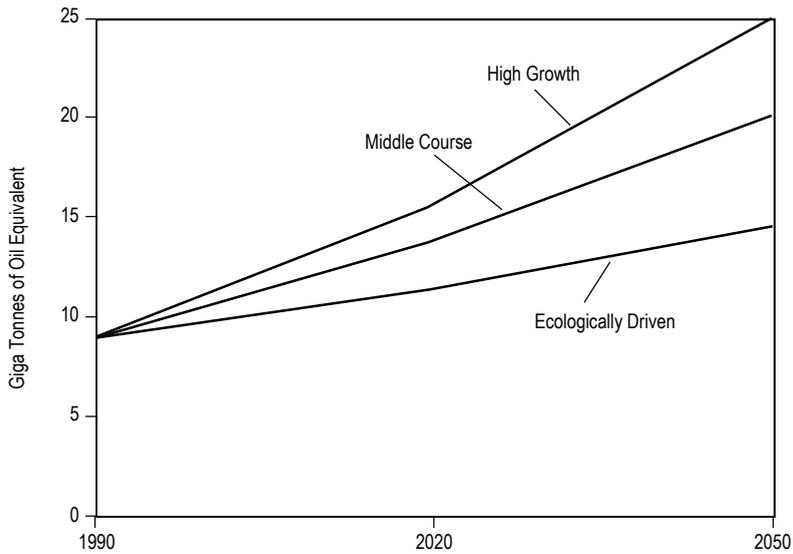


Figure 4. Future energy consumption.

Compared to the available resources it is can easily be foreseen that the depletion of energy resources is an imminent process that our civilization will face in the near future. Nevertheless, whatever is the accuracy of our prediction methods and models, it is obvious that any inaccuracy in our calculation may affect only the time scale but not the essential understanding that the energy resources depletion process has begun and requires human action before adverse effects may irreversibly come about.

2.3 Environmental degradation

Primary energy resources use is a major source of emissions [15,16,17]. Since fossil fuels have demonstrated their economic superiority, more than 88% of primary energy in the world in recent years has been generated from fossil fuels. However, the exhaust gases from combusted fuels have accumulated to an extent where serious damage is being done to the world global environment. The accumulated amount of CO₂ in atmosphere is estimated at about 2.75×10^{12} t. The global warming trend from 1900 - 1990 is shown in Figure 5 [18].

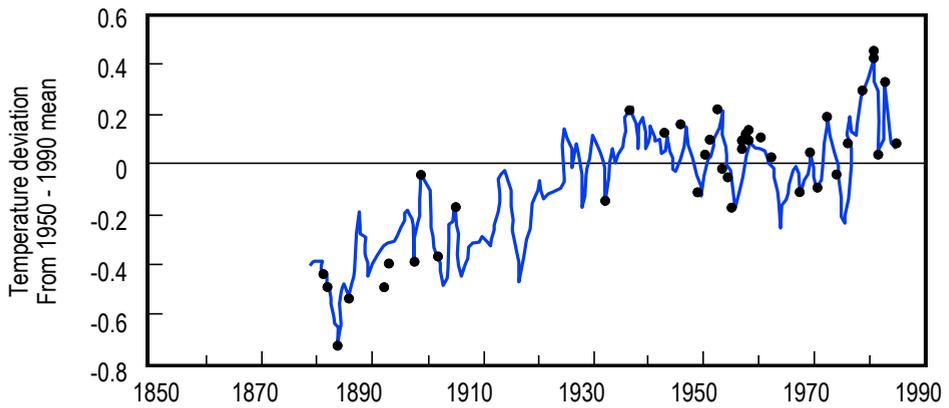


Figure 5. Global warming trend from 1900-1990.

The future trend of the carbon dioxide concentration in the atmosphere can be seen in Figure 6 [19].

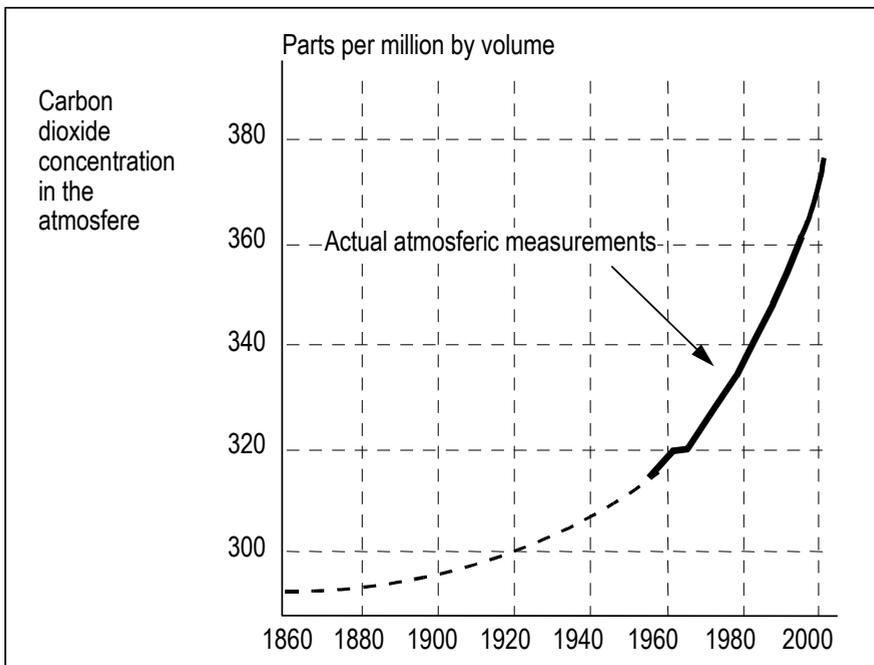


Figure 6. Carbon dioxide concentration in the atmosphere.

It is rather obvious that a further increase of CO_2 will lead to disastrous effects on the environment. Also, the emission of SO_2 , NO_x and suspended particle matter will exasperate the effect on the environment.

On a world scale, coal will continue to be a major source of fuel for electric power generation. Many developing countries, such as China and India, will continue to use inexpensive, abundant, indigenous coal to meet growing domestic needs. This trend greatly increases the use of coal worldwide as the economy in other developing countries, continues to expand. In this respect the major long-term environmental concern about coal use has changed from acid rain to greenhouse gas emissions - primarily carbon dioxide from combustion .It is expected that coal will continue to dominate China’s energy picture in the future. The share of coal, in primary energy consumption is forecast to be no less than 70 % during the period 1995 - 2010.

2.4 Water resources

In this part sustainability of desalination systems, essential component of human-made or built capitals is discussed with respect to its important contribution to life support systems [20,21]. Figure 7 shows the distribution of the global stock of water.

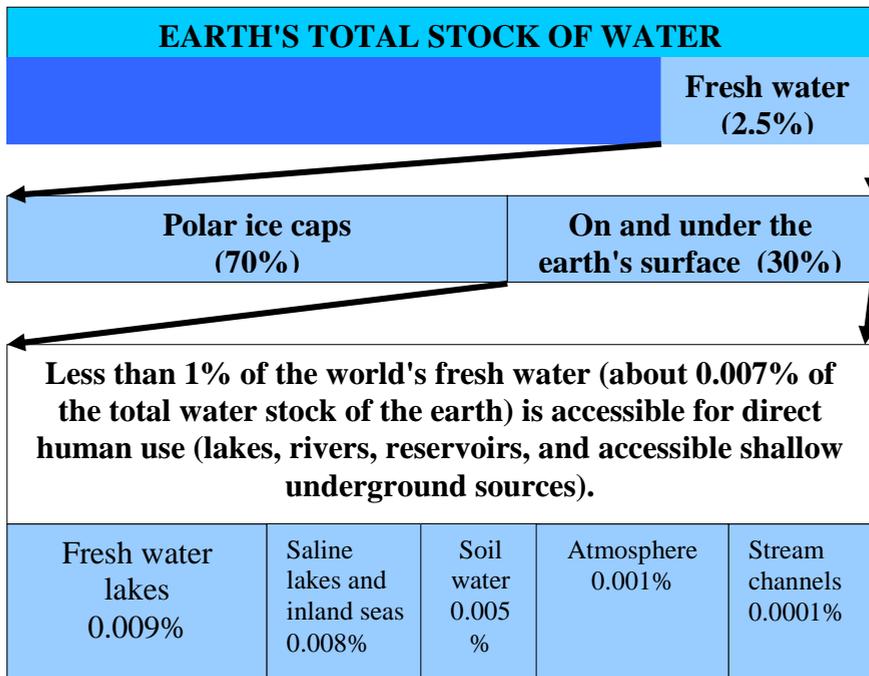


Figure 7. Global stock of water.

Ninety-seven point-five percent of the total global stock of water is saline and only 2.5% is fresh water. Approximately 70% of this global freshwater stock is locked up in polar icecaps and a major part of the remaining 30% lies in remote underground aquifers. In effect, only a miniscule fraction of the freshwater available (less than 1% of total freshwater, or 0.007% of the total global water stock) in rivers, lakes and reservoirs is readily accessible for direct

human use. Furthermore, the spatial and temporal distribution of the freshwater stocks and flows is hugely uneven. Hydrologists estimate the average annual flow of all the world's rivers to be about 41,000 km³/year. Less than a third of this potential resource can be harnessed for human needs. This is further reduced by pollution such as discharges from industrial processes, drainage from mines and leaching of the residues of fertilizers and pesticides used in agriculture. The World Health Organization (WHO) has estimated that 1000 cubic meters per person per year is the benchmark level below which chronic water scarcity is considered to impede development and harm human health.

Several countries are technically in a situation of water scarcity, i.e. with less than 1000 cubic meters of renewable water per year per head of population. Water shortage is predicted to increase significantly, mainly because of the increase in population. Table 2 provides figures, for these countries, showing predicted water availability per person in the year 2050, using the United Nations low and high population predictions. This does not consider the possible changes in rainfall or evapotranspiration because of global warming.

**Table 2. Projected water scarcity for selected countries,
by the year 2050 for selected countries
(World Resources Institute 1996-97)**

C O U N T R Y	Renewable water resources per capita		
	1990	2050 (low)	2050 (high)
Algeria	690	398	247
Bahrain	184	104	72
Djibouti	19	8	6
Egypt		644	398
Israel	461	300	192
Jordan	308	90	68
Kuwait	75	59	38
Lebanon		1218	768
Libya		276	213
Morocco		750	468
Oman		235	163
Qatar	103	68	47
Saudi Arabia	284	84	67
Somalia	980	658	473
Syria		667	454
Tunisia	540	363	221
United Arab Emirates	293	171	120
Yemen	460	127	90

To meet its needs of fresh water, humanity exploits all viable sources: erecting dams across rivers to hold flood waters, building reservoirs to store water for use during dry periods, digging canals to transport water from places

of abundance to places of scarcity, pumping water from the ground, and burning fossil fuels to desalinate seawater.

2.5 Material resources

Natural resources scarcity and economic growth are in fundamental opposition to each other. The study of the contemporary and historical beliefs showed that: (1) Natural resources are economically scarce, and become increasingly so with the passage of time; and (2) Scarcity of resources stunts economic growth. There are two basic versions of this doctrine. The first, the Malthusian, rests on the assumption that there are absolute limits; once these limits are reached the continuing population growth requires an increasing intensity of cultivation and, consequently, brings about diminishing returns per capita. The second, or Ricardian version, viewed the diminishing returns as current phenomena reflecting the decline in the quality of resources brought within the margin of a profitable cultivation. Besides these two models, there is also the so called “Utopian case,” where there is no resources scarcity. There have been several attempts to apply these models to the energy resources in order to define the correlation between specific energy resources and economic growth. The substantial questions related to the scarcity, its measurement and growth are: (1) Whether the scarcity of energy resources has been and/or will continue to be mitigated? and (2) Whether the scarcity has “de facto” impacted the economic growth?

Since the beginning of industrial revolution, different materials are used in/for the construction of the new systems. So it has become important to economic development to use new materials. In this respect a primary role was given to the different composition of iron material resources. Its use in everyday life has been essential for the economic development of our society. As a result of further economic development, it became obvious that many different materials have played important roles in the development of our society. The consumption of these resources has become also tied up to future economic development.

In order to take into consideration limits in material resources, we will focus our attention on iron [22], aluminium [23], copper [24], and silicon [25]. These materials have been in industrial use for a number of years and have substantially contributed to the development of our society. Presently available resources of these materials are reflected in Table 3.

Table 3. The availability of some materials (metals)

	Resources	Annual production	Years
	10^9 tones	10^6 t/ year	Year
Aluminium	13.8	46	300
Iron	88	580	152
Copper	0.59	11.4	52
Silicon	2.4	5.00	480

If compared to present production levels of these materials we can calculate the time period of their availability. As can be noticed, for some materials this period is rather short. For this reason, the future strategy resource of these materials has to be carefully planned. In the sustainability assessment of the material resource use, special attention has to be devoted to resource availability.

3 SUSTAINABILITY

3.1 What is sustainability?

Lately, “sustainability” became a popular buzzword in the discussion of the resources use and environmental policy. It is thus necessary to define and properly assess the term if we are going to use it [19]. So, what is sustainability? Among the definitions most often adapted are the following:

- (a) For the World Commission on Environment and Development (Brundtland Commission) [26], it is “development that meets the needs of the present without compromising the ability of future generations to meet their own needs;”
- (b) For Agenda 21, Chapter 35 [27], it is the “development (that) requires taking long-term perspectives, integrating local and regional effects of global change into the development process, and using the best scientific and traditional knowledge available;”
- (c) For the Council of Academies of Engineering and Technological Sciences [28], it means “the balancing of economic, social, environmental and technological consideration, as well as the incorporation of a set of ethical values;” and
- (d) For the Earth Chapter [29], it is “the protection of the environment (that) is essential for human well-being and the enjoyment of fundamental rights, and as such requires the exercise of corresponding fundamental duties.”
- (e) Thomas Jefferson, on 6 September 1889 [30], said of the same “...then I say the Earth belongs to each generation during its course, fully and in its right no generation can contract debts greater than may be paid during the course of its existence.”

Definitions (a) and (e) imply that each generation must bequeath enough natural capital to permit future generations to satisfy their needs. Even if there is some ambiguity in these definitions, it is meant that we should leave our descendants the ability to survive and meet their own needs. Also, there is no specification in what form resources are to be left and how much is needed for future generations, because it is difficult to anticipate future scenarios.

Definitions (b) and (c) set the actions to be taken at the global, regional and local levels in order to stimulate United Nations, governments and local authorities to plan development programs in accordance with the scientific and

technological knowledge. In definition (c), the ethical aspect of future development actions to be taken to meet sustainable development, is highlighted.

Definition (d) is based on religious beliefs in terms of responsibility and duty towards nature and Earth. In this respect, it is of interest to mention that the Old Testament, in which the story of the creation is told and is a fundamental basis for Hebrew and Christian doctrine, also touches on the environment. In the world of Islam, nature is the basis for human consciousness. According to the Qur'an, while humankind is God's vice-regent on Earth, God is the Creator and the Owner of nature. But human beings are His trusted administrators, they ought to follow God's instructions, that is, acquiesce to the authority of the Prophet and to the Qur'an regarding nature and natural resources.

3.2 Sustainability science

3.2.1 Background

Meeting fundamental human needs while preserving the life-support systems of planet Earth is the essence of sustainable development, an idea that emerged in the early 1980s from scientific perspectives on the relation between nature and society. During the late 80s and early 90s, however, much of the science and technology community became increasingly estranged from the preponderantly societal and political processes that were shaping the sustainable development agenda. This is now changing as efforts to promote a sustainability transition emerge from international scientific programs, the world's scientific academies, and independent networks of scientists [31].

3.2.2 Core questions

A new field of sustainability science is emerging that seeks to understand the fundamental character of interactions between nature and society [32]. Such an understanding must encompass the interaction of global processes with the ecological characteristics of particular places and sectors. The regional character of much what sustainability science is trying to explain means that relevant research will have to integrate the effects of key processes across the full range of scales from local to global. It will also require fundamental advances in our ability to address such issues as the behaviour of complex self-organizing systems as well as the responses, some irreversible, of the nature-society system to multiple interacting stresses. Combining different ways of knowing will permit different social actors to work in harmony, even with much uncertainty and limited information.

With a view toward promoting research necessary to achieve such advances, an initial set of core questions for sustainability science may be proposed. These are meant to focus research attention on both the fundamental character of interactions between nature and society and on society's capacity to guide those interactions along more sustainable trajectories.

3.2.3 Research strategies

The sustainability science that is necessary to address these questions differs to a considerable degree in structure, method, and content from science, as we know it. In particular, sustainability science will need to do the following [33]:

- (1) Span the range of spatial scales between such diverse phenomena as economic globalisation and local farming practices;
- (2) Account for both the temporal inertia and urgency of processes like ozone depletion;
- (3) Deal with functional complexity such as is evident in recent analyses of environmental degradation resulting from multiple stresses;
- (4) Recognize the wide range of outlooks regarding what makes knowledge usable within both science and society;
- (5) Define the criteria and indicators for the sustainability assessment of energy, water and environment systems that provide guidance for the efforts directed to a transition toward sustainability;
- (6) Recognise the limits of energy, water and the environment that mark irreversible changes on our planet; and
- (7) Make sustainability operational in everyday life through a paradigm manifesting interdisciplinary and multidisciplinary approaches.

Pertinent actions are not ordered linearly in the familiar sequence of scientific inquiry where action lies outside the research domain. In areas like climate change and scientific exploration, practical application must occur simultaneously. They tend to become entangled with each other.

In each phase of science research, novel schemes and techniques have to be used, extended, or invented. New methodological approaches for decisions under a wide range of uncertainties in natural and socio-economic systems are becoming available and need to be more widely exploited, as does the systematic use of networks for the utilization of expertise and the promotion of social learning.

3.3 Sustainability indicators

3.3.1 Reliability of indicators

Measuring sustainability is a major issue as well as a driving force of the discussion on sustainability development. Developing tools that reliably measure sustainability is a prerequisite for identifying non-sustainable processes and informing design-makers of the quality of products, and monitoring impacts to the social environment. The multiplicity of indicators and measuring tools being developed in this fast growing field shows the importance of the conceptual and methodological work in this area.

Sustainability analysis requires the use of a methodology that comprises specific criteria in the evaluation of the indicators. The first step in the

sustainability analysis is to perform the classification phase. There are two methods: cluster analysis and multivariate statistical method.

Cluster analysis is 'a technique for grouping indicators into clusters so that indicators in the same cluster are more like one another than they are like indicators in other clusters.' Thus its primary purpose is to group indicators based on the characteristics they possess. The resulting clusters of indicators should then exhibit high internal (within-cluster) homogeneity and high external (between-cluster) heterogeneity.

3.3.2 Definitions

For the sustainability assessment the following indicators are used:

- Resource Indicator - RI
- Environment Indicator - EnI
- Social Indicator - SI
- Economic Indicator – EcI
- Technology Indicator - TI

(a) Resource indicator

The resource indicator for the system will comprise four elements, including: iron resource, copper resource, aluminium resource and silicon resource. The indicator reflecting an individual element of the resource indicator is defined as the total amount of the respective material resource used divided by the total annual production.

The Iron indicator for example will comprise amount of available resources divided by the annual production. Similarly are calculated the copper, aluminium and silicon indicators.

(b) Environment indicator

The environment cluster indicator may be composed of number of elements, as: CO₂, NO_x SO₂ indicators. Following the same procedure used in the definition of the resource indicator, the environment cluster indicator is calculated. It is defined as the amount of specific specie per unit material production.

(c) Social indicator

The social cluster indicator reflects the social aspect of the options under consideration. It comprises a number of elements: job indicator, standard indicator and community indicator. The job indicator element represents the number of new jobs to be created corresponding to the respective option. The standard element reflects the potential increase in the standard of living in the community. The community indicator element takes into consideration the community benefits due to the individual option.

(d) Economic indicator

The economic indicator is based on elements that include: effectiveness indicator, investment indicator, and unit cost indicator. The effectiveness indicator element is defined as the thermodynamic efficiency of the system. It will include the efficiency conversion from the resources to the final product. The investment cost indicator is aimed to obtain valorisation of the investment per unit production. The product unit cost indicator will comprise the cost of the product per unit production.

(e) Technology indicator

Technology indicators comprise elements reflecting mining, processing and forming processes. Since every product is obtained by a specific technology, it is important to evaluate the contribution of each technology to the product quality. In order to make an assessment of individual processes contribution to the total quality of the product, it is anticipated that each process contribution can be measured by the amount of energy used per unit product.

3.4 Methods of sustainability assessment of material resources use strategy

3.4.1 Outline

Strategy development is a multi-criteria assessment of the potential options of the respective scenarios. In this respect the development of material strategy has to be based on the specific criteria, which reflect the complexity of the potential options characteristics to be taken into a consideration. It is obvious that the main consideration has to be devoted to those materials mostly used in the complex development of our society. In this analysis we will focus our attention on the metallic materials used in the industrial society.

In the history of industrial society development, the most important materials are: iron, copper, aluminium, and silicon. It is known that varieties of alloys are based on these materials and are used for the sophisticated structure in our society. For this reason in our analysis, the options under consideration are:

- (1) Iron technology development;
- (2) Copper technology development;
- (3) Aluminium technology development; and
- (4) Silicon technology development.

In order to compare these options and to obtain rating priority among the options, it is necessary to select common attributes with corresponding indicators. This part of the assessment procedure will require determination of the indicator numerical value for each option.

Once numerical values of indicators are defined, they can be used for the assessment of the respective options. It is obvious that different indicators will have different scales for sustainability. This will imply that there is a need for a

procedure to be adopted for the valorisation of the indexes and indicators. The first step in this direction is the definition of the criteria based on the indicators as a numerical scale to measure rating of the individual options under assessment.

3.4.2 Multi-Criteria analysis

At least six reasons can be given for the use of multi-criteria analysis as an appropriate tool in a sustainability study:

- It provides tools for analysing the complex tradeoffs between choice alternatives (e.g. classes of conflicting socio-economic and environmental criteria), simultaneously considering their different impacts;
- It allows one to deal with mixed (quantitative, qualitative) information, given the problem of the differences in the dimensions of the criterion used for economic-ecological modelling;
- It does not pose any restriction on the number and the nature of goals, but does require that the relative importance (priorities) of those goals to be indicated;
- It performs shifting from conventional 'one shot' decision making to institutional and procedural decision making where political aspects play a major role;
- It deals with the conflicting nature of modern planning problems and its various formal and informal decision-makers; and
- It fulfils the desire of modern public decision analysis not to be confronted with a single and 'forced' solution, but with a spectrum of feasible solutions.

The multi-criteria assessment is based on the decision-making procedure [34,35,36] reflecting the combined effect of all the criteria under consideration and is expressed in the form of the General Index of Sustainability. Selected numbers of indicators are taken as measure of the criteria comprising specific information of the options under consideration.

The next step in the preparation of data for the multi-criteria sustainability assessment is calculation of the date.

This step consists of the formation of particular membership functions $q_1(x_1), \dots, q_m(x_m)$. For every Indicator x_i we have: (1) To fix two values $MIN(i)$, $MAX(i)$; (2) To indicate the function $q_i(x_i)$ decreasing or increasing with argument x_i increasing; (3) to choose the exponent's value λ in the formula:

$$q_i(x_i) = \begin{cases} 1, & \text{if } x_i \leq \text{MIN}(i), \\ \left(\frac{\text{MAX}(i)x_i - x_i}{\text{MAX}(i) - \text{MIN}(i)} \right), & \text{if } \text{MIN}(i) < x_i \leq \text{MAX}(i), \\ 0, & \text{if } x_i > \text{MAX}(i) \end{cases}$$

For the decreasing function $q_i(x_i)$.

The functions $q_1(x_1), \dots, q_m(x_m)$ formation process being finished with a matrix $(q_i^{(j)})$, $i = 1, \dots, m$, $j = 1, \dots, k$, where an element $q_i^{(j)}$ is a value of i -th particular criterion for j -th option. In this analysis, it assumed that the linear functions $q_1(x_1), \dots, q_m(x_m)$ are used. For q_1, q_2 and q_4 membership function, the decreasing function is adopted.

General indices method comprises the formation of an aggregative function with the weighted arithmetic mean as the synthesizing function defined as:

$$Q(q; w) = \sum_{i=1}^m w_i q_i$$

Where,

w_i – weight-coefficients elements of vector \mathbf{w} ;

q_i – indicators of specific criteria.

In order to define weight-coefficient vectors, the randomisation of uncertainty is introduced. Randomisation produces a random weight-vector. It is assumed that the measurement of the weight coefficients is accurate to within a step of $h = 1/n$, with n being a positive integer. In this case the infinite set of all possible vectors may be approximated by the finite set $W(m, n)$ of all possible weight vectors with discrete components. The nonnumeric, inexact and incomplete information is used for the reduction of the set $W(m, n)$ of all possible vectors \mathbf{w} to obtain the discrete components set $W(I, n, m)$. It is defined as a number of constrains reflecting nonnumeric information about mutual relation among the criteria under consideration.

3.4.3 Demonstration of multi-criteria analysis

The application of multi-criteria analysis in decision-making procedures [36,37,38] for the sustainability assessment of different options of the material development strategy is presented below. This leads to the determination of the criteria and respective indicators for the options under consideration, and application of the procedure for the multi-criteria analysis, and the determination of the sustainability index for the options under consideration and finally forming the priority list of the options.

In this respect, a simplified procedure is adopted with the following criteria with respective indexes: Resource Indicator, Energy Indicator, Environment

Indicator, Social Indicator, and Economic Indicator. Table 4 shows the indicators values for the options under consideration.

Table 4. Indicator values

	Resource Indicator RI	Energy Indicator EI	Environment Indicator EnI	Social Indicator SI	Economic Indicator Eci
Options	Years	kWh/kg	kg _{CO2} /kg	h/tons	u/kg
Iron technology development	152	308	16.3	2.5	0.326
Cooper technology development	72	19.4	16.3	8	1.32
Aluminium technology development	300	13	4	4	1.16
Silicon technology development	480	4.5	8.9	3.5	0.7

By the normalisation of these indicators with the maximum value of indicator, the normalised indicator matrix is obtained. In order to obtain Sustainability Index an aggregative function with the weighted arithmetic mean as the synthesizing function defined as:

$$Q(q; w) = \sum_{i=1}^m w_i q_i$$

Where,

w_i – weight-coefficients elements of vector w

q_i – normalized indicators of specific criteria

The weight-coefficients are obtained by the randomization of numerical scale and number of criteria leading. From the number of possible combination obtained under specific constrains, the average value of the weight-coefficient is calculated. In the randomization process the scale between 0-1 is divided by $n=40$ so that $h = 0.025$ and total number of possible combination is $N = 23751$.

In this analysis, the following non-numerical constrains are used in the evaluation of priority rating of Sustainability Index.

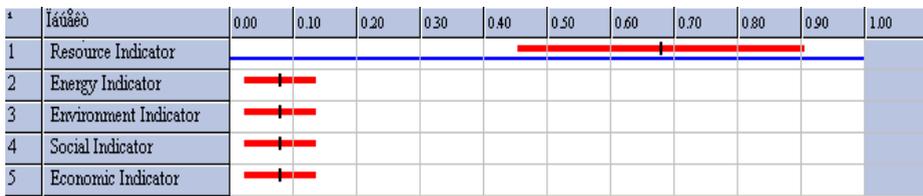
Evaluation procedure is based on the following cases:

- Case 1** $RI > EI = EnI = SI = EcI$
- Case 2** $EI > RI = EnI = SI = EcI$
- Case 3** $EnI > RI = E = SI = EcI$
- Case 4** $SI > RI = EI = EnI = EcI$
- Case 5** $EcI > RI = EI = EnI = SI$

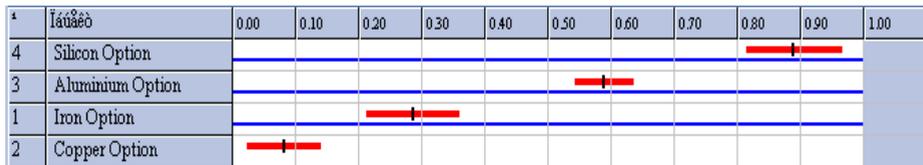
Case 1 $RI > EI = EnI = SI = EcI$

Case 1 is designed to give priority to the Resource Indicator with other indicators having the same value of average value of weight-coefficient. In this case, priority is obtained for the Silicon option followed by Aluminium, Iron and Copper options. As it can be noticed, there is no difference in rating if compared with single resource Indicator.

Weight-coefficients



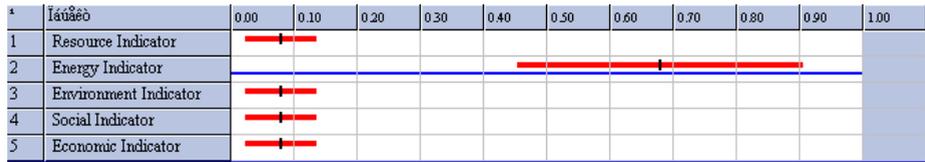
Sustainability Index



Case 2 $E \triangleright RI = EnI = SI = EcI$

Case 2 reflects the situation when priority is given to Energy Indicator with the other indicators having the same values. Such changes in the priority given to Energy Indicator, Silicon and Iron options gain priority in comparison with other two options. Under this constrain, there is substantial difference in comparison with the single Energy Indicator. This reflects the influence other indicators have on the rating list.

Weight-coefficients



Sustainability Index



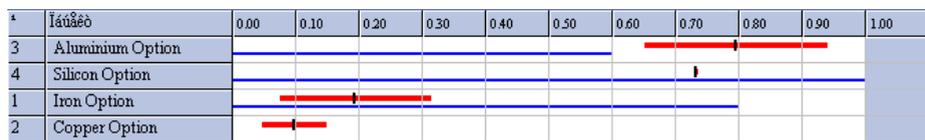
Case 3 $EnI > RI = E = SI = EcI$

Case 3 aims to investigate the effect of Environment Indicator on the priority of the Sustainability Index. Placing the Aluminium option on the priority list reflects a strong influence of the Environment Indicator on the priority of the rating list.

Weight-coefficients



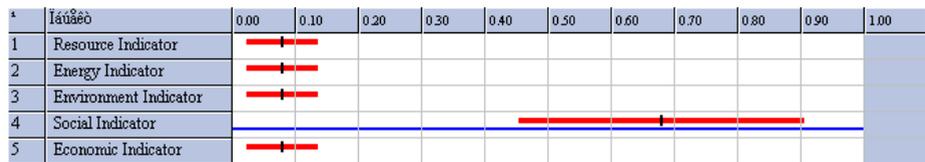
Sustainability Index



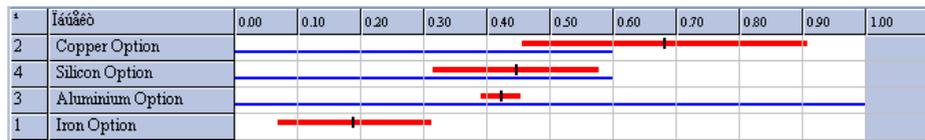
Case 4 $SI > RI = EI = EnI = EcI$

Case 4 in this analysis is devoted to the effect of Social Indicator on the priority list. It can be noticed that very high dispersion of Sustainability Index is characteristic of this case. It is a result of a rather small number of the combination used in the determination of the average value of weight coefficient.

Weight-coefficients



Sustainability Index



Case 5 $EcI > RI = EI = EnI = SI$

This Case reflects rating among options under consideration with strong influence of Economic Indicator. High dispersion of weight coefficient of Economic Indicator

Weight-coefficients



Sustainability Index



Second group of evaluation cases are those where priority is given to the selected group of indicators. Among those are:

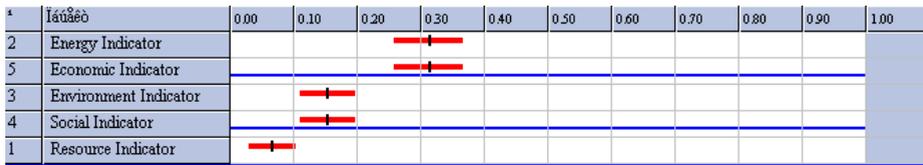
Case 6 $EI = EcI > EnI = SI > RI$

Case 7 $EnI = SI > RI = EI = EcI$

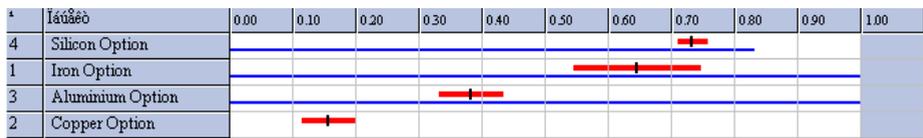
Case 6 $EI = EcI > EnI = SI > RI$

In the design of this group, attention is focussed on the two groups, namely, Energy and Economic indicators as the representative of techno-economic characteristic of the options, and socio-environment group reflecting non-economic parameters. Silicon and iron options have priority in comparison with aluminium and copper options. Characteristic of this case is that it has high probability of dominance between options under consideration, and it may be used as the most probable case we have considered in this evaluation.

Weight-coefficients



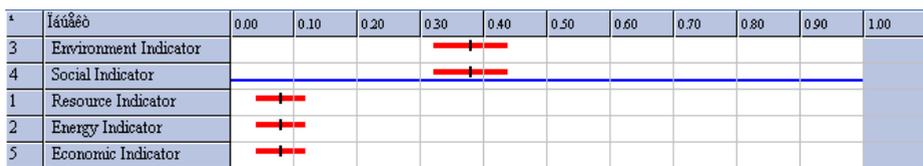
Sustainability Index



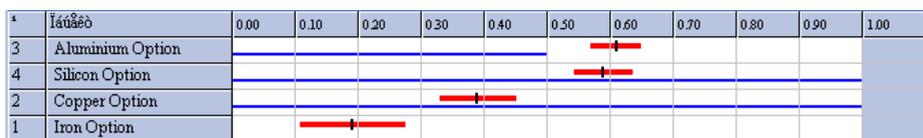
Case 7 $EnI = SI > RI = EI = EcI$

If we give priority to the Environment and Social Indicators, the result obtained gives priority to the Aluminium and Silicon options. It should be noticed that the probability of dominance between Aluminium and Silicon option is rather low which is characteristic of the very probability of this case.

Weight-coefficients



Sustainability Index



The presented cases are only a demonstration of the potential use of the multi-criteria assessment method for the design of the future strategy of material resource use and development. This evaluation is a simple example of the presented method and can be used as a tool for the decision-making procedure.

CONCLUSION

The sustainability concept has proven to be a leading strategy in the future development of human civilisation. Natural capital limits are recognised in energy, water, environment and material resources. In this respect, a complex system approach is envisaged as possible route in sustainable development. As was demonstrated, this approach requires selection of appropriate criteria and respective indicators to monitor resources, energy, economic, environment and social characteristics of the system under consideration. In particular, the selection of the route for material resources utilisation and development is important in order to meet present need and preserve available resources for future generations. Also, it is of great importance to plan future strategy taking into consideration multi-criteria approach in evaluation of the potential options.

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Polyaromatic Hydrocarbons, Pollutants and Molecules of Technological Interests

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1 ABSTRACT

Polyaromatic Hydrocarbons (PAHs) are molecules of great ecological interest due to their carcinogenic activity. The mechanism of their carcinogenic activity was subject to various experimental and theoretical chemical treatments during the last 50 years. Of particular importance were the theoretical treatments that involved applying quantum mechanical methods. Hückel Molecular Orbital theory and perturbation treatments were the most prominent tools in these studies. They allowed a proper understanding of their carcinogenic activity.

Besides their environmental importance, PAHs are gaining increasing industrial importance, they compose 3-4% of the heavy cut of mineral oils! Current studies are done to investigate the possibility of converting PAHs to simpler molecules which might serve as basis for the chemical industry, such as acetylene, ethylene or benzene.

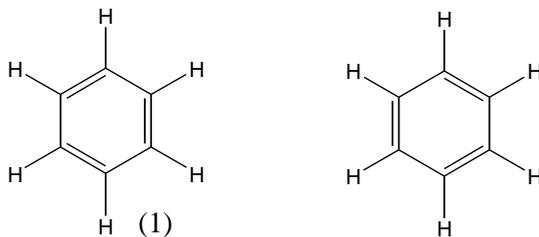
In the recent years PAHs were found suitable for nanochemistry and nanotechnology. For this purpose, PAHs of dimension $>10\text{nm} < 100\text{nm}$ are currently synthesized and investigated. The success of these efforts is mainly due to two reasons: (a) The ease of their deposition on solid surfaces and, (b) The convenient understanding of their chemical and physical properties on the basis of the Hückel MO theory. The possibility of their properties' manipulation makes them very suitable for different applications in modern nanochemistry.

2 THEORY

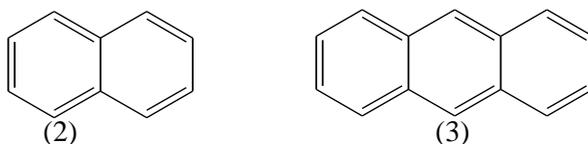
Aromatic hydrocarbons are cyclic conjugated (unsaturated) molecules with considerable chemical stability, lack of reactivity and some common physical properties. In many cases an aromatic molecule may contain one or more

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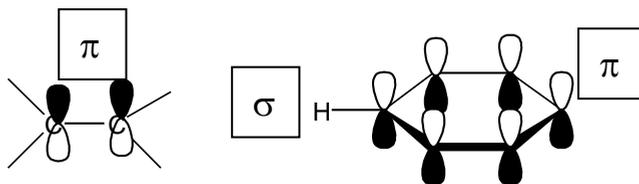
heteroatoms (other than C) such as N, O, S, P..etc. The cyclic conjugated structure was first introduced to organic chemistry by the German chemist August Kekule [1], who assigned the following structure for the most prominent aromatic molecule, benzene:



Similar structures are assigned for the other members of this family of molecules such as naphthalene (2) or anthracene (3).



The concept of aromaticity was very useful for chemists and helped them in dealing with such molecules, on the synthetic or structural elucidation levels or on studying their physical properties. Definitely, it was an accelerating factor in the growth and development of chemical industries at the time which followed Kekule`s work. However, it was later discovered, that the application of the newly discovered methods of quantum mechanics [2,3] lead to a more precise understanding of the aromatic character. The major breakthrough in the quantum mechanical treatment for organic conjugated molecules in particular and molecules in general was due to the work of E. Hückel [4], who classified the electrons of conjugated molecules, and consequently aromatic molecules, in two classes, the π - and the σ - electrons;



He was able then to describe mathematically the Schrödinger eigenvalue equation for the π - electrons;

$$\underline{H}^{\pi} \Psi^{\pi} = E^{\pi} \Psi^{\pi} \quad (1)$$

He described H^{π} as an effective mathematical operator for the total energy of the π -electrons and Ψ^{π} in terms of linear combinations of the C atomic wave

functions for the p_z orbitals of similar symmetry as Ψ^π . It is important to realize that the solution of the eigenvalue equation (1) provides us with;

- (1) The energy eigenvalue (or quantized energy level) for each π - electron in the molecule E_i^π ;
- (2) The wave function (eigenfunction) ψ_i^π for each π -electron in the molecule.

The second result, No. 2, was of great importance to chemists, since ψ_i^π is the key for all physical and chemical properties of the electron that one could imagine. Hückel extended his work and defined the electronic configuration $(4n+2)$, for one single aromatic ring, as a requirement for the aromatic property [5]. In this, Hückel rule, n represents an integer and the sum $(4n+2)$ the total number of π -electrons in the ring. Other configurations $(4n)$ or $(4n+1)$ are either anti-aromatic or non-aromatic unstable structures.

Two prominent interpretations of aromaticity followed the Hückel MO picture. The first was that of L. Pauling [6], who accepted the σ - π separation, applied a different mathematical picture for the wave function ψ^π , the so-called valance bond picture, and ascribed the aromatic character to the cyclic conjugation of the C-C double bonds. He defined the aromatic stabilization energy as the difference in energy between the ring with an assumed non-interacting C=C bonds and the same ring with complete interaction between them;

$$\Delta E_{\text{Pauling}} (\text{aromatization}) = E^\pi_{\text{delocalized}} - E^\pi_{\text{localized}} \quad (2)$$

$$= E^\pi_{\text{benzene}} - E^\pi_{\text{1,3-cyclohexadiene}}$$




The second explanation was that of M. Dewar [7], who defined the thermodynamic stabilization of aromatic compounds as the difference in π -electronic energy between the cyclic conjugated ring and the corresponding open chain structure with the same number of electrons;

$$\Delta E_{\text{Dewar}} (\text{aromatization}) = E^\pi_{\text{delocalized}} - E^\pi_{\text{open chain}} \quad (3)$$

$$\Delta E_{\text{Dewar}} (\text{aromatization}) = E^\pi_{\text{benzene}} - E^\pi_{\text{1,3,5-hexatriene}}$$

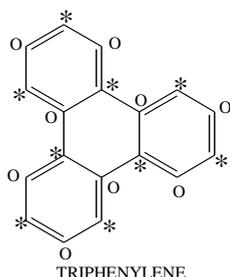



He developed then a simplified “first order perturbation” treatment to calculate ΔE_{Dewar} (aromatization) for any conjugated ring molecule and distinguished the aromatic from the anti- or non-aromatic rings. This simplified quantum mechanical treatment was so powerful that it replaced the older resonance theory of Pauling and Wheland [6] in all its domains.

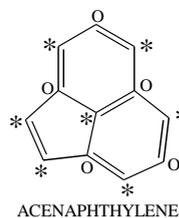
The quantum mechanical treatment, based on the Hückel MO theory, was extended then by C.A. Coulson and Longuet-Higgins [8] to the treatment of most major chemical problems of aromatic compounds. They developed the mathematical treatments for the following phenomena:

- The electron densities at the C atoms, ρ_i ;
- The bond orders $P_{i,j}$ between any two C atoms of the ring;
- The bond distances between any two neighbored C atoms of the ring, according to a linear relation between distance and bond order; and
- The atom and bond polarizabilities.

Classifying the conjugated molecules into alternate (a) and non-alternate (b) hydrocarbons, they could even simplify the effort in obtaining the wave functions ψ_i^π and eigenvalues E_i^π for the electrons.



(a) alternate HC

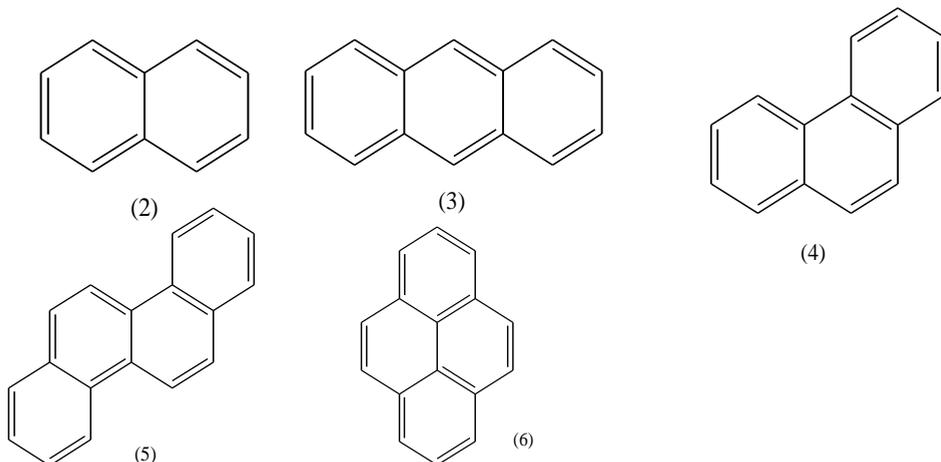


(b) non-alternate HC.

In conclusion, one may state that the pioneering work of E. Hückel, C.A. Coulson, H.C. Longuet-Higgins and M.J.S. Dewar established a convenient, correct and practical way of treating the chemistry of aromatic hydrocarbons in particular and conjugated organic molecules in general. Not only were their ground state chemistry studied so thoroughly, but also their excited states. Basic research was done by Th. Förster [9] and others, which helped in understanding their electronic configuration, spectroscopic properties and energy release processes.

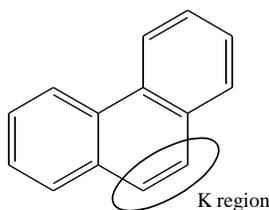
3 CARCINOGENIC AND MUTAGENIC ACTIVITY OF PAH

Polyaromatic compounds are multicyclic molecules with aromatic character, of the following shape:

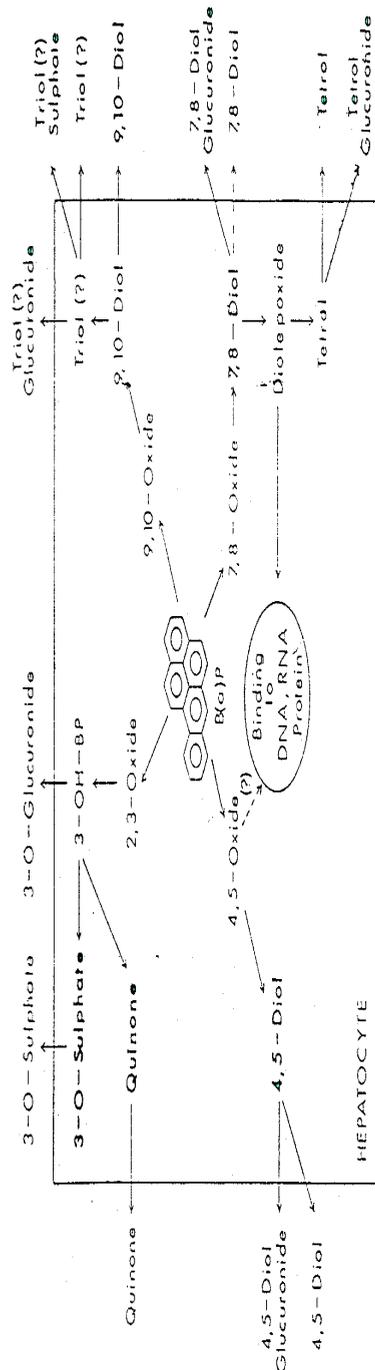


They are not limited to six member rings only, but also four- five- and seven- member rings too. They may include other atoms besides C such as N, O, S etc. Hundreds of such PAH's have been isolated, synthesized, characterized and utilized chemically till now. Many of them are known to be strong carcinogenic, mutagenic and hazardous pollutants [10,11]. Their dangers are very acute, since they are formed through a process of incomplete combustion. They are emitted from the combustion engines, refineries, power stations, forest burns, and military bombardments, and are formed even on grilling meat. They form 3-4% of heavy mineral oil cuts [12]. Since the sixties of the last century, tremendous efforts were done internationally to eliminate their hazards in the environment. As a result, thousands of scientific papers and Internet reports emerged dealing with their pollution problems.

Besides the many studies of their ecological properties, basic research was done to elucidate the mechanisms of their carcinogenic and mutagenic activity. Even here, the pioneering work of A. & B. Pullman [13] was based on quantum mechanical concepts, derived from the Hückel MO theory forming the starting point of the investigation. They ascribed the carcinogenic activity of PAH to the presence of an “active” C=C bond in a so called K-region.

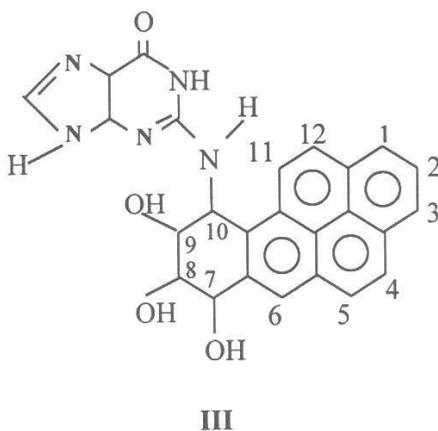
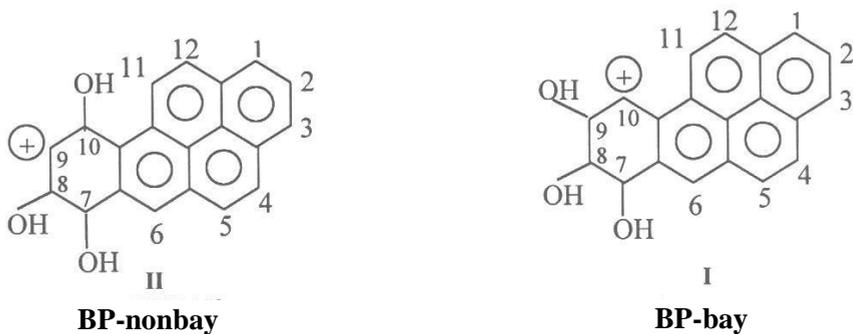


Later, other scientists introduced similar treatments to conclude the presence of other, L-, M-, Bay-, and Fjord-regions [14], that facilitate their carcinogenic and mutagenic activity. Experimental chemical evidence proved that the PAH's are oxidized in the living cell according to the following scheme [15].



Scheme 1. Extracellular medium.

The resulting epoxides, diols and triols in their turn undergo condensation reactions with a DNA base, forming an addition product and an unnatural DNA, which as expected leads to the mutagenic or carcinogenic appearance [16].



Scheme 2. Benzo (a) pyrene Triol-guanine adduct.

4 INDUSTRIAL ASPECTS OF PAHS

Polyaromatic hydrocarbons are constant components of the heavy cuts of mineral oils, the different components of which are given in the following Table 1 [12].

**Table 1. Composition of the 370- 535 C distillates of crude oil [12]
Wt% of crude oil (of distillate)**

	Gach Saran Iran	Swan Hills Canada	Wilmington California	Recluse Wyoming	Prudhoe Alaska
Acids	0.34	0.33	1.38	0.25	0.61
Bases	0.42	0.40	1.67	0.21	0.53
Neutral nitrogen cmpds.	0.23	0.08	1.04	0.17	0.19
Saturates	9.54	12.10	9.12	10.16	10.45
Mono- aromatics	3.31	2.30	4.15	2.09	3.67
Diaromatics	2.30	1.15	3.05	0.94	2.58
Polyaromatics-polar	3.54	1.99	4.28	1.14	3.59
Whole distillate	19,67	18.35	24.69	18.58	21.63

The table shows that the average percent ratio of PAHs in these cuts is 3-4%. According to these figures, the world presence of these compounds amounts to millions of tons. However, their present industrial consumption is very limited. This is due to the fact that at present the petrochemical industry is based mainly on earth gas or light to intermediate hydrocarbons. The question arises about new resources for the petrochemical industries once the earth gas or light hydrocarbons are no more available on a feasible price scale. By then PAHs may form an adequate substitute for them. Thermal decomposition of such compounds could yield small hydrocarbon molecules, ethylene or acetylene that are suitable for this purpose. Ethylene is a petrochemical starting material at present; acetylene is appropriate too, considering the possibilities of the well-known Reppe synthesis [17]. In our laboratory we have carried out quantum mechanical study of the thermal decomposition of some PAH molecules, applying the so-called Self Consistent Field methods. The study included both C...H bond rupture as well as HCCH elimination reactions of the following type;

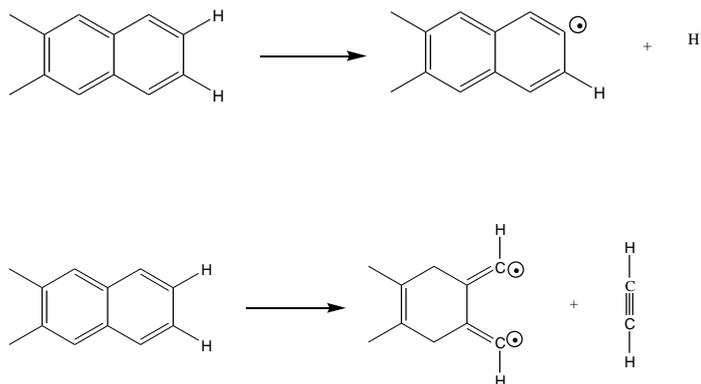


Figure 1 shows the calculated reaction paths for the C...H bond rupture reaction of phenanthrene PAH molecule. It is seen that the reaction is endothermic and that the calculated activation energy is ~ 99.2 kcal/mol.

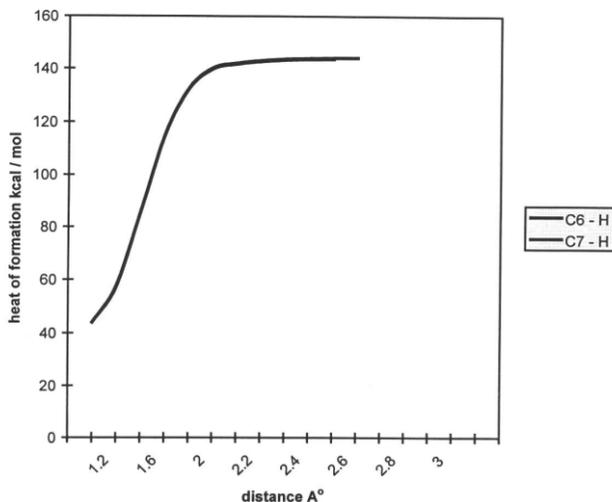


Figure 1. SCF-MO calculated reaction path for the C-H rupture reaction of phenanthrene PAH molecule.

The acetylene elimination seems, according to the calculation results, less facile and requires higher activation energy, ~ 223.7 kcal/mol (Figure 2).

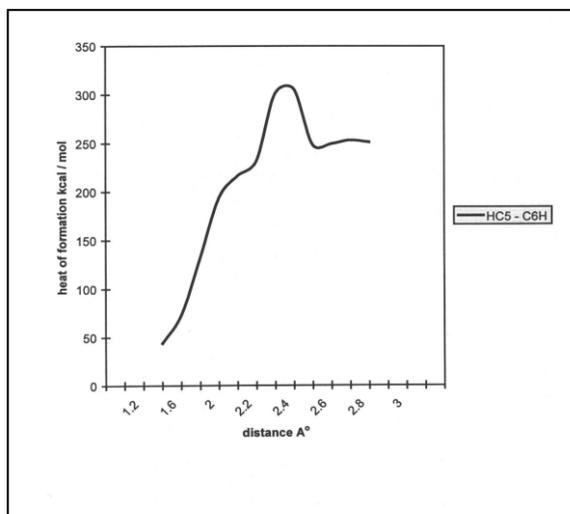


Figure 2. SCF-MO calculated reaction path for the acetylene elimination reaction of phenanthrene PAH molecule.

The difference in activation energy is ~ 133.5 kcal/mol., for the favor of C-H rupture reaction. The possibility of catalyzing the elimination reaction was studied then according to the following model. SCF calculations were done for the radical cation of the PAH resembling the case of electron withdrawing catalysts such as Lewis acids, and radical anions, resembling the case of electron releasing catalysts such as amine or phosphine derivatives. Figure 3 shows the calculated reaction paths for the decomposition of the radical ions of the same PAH molecule.

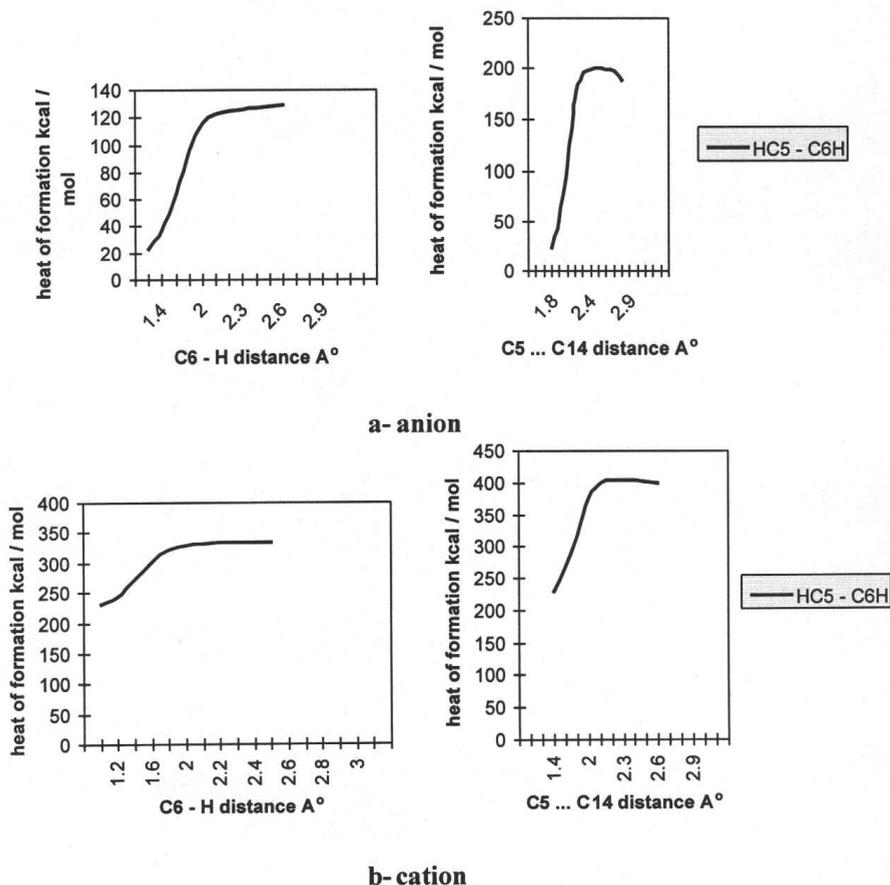


Figure 3. SCF-MO calculated reaction path for the C-H rupture and acetylene elimination reactions of phenanthrene radical anion and cation.

Interesting is the decrease in the activation energies of acetylene elimination reactions in both cases. The decrease in energy is ~ 53.4 kcal/mol. The calculated activation energies for the catalyzed reactions are smaller than the activation energies of the noncatalyzed reaction.

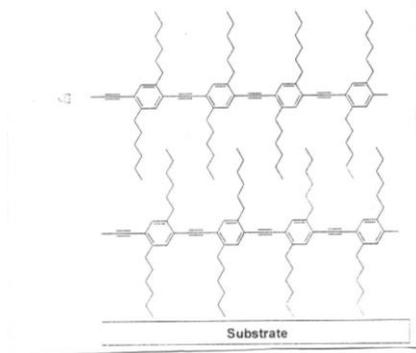
5 NANOCHEMISTRY

In recent years much has been written about the so called Nanotechnology[18]. The required materials for this technology are a challenge for chemists. For this reason the term “ nanochemistry” emerged in the literature [19]. It might be easily defined as the chemistry of the single molecules. It requires molecules of “big size” 1-100nm, and strong magnifying microscopes such as Scanning Tunneling Microscope (STM) or Atomic Force Microscope (AFM). The chemical and physical manipulations are to be carried out then for single molecules under strong magnifying devices.

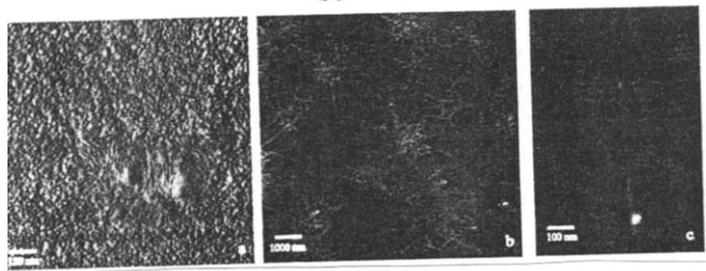
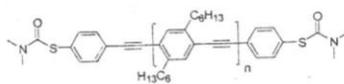
Polyaromatic hydrocarbons seem very suitable for nanochemistry for two important reasons;

- (1) The excellent theoretical understanding of their physical and chemical properties on the bases of quantum mechanics as shown in the former paragraphs; and
- (2) The existing experimental knowhow of forming different molecular structures such as discs, chains, with the basic aromatic molecule as a building block, and of depositing them on solid surfaces.

Chemists repeated their efforts in recent years to design and synthesize such nanomolecules and study their physical properties [20]. Different types of PAH chains were synthesized and studied. Figure 4 shows a representation of molecular packing of a polyphenylen-ethynylene chain [21].



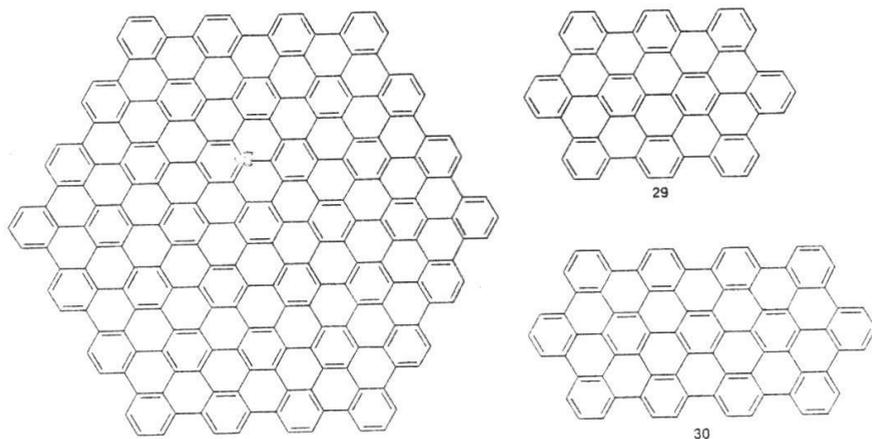
a-



b-

Figure 4. Molecular packing of polyphenylene-ethynylene chain.

Figure 5 shows some “disc” molecules built from benzenoid units, and Figure 6 shows STM picture of a rhombus type PAH [21].



a-

b-

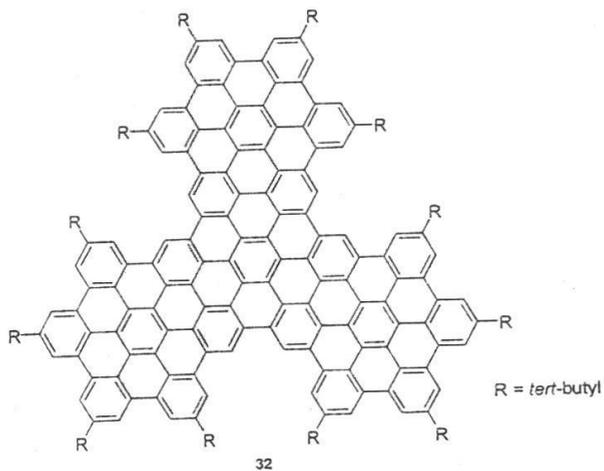


Figure 5. a- Giant disc molecule built from benzenoid units; b- Examples of PAH molecules with D_{2h} symmetry.

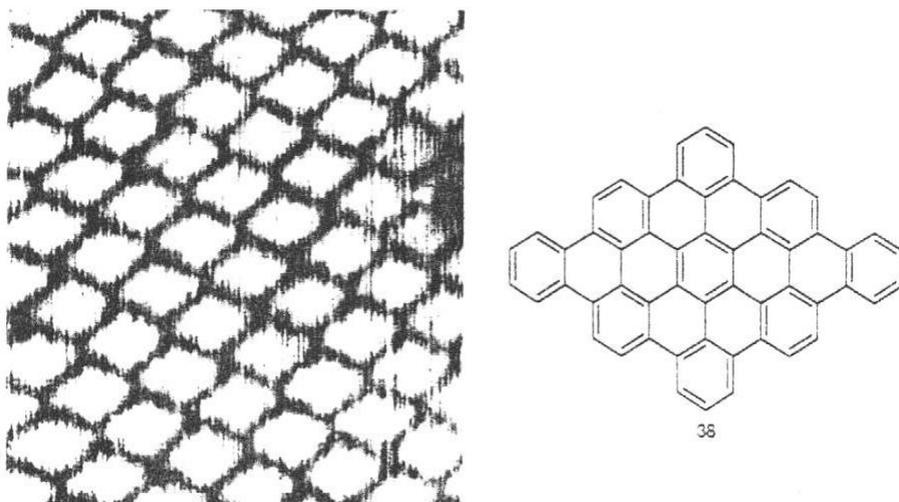


Figure 6. Scanning tunneling microscope (STM) of a rhombus type PAH [21].

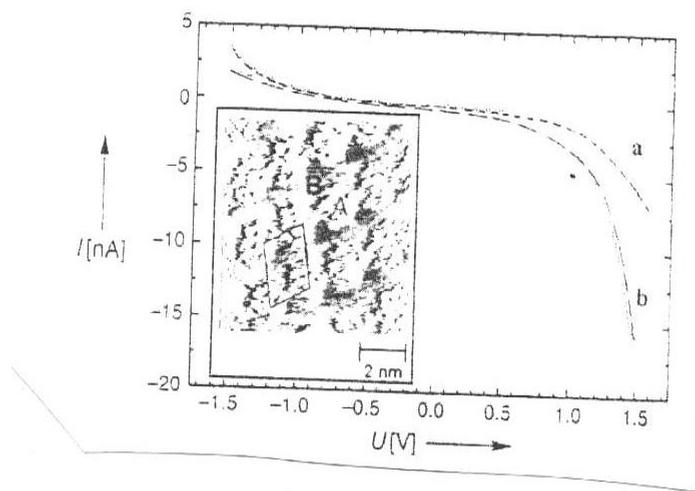


Figure 7. Current-voltage curves of hexadodecyl substituted hexabenzocoronene (HBC) nanomolecules[22]; a- for the aliphatic part of the molecule; b- for the aromatic part.

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* As listed by author.

Nanotechnology: An Overview

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1 ABSTRACT

The properties of the same material may drastically change when measured at bulk scale and the micro or nano-scale in physical dimensions. A material fabricated with small grain size shows higher strength than the same material prepared with larger grain size. The properties would also change when studied under different temperatures. An electrically insulating material at room temperature may behave as a superconductor at very low temperatures, such as in the case of high temperature conductors of $YBa_2Cu_3O_7$ ceramic compounds. In this overview, the extensive use of the materials at the nano-scale of dimensions will be given. The area of the so-called “Nano-technology” of materials has found a variety of applications in many areas of science, be it Physics, Chemistry, Biology, Medicine etc. Nano-science is the topic of today and holds great hope of future.

The handling and control of materials at the nano-scale is the “Nanotechnology.” One nano-unit, i.e. 10^{-9} m would thus contain about 10 atoms (an atom size being about 10^{-10} m). Thus handling and experimentation of material sizes of a few atoms in all areas of science; Metallurgy, Biology, Physics, Medicine, Chemistry and so on, is what has become to be known as “Nanotechnology.” Therefore, “Nanotechnology” is not restricted to one speciality - it is an opportunity for specialists in a variety of disciplines of science. It is indeed a true meaning of multi-disciplinary nature. The exotic applications of nanotechnology in various areas such as lithography, information technology, metallurgy, medicine, etc. will be briefly illustrated. An attempt has been made to explain that Nanotechnology belongs to all sciences; it is not in the possession of one discipline of science. It belongs to all. Nanotechnology belongs to a medical specialist, a chemist, a physicist, and a biologist or even to a mathematician who builds the protein models or a computer specialist who makes the relevant computation.

It has applications ranging from the drug engines in medical treatment of tumours to the surface hardening of metals in ion implantation. From the technology of lithography where on the head of a pin one should be able to print

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all of the Encyclopaedia Britannica, to the self-assembly of biological molecules to understand the process of life mechanism or to the communication technology where the silicon chip will be replaced by molecular switching system 10 times smaller than the existing size of chip used today.

2 NANO-SCIENCE AND NANO-MATERIALS

2.1 General

Nanotechnology basically deals with the Science and Technology of Materials. Materials have been from time immemorial the hub of physical and economic strength in our lives. He was right when an excommunicated and primitive tribesman said, “*I have got the might of God, and I will conquer the world,*” when he found an iron bar. This is true even of today when history has transgressed over the centuries various “ages” such as the stone age, the bronze age, the iron and steel age, the semiconductors age, the nuclear materials age, advanced materials or new materials age (composites, ceramics, polymers) and now the nano size materials age; the “Nanotechnology age.”

The concept of nano science was evolved when Feynmann gave the famous lecture, “*There is a plenty of room at the bottom,*” and made the remark that “*why cannot we write entire 24 volumes of the Encyclopaedia Britannica on the head of a pin,*” at the Annual American Physical Society Meeting held at the California Institute of Technology, California, December 1959 [Feynman, 1959].

The term “nanotechnology” was then coined by the Japanese Professor Norio Taniguchi in 1974 [Taniguchi 1974], while describing “*the processing of materials to nanoscale precision,*” in reference to precision machining of hard and brittle materials like Quartz, Silicon and Al_2O_3 etc. by ultra-sonic machining. K.E. Drexler’s PhD thesis at MIT led to his book “Engines of Creation” in 1986 and brought in the possibilities of molecular manufacturing technology and the revolution in and popularity of the field of nanotechnology [Drexler 1986, 1992]. While nature has nano-size things like DNA (diameter of the order of 2.5nm, ATP Synthase with diameter ~10nm and atoms of silicon spacing ~ 0.1nm etc.) the production of man-made things of nanometer size (Carbon nano-tube ~ 2nm diameter, Zone plate X-ray “lens” outer most ring spacing ~35nm etc.) is the beginning of nanotechnology for man.

The nano-science seeks to understand the new properties of materials on the nano-size scale while “nanotechnology” seeks to develop materials and structures that are novel and have significantly improved physical, chemical, tribological properties and functions due to their nano-size. The goals of nano-science and nanotechnology are:

- (1) To understand and predict the properties of materials at nano-scale;
- (2) To manufacture nano-scale components from the “bottom up;” and

- (3) To integrate nano-scale components into macroscopic scale objects and devices for real world uses.

2.2 Preparation of nano-crystalline materials

There are five widely known methods for synthesis of nano-materials:

- (1) Sol gel synthesis;
- (2) Inert gas condensation;
- (3) Mechanically alloying or higher energy ball milling;
- (4) Plasma synthesis; and
- (5) Electro deposition.

Among these, sol gel synthesis [Hunt and Ayers, 2003] is commercially very versatile and useful. It can synthesise materials of ultra high purity of 99.9999%. When the compacted specimen grain size is about 5nm the crystalline and interfacial “phases” have nearly the same volume fraction assuring a grain boundary thickness of 1-2 nm.

2.3 Multidisciplinary nature of nanotechnology

The strong point of nano-science and nanotechnology is their multidisciplinary nature. It is strongly interconnected and requires the optimum use of multidisciplinary subjects involving engineering (mechanical, electrical, chemical), physics, chemistry, biology, materials sciences, information technology and computer sciences [Figure1]. The multidisciplinary aspect is well represented by the “Nanotechnology Tree” [Figure2].

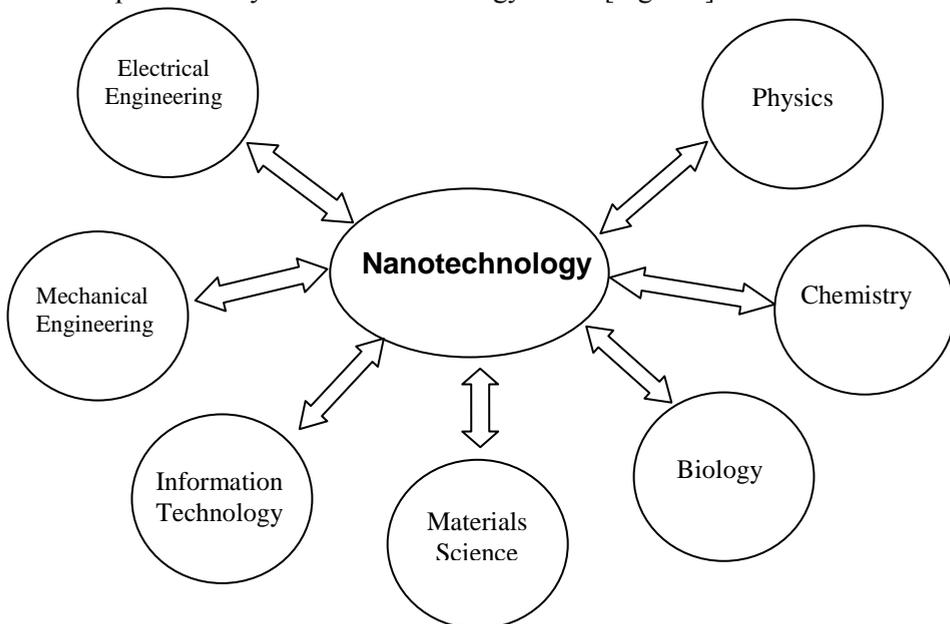


Figure 1. Multidisciplinary aspect of nano-science and nanotechnology

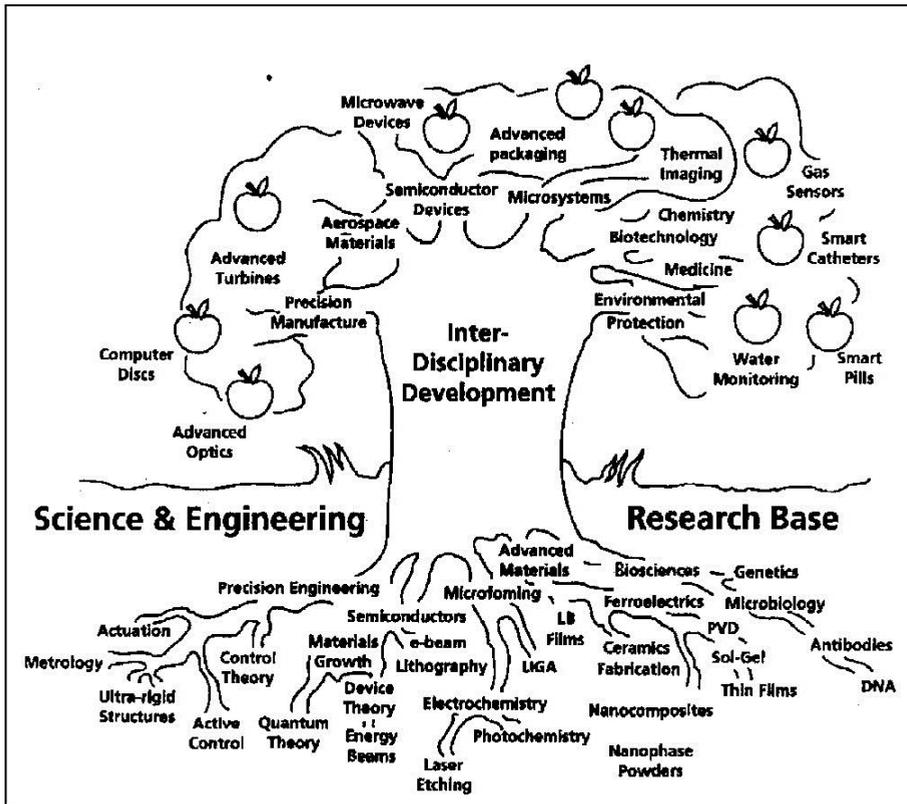


Figure 2. Nanotechnology tree.

2.4 Analysis and characterization of nano-sizes

No doubt synthesis and preparation of nano-size materials is one of the important aspects of nanotechnology both from the development point of view and for the fabrication of products for commercial purposes, but the characterization of the nano-size materials produced is essential before fabrication of the products. Basically the techniques of particle size measurements using microscopes (optical, electron, transmission and scanning) and spectroscopic techniques are already used in materials science. New high resolution scanning micro probes along with the nuclear techniques of neutron scattering, NMR and synchrotron radiation (SR), etc. can be used in the characterization of the nano-particles [Figure3]. All these experimental techniques are today in use for extensive characterization of nano-materials.

Some useful physical techniques are:

- (i) Scanning Probe Microscopy (STM);
- (ii) Atomic Force Microscopy (AFM); and
- (iii) Energy Beam Processes:

- EBM (electro-discharge-machining);
- FIBM (Focused Ion Beam Machining);
- RIE (Reactive Ion Beam Etching).

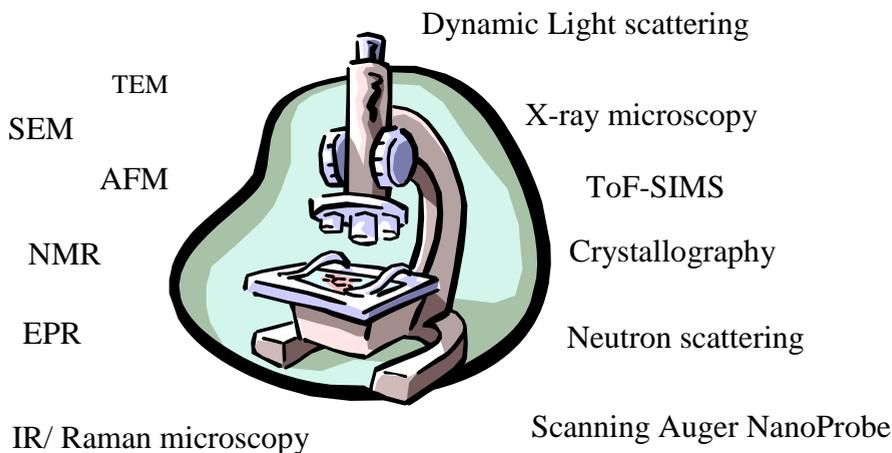


Figure 3. Nano-characterization tools.

One of the most important instruments with a resolution to see and handle single atoms and molecules is the atomic force microscope (AFM). It is extensively used for biological samples [Figures 4-5].

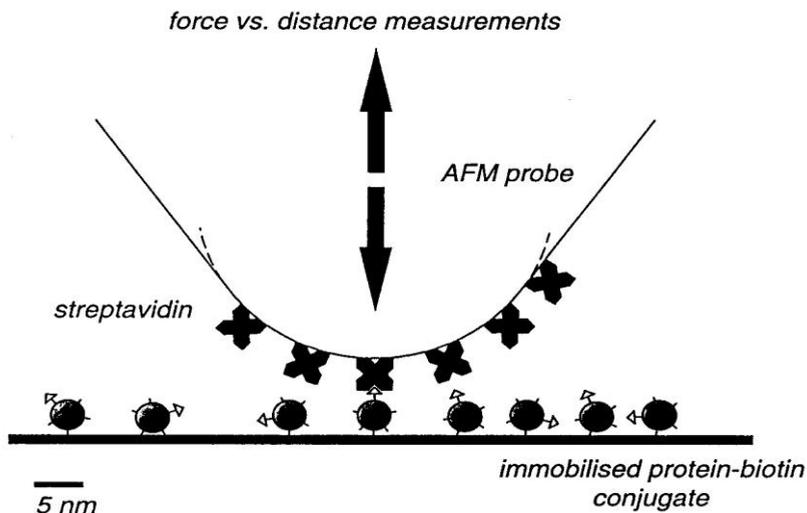


Figure 4. Schematic representation for measurement of single molecule interaction using atomic force microscope (AFM). The AFM has the ability to measure forces in the range of nanonewtons and less.

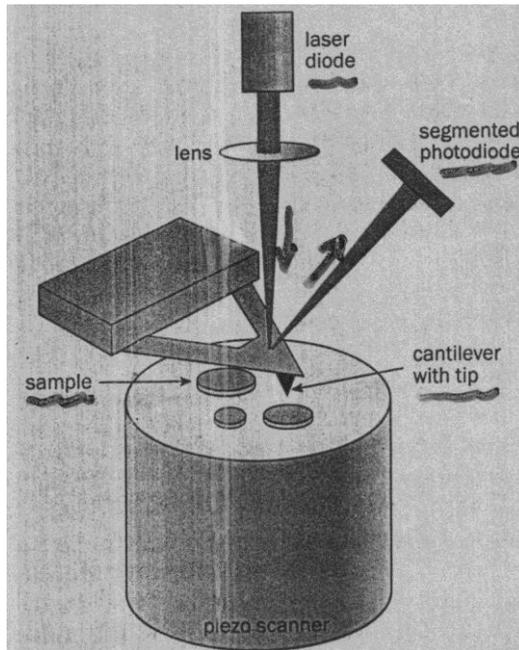


Figure 5. The atomic force microscope (AFM) comprises a sharp tip about 10^{-10} m in diameter mounted on a soft cantilever spring. The small diameter of the cantilever tip limits the number of molecules able to interact to only a few, of even a single molecule.

The cantilever tip of AFM attached to a spring could be precisely controlled to handle the single protein molecules of a biological sample and thereby the force between these molecules could be measured. Typically a force of 200 piconewton with an accuracy of about 5 piconewton could be measured. The electron beam (EB) techniques are good tools for miniature work. The concept of writing encyclopaedia on tip of a pin introduced by Feynman is practically in hand through these EB tools [Figure 6].

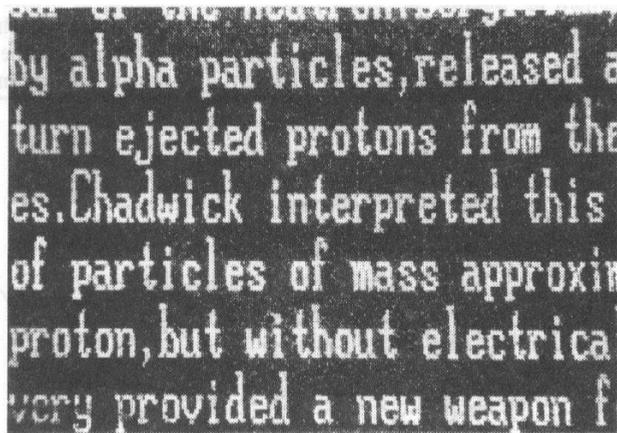


Figure 6. Electron beam lithography: Writing the Encyclopaedia Britannica on the head of a pin. The line width of each letter is two electron beam drilled holes, each hole is 4 nm diameter, the substrate is silicon fluoride.

2.5 Industrial Scale Production

With proper synthesis and characterization of the nano-size materials, enormous applications have been made, exploiting the basic fact that at nano-sizes the properties of materials are greatly changed. On the one hand “miniaturization” of products has been affected by what is now called molecular engineering and on the other “bulk products” have been produced from these nano-size materials on commercial scale. Specific institutes of “Molecular Manufacturing” have been established to concentrate attention for fabrication of products on molecular scale. [Ref. Inst. for Molecular Manufacturing (IMM), Los Altos, Ca 94022, USA, Fax: 650-917-1123; e-mail: admin@imm.org; Website: <http://www.imm.org>, May 2003].

2.6 Molecular Manufacturing

Handling at the molecular level has led to a number of nano-scale and micro-scale fabrication of products in a number of areas such as micro and nano-electronics, and molecular rotors. An electric rotor has been built [Figure 7] which is “2000 times smaller than the width of a human hair”. Its gold blade is 300 millionths of a millimetre long [Zettl, 2003].

Figure. 7 World's Smallest Rotor (Nanotube-mounted blade to drive switching and sensing).

Nature already provides nano-motors, for example, in the form of many bacteria propelled by nano-motors. The tiny biochemical motor turns a rotor shaft that spins the tails or *flagella* and allows bacteria such as the *E-coli* to move through liquid [Figure 8].

Gold Blade



Figure 8. Nanomotors in bacteria.

Molecular sensors and targeted drugs for cancer treatment and other diseases, and defence areas are examples of this. Micro-electronic circuits with just a few molecules; a few thick lines onto gold have been drawn using atomic force microscope as “pen,” gold as paper and the chemicals of “alkanethiols” as ink. That was the world’s smallest pen as claimed by the team of researchers in Northwestern University, Chicago [Science, 1999].

The machining accuracy in mechanical parts has greatly improved due to the use of electron-beam technology [Figure 9], used in molecular engineering.

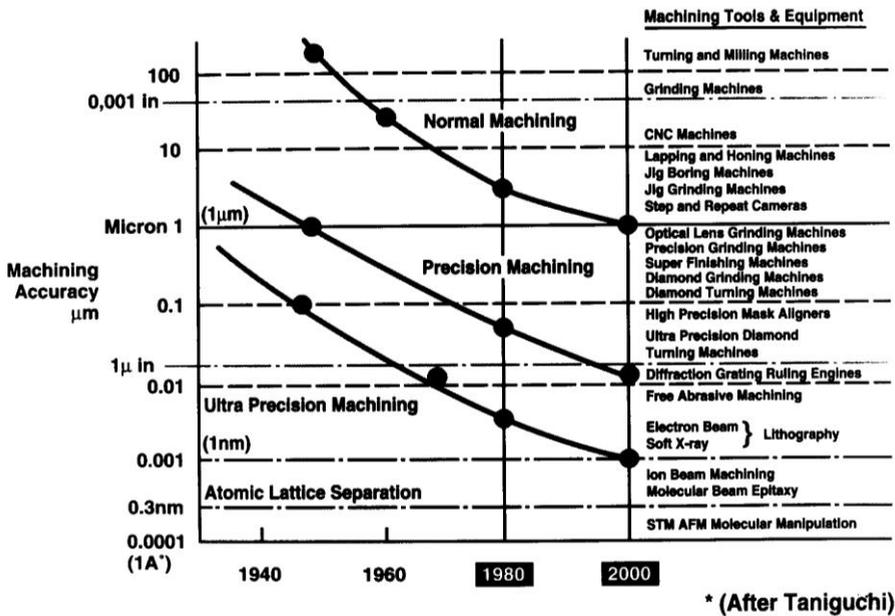


Figure 9. Achievable machining accuracy over about 60 years.

2.7 Carbon Nano-tube Technology

A great promise in molecular manufacturing has come up due the manufacturing of carbon nano-tubes. The discovery of C_{60} , the Fullerene, led to a number of such promises because of the exotic properties of carbon nano-tubes such as high mechanical strength, high electrical conductivity and energy storage capacity. The C_{60} nano-tube and a variety of such nano-tubes are shown in [Figure. 10].

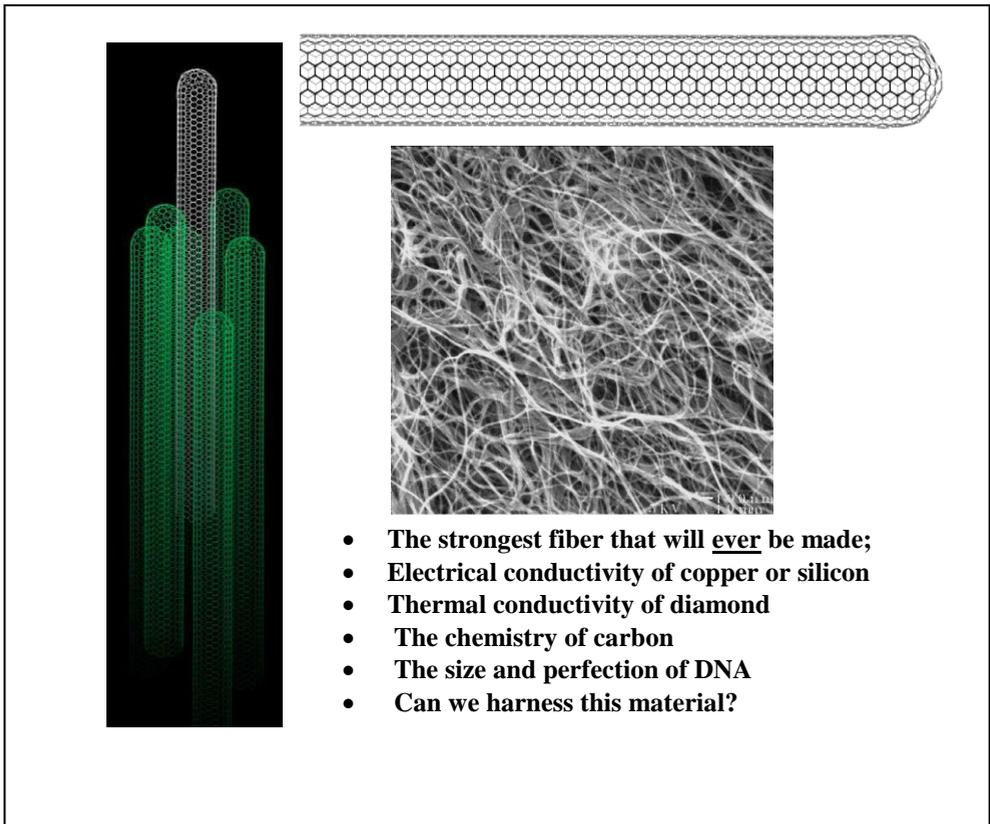


Figure 10. Fullerene (C₆₀) Carbon Nanotubes.

Carbon nano-tube technology revolution is occurring in the miniaturization of electronic products and the speed in electronic communication and information [Figure 11].

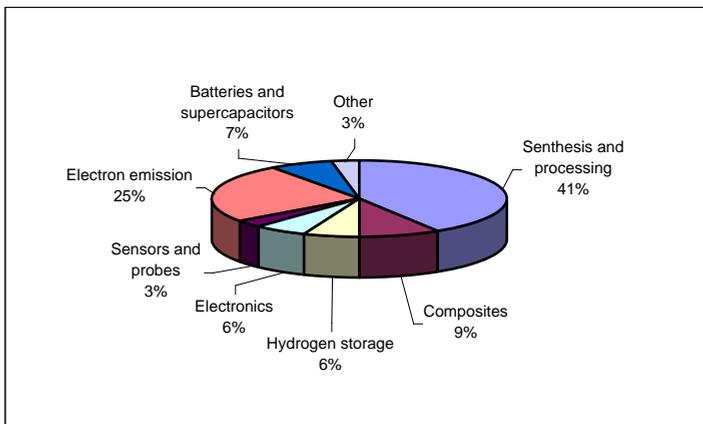
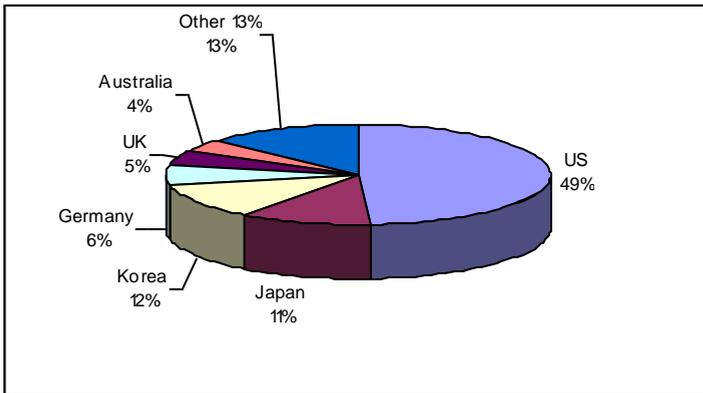
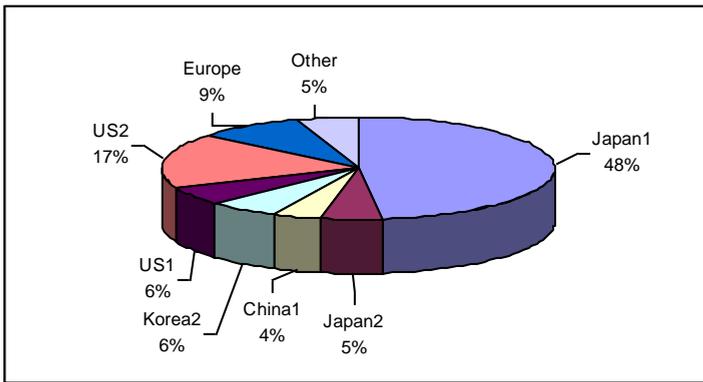


Figure 12. Publications and patents in nanotechnology, (A: Years-wise increase, B: Percentage total patents by individuals in a country or a region, C: Percentage of patents of different countries, D: Percentage of inventions in different areas of nanotechnology).

3 NANOTECHNOLOGY IN ACTION

3.1 Applications of nanotechnology in defence

- (1) New nanotechnology materials might be developed that offer improved stealth, spanning the electromagnetic spectrum from the visible, through the infrared and into the radar bands;
- (2) Specially prepared clouds of nanotechnology particles could be used to disrupt electronic systems;
- (3) A molecule consisting of carbon atoms in the form of a geodesic ball (a buckyball) could be used to deliver a specific type of atom or a single molecule to a site at which it might be required;
- (4) New forms of sensors, information processing and communication will enable small unmanned systems and autonomous weapons to reach their target with the ability to adapt to unexpected changes in weather and also the ability to detect and counter threats directed at them;
- (5) A whole range of military equipment including clothing, armour, weapons, personal communications equipment may have their characteristics optimised, operation and performance enhanced to meet changing conditions automatically;
- (6) Kinetic Energy (KE) penetrators with enhanced lethality (replacement of depleted Uranium penetrators); and
- (7) Better and future weapons platforms.

3.2 World interest in Nanotechnology

3.2.1 *In the USA*

In addition to the allocation of specific funds and setting up specific institutes in the advanced countries in the area of nanotechnology, there is a specific approach of “ a network” of various laboratories and centres involved in the techniques used in nanotechnology.

In the USA, the amounts of funds allocated in recent years to nanotechnology show increasing trends in investment [Tables 1 and 2]. Table 1 shows the allocation of budget for the years 2001-2004 in the important areas of defence, energy, commerce, health, NASA, environment, transportation, agriculture and justice. Almost 100 per cent increase in budget has been made from 2001-2003 in defence and commerce.

Table 1. Breakdown of Spending in the US's National Nanotechnology Initiative from 2001 to 2003 (all figures in millions of dollars)

	2001	2002	2003	Increase in 2 years	2004
National Science Foundation	<u>150</u>	199	<u>221</u>	47%	247
Defence	<u>123</u>	180	<u>243</u>	100%	222
Energy	<u>88</u>	91	<u>133</u>	51%	197
Commerce	<u>33</u>	38	<u>69</u>	109%	62
National Institute of Health	40	41	65	62%	70
NASA	22	22	33	50%	31
Environment Protection Agency (EPA)	5	5	6	20%	5
Department of Transportation	-	2	2	-	-
Department of Justice	1	1	1	-	1
Agricultural	-	-	1	-	10
Total	<u>464</u>	579	774	67%	<u>874</u>

A number of US departments and agencies cooperating in this National Nanotechnology Initiative Programme (*Ref: National Nanotechnology Initiative: leading to the next industrial revolution: A report by the Interagency Working Group on Nanoscience Engineering and Technology, Committee on Technology, National Science and Technology Council, Washington, DC, USA, February 2000, <http://www.nsf.gov/home/crssprgm/nano/nni.html>*) are listed below:

- Department of Agriculture (USDA);
- Department of Commerce (DOC);
- National Institute of Standards and Technology (NIST);
- Department of Defence (DOD);
- Department of Energy (DOE);
- Department of Justice (DOJ);
- Intelligence Community (IC);
- Department of Transportation (DOT);
- Department of Treasury (DOTreas);
- Department of State (DOS);
- Environmental Protection Agency (EPA);
- Food and Drug Administration (FDA);
- National Aeronautics and Space Administration (NASA);

- National Institutes of Health (NIS);
- Nuclear Regulatory Commission (NRC); and
- National Science Foundation (NSF).

3.2.2 In Europe and the far East

Even in Europe and the far East, countries have made specific budget-allocations to concentrate on nanotechnology development. Tables 2 and 3 below show the allocations made by some countries that have made considerable investment in this area.

Table 2. European nanoscience and nanotechnology spending, 2000 (in millions of Euros)

Country	Spending	Country	Spending
Austria	2.5	Ireland	3.5
Belgium	1.2	Italy	6.3
Denmark	2.0	Netherlands	6.9
Finland	4.6	Portugal	0.4
France	19.0	Spain	0.4
Germany	63.0	Sweden	5.8
Greece	0.4	United Kingdom	39.0
European Commission	29.0		

Table 3. Government nanotechnology spending in the far East, 2002 (Million of Dollars)

Japan	680
China	200
Taiwan	150
Korea	150
Singapore	40

In Germany, an institute of nanotechnology was established in Karlsruhe and a project “NanoMat” has been organised where the universities, industry and research centres collaborate [see below] in a concerted effort on national basis. Even the concept of Nano Valley has been initiated with the collaboration of the Institute of Nanotechnology, Karlsruhe, and the University of Strasbourg in France [Figure 13].

This two nation joint venture is another example of the coordinated efforts which are being made in the area of Nanotechnology (*Ref: Institute for Nanotechnology, Report (1998-2001), Forschungszentrum Karlsruhe GmbH,*

Postfach 3640, 76021-Karlsruhe, Germany. [Fax: 07247-82-6368, e-mail: office@int.fzk.de).

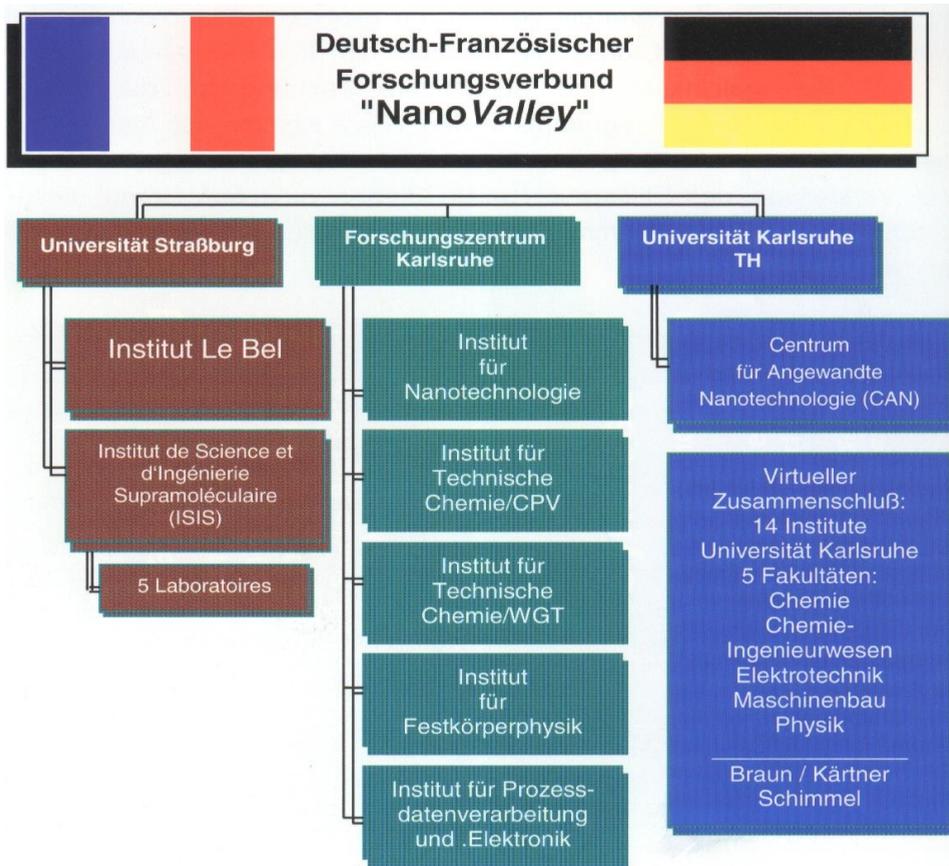


Figure 13 German-French Nano Valley Project.

3.3 Applications of Carbon Nanotubes

- (1) Use in electro chemical devices, electrodes, super-capacitors etc.;
- (2) Hydrogen storage for fuel cells in electric vehicles, laptop computers etc.;
- (3) Field (electron) emission devices for flat panel displays, lamps (life: 8000 hrs), gas discharge tubes, x-ray and microwave generators etc.;
- (4) Nanometer-size electronic devices: NT - field effect transistors, single walled nanotube (SWNT) devices, nano-volatile memory devices etc.; and
- (5) Sensors and probes for scanning atomic microscope tips.

3.4 Other applications of Nanotechnology

As the applications of nanotechnology are very wide and are expanding everyday, it is useful to mention only the titles of the applications, instead of going into the academic basis and interpretation of the applications, so as to appreciate the extent of such applications in almost all areas of life.

Some of the applications are listed as under:

- Next - generation computer chips;
- Better insulation materials;
- Phosphors for high definition TV;
- Low-cost flat-panel displays;
- Tougher and harder cutting tools;
- Elimination of pollutants;
- High energy density batteries;
- High-power magnets;
- High-sensitivity sensors;
- Automobiles with greater fuel efficiency;
- Aerospace components with enhanced performance characteristics;
- Longer-lasting satellites;
- Ductile, machinable ceramics; and
- Large electrochromic display devices.

3.5 Bio-medical applications

- Longer-lasting medical implants;
- Diagnostic sensors that can detect if clothing has been in contact with Anthrax;
- Laboratory or chip techniques for blood analysis and other samples;
- Anticancer drugs, implanted insulin pumps, gene therapy etc.;
- Work on prostheses and implants of nanostructured materials;
- Synthesis and use of nanostructures;
- Applications of nanotechnology in therapy;
- Biomimetics: Synthetic Products;
- Biological nanostructures;
- Electronic biological interface; and
- Easy detection of diseases;
- Instruments for studying individual molecules;
- Nanotechnology for tissue engineering;
- Longer lasting medical implants;
- Capability of mapping the individual's genetic code immediately;
- Ability to extend life by 50%;
- Lab-on-chip diagnostics;

- Light and strong materials for defence, automotive, aerospace and medical applications;
- Sensors for pharmaceuticals and chemicals in the environment;
- Nano-carbon buckyballs and nano-tubes as “drug delivery vehicles” because of their nano-size;
- Nano-particle delivery system for anti-cancer drug;
(130nm ABI-007 drug nano-particle engineered protein containing “paclitaxel” used for breast, bladder and other cancers.). Expected in market in a few years;
- Nano-size UV absorbing particles of Zn-oxide as sun-screen products (Particle size about 3-200nm);
- Manufacture of quantum dots of 3-5nm suitable for binding biomolecules;
- Tissue engineering: From MESA+ to replace damaged tissue or to replace the missing ones;
- Self growth of materials with nano-materials as “seeds;” and
- Artificial sensors for eye, ear or a nerve.

4 NANOFUTURE

4.1 Twenty-First century miscellaneous nanotechnology applications

- *Coupling between mechanical processes and bio-chemically well-defined processes*

The measurement of nanometer displacements and piconewton forces in actin-myosin interaction system will lead to the use of these molecules as the components of “nano-engines.” These have potential applications as components of “*artificial muscles*”. This provides direct coupling of bio-chemical energy (ATP) and mechanical energy of movement.

- *Insights into catalysis*

Study of oxidation of CO at the surface of Oxygen covered Rh surface (like removal of CO from exhaust fumes).

- *Approaches over “positional control” of atomic and molecular arrangements*

- (1) “Top-down approach” as in refining modern lithographic techniques to make finer divisions;
- (2) “Bottom-up approach” as in “self-assembled molecules” as in DNA “*to form range of geometric shapes,*” polyhedrons: octahedron, square etc. *A great stride in “Bio-synthesis.”*

- *Molecular engineering*

This involves (the hair-diameter) the control of atoms and molecules to build up shapes like LEGO (*Atomic/Molecular LEGO*), the way nature does. The “bottom-up approach,” can lead to build up structures into larger dimensions like automobiles, jet planes etc.

- *Attachment of molecules to outside of cages*

Attaching “proteins” to the edge of polyhedron would construct “*artificial multienzymes*.”

- *Injection possibilities*

Possibility of injecting a particular shape into the body or circulatory system to docking sites of particular cells, thus injecting microdoses of toxin into cancer cells - true healing at the molecular level.

- *Carbon atoms arranged in precise diamond-like fashion*

This to create a material 100 times strength-to-weight ratio than steel but 10 times stronger and 10 times lighter.

- *Material preparation with high electrical conductivity*

Electrical conductivity more than copper for materials like polymers, plastics etc.

- *“Self-assemble” systems challenge*

The handling of atoms and molecules by AFM & STM, at nano-levels has the challenge of imparting intelligence to them through the mechanism of “Self-assemble System” – nature’s way of self-organisation - nature’s way of building life. This challenge of “self-organisation,” when understood, may unravel nature; forming incredibly complex organisations such as trees, complete ecosystems and human beings. This understanding of self-organisation in molecular-engineering may lead to understanding self-organisation of large-scale socio-economic systems such as transportation, communication, power distribution, traffic etc.

- *Atomic scale electronics*

Ultra-miniaturized electronic systems through atom by atom at a time - paving the way for atomic-scale electronics.

4.2 Future Trends

Future trend for the next decade is summarised in Figure 14.

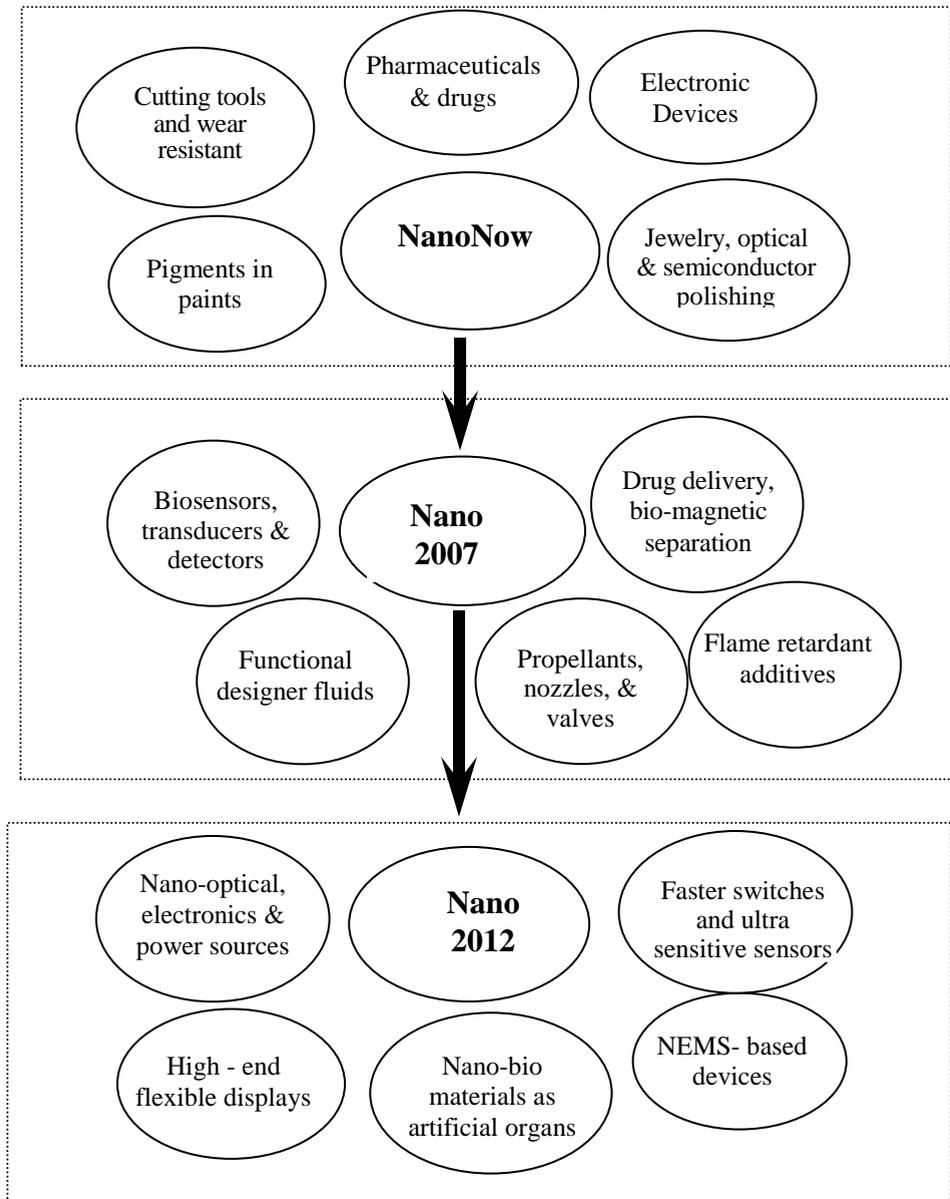


Figure 14. Nano Future!

4.3 Nanotechnology for OIC countries

4.3.1 General

It is imperative that OIC countries pay urgent attention to this fast growing area of extensive applications both from the high technology and the defence points of view. Once a stage is reached whereby advanced countries acquire the exclusive control of this know-how, OIC countries will be at the mercy of advanced countries.

Nanotechnology at present is in its early stages of its development and considerable research on nano-science is to be done. At the research stage, some OIC countries already have some basic research tools of nanotechnology. These tools or techniques are basically those of precision materials science and those used in nuclear sciences. Some of these are: electron microscopy, neutron scattering, Mossbauer spectroscopy, ion-beam methods, spectroscopic methods, nuclear magnetic resonance and x-ray diffraction techniques etc. OIC countries that have materials science laboratories are well suited to slide into the area of nanotechnology.

Countries like Turkey, Pakistan, Egypt, Malaysia, Indonesia and Iran could concentrate such efforts through the Islamic Academy of Sciences (IAS).

4.3.2 Ethical and Safety aspects of nanotechnology

The issues of safety and ethics are very essential in nanotechnology. Since nanotechnology deals with handling of nano-size materials, i.e. the sizes are of the order of the sizes of viruses, bacteria etc., then handling of any dangerous materials would need strict safety standards. Not many harmful effects are known of nanomaterials, and thus need precaution in handling. The nano-size materials have greatly enhanced reactivity and a lot is not known about the dangers during handling by human beings [Kleiner and Hogan, 2003].

The matter of ethics is also important because of self-assembly characteristics of bio-nano-materials. The nano-bio-technology based on self-assembly of bio-molecules will deal with products of the creation of life and life processes and will certainly involve great ethical problems.

4.3.3 Potential risks of nanotechnology

Nanotechnology may pose some risk to health as nano-particles may enter pores of the body and may have dangerous effects so far unknown. Viruses are of nano-size and are dangerous, nanotechnology may thus cause unforeseen health hazards.

5 CONCLUSION

It is well known that the properties of materials; physical, thermal, electrical, magnetic or structural, are found to change when conditions like temperature vary. Also the properties of materials have been found to change for the same material when its grain size changes. In recent years, extensive research in physical metallurgy has been done on the dependence of strength of materials on the grain size of alloys and metals. The smaller the grain size, the stronger the material.

Grain sizes could be a fraction of a millimetre to some microns (10^{-6} m). Extending grain sizes to such micro-size (10^{-8} m) particles to still smaller sizes such as nano size (10^{-9} m) or even smaller, we have to deal with a size corresponding to a few atoms (5 atoms or so) such as molecules, or even to single atoms, the size of a single atom being about 10^{-10} m or about one tenth of a nano meter ($1\text{nm}=10^{-9}$ m).

The mechanical, electrical, thermal or magnetic properties change drastically when the particle sizes being studied are in the range of nano-meter (10^{-9} m- 10^{-7} m). The smaller the size, the greater the mechanical strength of fabricated materials, the smaller the size the greater the thermal insulation, the smaller the size the more sensitive the magnetic devices, and the smaller the size the smaller and more sensitive the electrical and electronic devices. Nano-science, has led to exotic applications and handling of nano-size materials in the laboratories which has developed into the current field of "Nanotechnology." Even the handling of nano-sizes, i.e. "atoms and molecular sizes" of materials has taken to the stage and to the building of factories for mass-scale production of consumer goods, be it textiles or magnetic sensors or nano-electronics products. Already trousers of stain-resistant cloth and dust resistant kitchens are on the market, apart from sophisticated high precision lithographic products and electron beam precision machining products. While nano-science has brought nanotechnology in factories, complexity is however one of the main features of nano systems such as, nano-structural alloys and composites, advanced functional polymeric materials, ultrathin films, quantum dots, nano-tubes, nano-crystals etc. On the other, nano-science covers the complex systems, which determine our life such as protein complexes, viruses, colloidal particles in water, and aerosols, and the process of self-assembly of these organic as well as inorganic materials. A review by McKeown [McKeown, 1997] gives an extensive picture of "nanotechnology," while exotic advances are being reported all the time [Zettl, 2003].

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Culture of Science

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1 INTRODUCTION

History has shown the pivotal role of science in overall human development. With the dawn of the new millennium has come the realization that all aspects of our social and cultural life, art, politics, leisure, information and even consciousness itself are being rapidly transformed by different areas of scientific discovery and technological development.

To belong to today's world, survive successfully, benefit fully from the advances of science and technology and contribute to sustainable development, every person must understand the basic principles of science and technology and put them into practice as familiar companions and daily tools in the continuous drive to make life and environment better. Science and technology education has become a universal requirement of modern living.

Globalisation is leading to "technology," a form of totalitarian technocracy that eliminates alternatives, making them invisible and therefore irrelevant, by redefining prevailing concepts about art, family, politics, history and religion, to fit technology's new requirements.

This in turn is continuously threatening cultural diversity and distinctiveness through altering almost every aspect of daily life. The distinction between what is natural and what is artificial, between what is authentic and what is deception, is becoming increasingly blurred. People are becoming so dependent on technology that many lose the ability and knowledge to perform basic physical and mental processes that were routine in the past.

The evolution and developments in science produce knowledge that is translated into products. Unfortunately, science can neither determine the use of nor control of such products or outcomes. Science works on the principle of trying to understand, and in many ways to dominate, nature. It is the result of an intricate interaction between scientific, social and cultural environments, ultimately influencing morals, values and ethics that determine the use (or misuse) of scientific knowledge within societies.

It is true that the recent Western scientific revolution is based on the excellent contribution and achievement of Islamic scientists in various disciplines. However, data have clearly shown that developing countries,

including Islamic countries, have contributed very little to scientific development during the 20th century. The national science systems in Islamic countries need to face the challenge and develop comprehensive national science policies and comprehensive national strategies on scientific research in priority areas.

The strengthening of capacities for scientific research must have support from the leadership backed by an informed and supportive public. Such commitment is necessary to mobilize national support to build career structures, incentives, and funding for creating and sustaining research capacities. A proposed target of 2% of the GNP is considered a necessary minimum investment to develop a nation's science and technology capacities. Of this, at least 10% must be dedicated to investment in health related research and development programmes. Strong national commitment is indispensable to secure resources and to create a positive environment for research capacity building.

2 PRINCIPLES OF A SCIENCE CULTURE

National scientific communities cannot overcome various problems unless an appropriate science culture is developed and promoted. From Islamic perspectives, a science culture particularly in the field of health, should be based on the following principles:

(a) Islamic science culture should be based on the concept of useful science and avoid harmful science

Muslim scientists have the duty to reorient science and technology to clarify the distinction between means and ends, between tools and objectives, between technologies and learning who we really are, and redirect science and technology to achieve their purpose in helping human beings to live in full harmony with the universe. The moral and cultural dimensions of education should receive a new emphasis to enable each person to achieve self-understanding through an inner voyage the milestones for which are knowledge, meditation, and the practice of self-criticism.

The Qur'an is full of references to natural phenomena inviting people to think, seek knowledge, and contemplate in God's creation. The first verse of the Qur'an is an invitation to seek knowledge. Science is a corollary to power, according to verse 40 of *sura* 27, entitled The Ants (*An-naml*):

"قال الذي عنده علم من الكتاب أنا آتيتك به قبل أن يرتد إليك طرفك فلما رآه مستقراً عنده، قال هذا من فضل ربي ليبلوني أأشكر أم أكفر ومن شكر فإنما يشكر لنفسه، ومن كفر فإن ربي غني كريم" . .

Those endowed with knowledge, according to verse 18 of *sura* 3 (*Al Imran*), rank immediately after the angels as witness to the unity of God:

"شهد الله أنه لا إله إلا هو والملائكة وأولو العلم قائماً بالقسط، لا إله إلا هو العزيز الحكيم".

Maurice Bucaille, in his book *The Bible, the Qur'an and Science*, provides striking examples of the total concordance of Qur'anic verses with modern science.

In another verse of the Qur'an, (8:60), believers are urged to be ready to the utmost of their power to deter the enemies and intimidate them in order to prevent transgression:

"وأعدوا لهم ما استطعتم من قوّة ومن رباط الخيل ترهبون به عدو الله وعدوكم وآخرين من دونهم لا تعلمونهم، الله يعلمهم، وما تنفقوا من شيء في سبيل الله يوفّ إليكم، وأنتم لا تظلمون".

Science and technology represent power in the modern world; therefore seeking knowledge is a collective duty (*fard kifaya*) superior to individual duty (*fard ain*) in that the person performing it fulfils the need of the Islamic nation (*umma*). It is to be noted that when no one fulfils this collective duty, the whole community is considered sinful until the duty is fulfilled by a member of the community. This is why it is necessary, among other things, to familiarize children at an early age with science and the uses of science, and with the difficult task of assimilating progress in such a way that human dignity and integrity are fully respected. Here, too, ethical issues must not be overlooked.

The Prophet Muhammad (peace be upon him) encouraged his followers to seek knowledge through education. Indeed, he made it a duty requiring, like all other religious duties, purity of purpose and dedication. In one *hadith*¹, he is quoted as saying: "Seeking knowledge is a binding duty on every Muslim." All scholars agree that the term Muslim includes both men and women. Needless to say that making education a binding duty imposes on every Islamic state an obligation to make education a requirement for all Muslims, boys and girls, men and women.

(b) Science culture should ensure adherence to clear and strong ethical values governing the design, conduct and use of research

The *10/90 Report on Health Research 2000*, published by the Global Forum for Health Research, highlighted the enormous disparities in health worldwide that have been a source of global debate and concern for some time. Misallocation of resources and the resulting inequities have drastically affected the quality of life in the developing world. The disparities between the levels of health across the world in general correlate very closely with socioeconomic development.

While it is important to understand the difficulties confronting those who need to improve public health, and the barriers to sustainable development, it is also important to know that within the constraints, there are choices and options available. The moral burden of these choices weighs especially heavily on those

¹ Related by Ibn Majah following Anas Ibn Malik.

who enjoy a privileged position, because by definition, they have the greatest capacity to induce change. It is important to ensure that principles are applied by individuals and organizations when they make decisions or adopt policies which constitute a framework for articulating the duties, obligations, claims and expectations of those involved in research related to health care. The four main principles in particular are as follows:

- ***The duty to alleviate suffering.*** *Science research, particularly health science research, is fundamentally enshrined by duty to alleviate suffering of fellow beings. A duty that has been acknowledged in moral codes and practices since ancient times. This duty obliges us to do what we can to reduce suffering, first within our communities and then in the rest of the world;*
- ***Respect for people.*** *All individuals are worthy of respect, and are the best guardians of their own interest. Their integrity must never be violated. They must not be misinformed or treated with indifference and they must not be exposed to unnecessary risk;*
- ***Sensitivity to culture differences.*** *Individuals live within particular societies and with cultural values and practices that shape their understanding of themselves and others. Ethical judgements are about being able to do the right thing bearing in mind the local culture; and*
- ***The duty not to exploit the vulnerable.*** *As a matter of principle, the powerful have a duty to refrain from taking advantage of the vulnerability of the weak. Just as it is unacceptable that local political and economic elites should seek their own goals at the expense of the weak, it is unacceptable that researchers should select populations, which are economically or politically weak in order to test therapies more cheaply to benefit other wealthier communities. The wider roles and obligations of all those involved in research, pharmaceuticals, national and international agencies involved in reducing global inequities must be borne in mind. Researchers have a responsibility to enable those who participate in research to benefit wherever possible from this research.*

(c) Science culture should ensure that knowledge generated from scientific research should be accessible and affordable to all

The social values and norms of different cultural environments necessitate the need for developing ethical standards and codes that protect the weak, vulnerable and marginalized to prevent the abuse or misuse of the emerging new genetic knowledge and associated technologies.

According to the World Science Report 1998, science as a public good versus science as a market good are two perceptions of science that are based on different logics: that of disclosure, open knowledge and thus the free circulation of information; and that of intellectual property and knowledge as private property and thus the retention of information.

Science constitutes an important aspect of our cultural domain and has historically played a progressive role in socioeconomic development. In the ongoing process of globalisation, the perception of science as a market good has permeated developing countries, challenging the prevailing mode of science as a public good with long-term consequences for the structure of their scientific research systems. This is indeed a serious problem in developing countries.

(d) Science culture should promote scientific methodology and logical framework as part of basic education and research activities

A broad-based scientific culture, beginning with basic literacy, is an underlying requirement for effective research generation, demand, and use. All students should be provided with:

- *The foundational skills that will facilitate future learning;*
- *Broad experience with the methods and results of the most widely employed approaches to knowledge; and*
- *A sense of how to integrate these approaches to knowledge in ways that cross-traditional disciplinary boundaries.*

There should be at least as much emphasis on how we know what we know as on the facts themselves. Examples of the scientific method at work should be highlighted. How is science done? How can it be distinguished from pseudo-science? The development of hypotheses, design of experiments that critically test them and the need to constantly refine hypotheses should all be taught by example. Students should learn to determine how tightly an investigator's conclusions follow from experimental data. Are there alternative explanations for an experimental finding? Was there a better way to design an experiment so that alternative interpretations could be ruled out? Does an experimental result suggest a general law of nature, or do the conclusions apply only to a specific model system?

(e) Science culture should support the development of the national science system working within a national science policy and contributing to the overall national socioeconomic development

The fundamental aim of the policy for science and technology is to improve the quality of life of citizens and provide opportunities for all citizens for a life of joy and creativity, embracing physical, mental, moral and spiritual well being and values. The world, and more so developing countries, faces a fundamental challenge: harnessing the power of science and technology for equitable access to health. The development of national science systems is therefore crucial to national development. Good health is recognized as the key to human development and economic growth. Its central role in the overall national development agenda is now well acknowledged.

In this respect, reference should be made to the strategy for science and technology development in Islamic countries endorsed by the Eighth Islamic

Summit held in Tehran in 1997. The strategy document provides a comprehensive analysis of the science and technology situation in Islamic countries and provides well-formulated recommendations that encourage Islamic countries to develop national science and technology policies and provide necessary financial and other resources for strategy implementation.

A research policy is essential for guiding action, and any action without necessary tools, intelligence and information, can be ineffective and wasteful. Appropriate research can inform and accelerate the efficiency and effectiveness of action for better health. This is exemplified by changes in lifestyles, diet and activities, which result from better understanding of risk factors for diseases, improvements in health services and disease prevention. Health policies and strategies of those involved in health care can be strengthened through research. Even when appropriate tools are available, operational research is necessary for their application in the diverse real-world settings.

Health research should be an integral component in policy formulation. All countries need to focus on country-specific health problems and frame policies and plans for action on the results of such research. This has been neglected in most developing countries and deserves the highest priority. The demand for research among those responsible for policy formulation can be fostered by good communication between the research groups and the users of research.

In order to draw up policies for the promotion of scientific research, it is necessary to understand it in its totality and to identify important research fields to be promoted on a priority basis. For this purpose, while consideration should be given to varied social demands for scientific research, efforts should be made to understand the trends of research in specific scientific fields, in terms of the current situation, future directions, issues to be tackled, and the areas and subjects which are important for the development of research in the fields concerned. For the health sector, one challenge in setting a research agenda is the trade-off between meeting current health needs and generating future health benefits.

Most developing countries are burdened heavily with diseases and have scarce resources, whether human, capital or financial, and poor governance. It is therefore paramount that countries use these with great care to benefit those who are most in need, and at the same time identify ways to invest more in health research.

(f) National policy system should promote science culture and make available to the national science system necessary resources, incentives, and good working conditions for scientists

Research on health matters in most developing countries suffers serious constraints, including limited opportunities for career advancement and professional development, weak and unstable institutional environments and insufficient and erratic funding. The lack of appreciation of the importance of

research has resulted in low social esteem and poor salary structures for scientists.

In the Eastern Mediterranean Region, which includes many Islamic countries, the overall output in health research is low. A glimpse of published health research shows that almost 90% of the health research information in the Region comes from 12 countries. Although there is additional information available in some local languages, the access to this information is very limited and the quality is not well assured.

Strengthening research capacity in developing countries is one of the most powerful, cost-effective, and sustainable means of advancing science and development. The overall goal of capacity building is to improve the capabilities of individuals and institutions to address socioeconomic issues through research. Capacity building should be undertaken at a national level, adapted to the unique circumstance of each nation. Building capacity for science-based development involves at least the following two components:

- **Individual competence.** *Competence includes not only the skills needed to use particular disciplines, but also a systematic and scientific approach to problem solving; and*
- **Institutional infrastructure that supports research.** *Examples of capacity building include upgrading career structure incentives, scientific information, equipment supplies, research management, training and building operational linkages with other national research units. This capacity must be strengthened in universities, research institutes, relevant departments, and ministries of the government as well as nongovernmental organizations.*

3 CONCLUSION

Science culture worldwide should promote international collaboration, as reflected in the following statement by Professor Abdul Salam, 1979 Nobel laureate in physics.

Science and technology are a shared heritage of all mankind. East and West, South and North have all equally participated in their creation in the past as, we hope, they will in the future - the joint endeavour in science becoming one of the unifying forces among the diverse peoples on the globe.

The health sector both at national and global levels is facing serious challenges. To respond to these challenges, health science culture should be developed to promote equitable health and health care through a sustainable health research system focused on knowledge production and efficient and effective use of available knowledge.

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Science for *Taqwa*

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1 ABSTRACT

Believing in the existence of God is considered as a universal culture. What is lacking seems to be in the dedication to the belief. Science has been suggested as a tool to achieve the highest level of this dedication, i.e. *Taqwa*.

The main theme proposed is not to manipulate the *Qur'an* to fit an experimental finding through philosophical interpretation but to reconsider experimental results to confirm what has been revealed. Reason? Scientists are preachers of the truth and the substance preached therefore must be the truth.

2 INTRODUCTION

In the creation of Heaven and Earth, the alternation between night and day, the ships which plough the sea with something to benefit mankind, and any water God sent down from the sky with which to revive the Earth following its death, and to scatter every kind of animal throughout it, and directing the winds and clouds which are driven along between the sky and Earth, are (all) signs for folks who use their reason. Al-Baqarah, 164.

All of us agree fully with the above Revelations**. However, the problem of our modern generation is not simply believing but finding how to act positively on it as well, i.e. how to heighten our *taqwa* to God because there are so many things that distract us from remembering Him in our everyday life.

Having faith in Him is one thing but having a clear idea about His love for us, His creations and His power is another thing altogether. In other words, scientists are especially concerned with whether our scientific theories, our belief in the nature of things, are in line with what He wants them to be. We cannot afford to have a dichotomy in science and Islam because in a way we as

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** Revelations in the context of the paper means *Wahi...* وحى

scientists are preachers, be it limited to our scientific belief. We teach people, we influence them and we convince them with our belief. Those actions on our part will have a strong effect on the *taqwa* of future generations. If we teach them something, which is not correct, we will be held responsible. The value of our scientific knowledge is determined by how close it brings our disciples to God. Even a mundane fact such as the reaction of hydrogen with oxygen to form water, if taught correctly, can reveal God's intervention and induce them to say "Praise be with Him!"

Scientists use science as a tool in their effort to search for the truth whereas the Revelations in their originality represent the truth. Therefore, it is most appropriate that science be used to rediscover the truth. Theories and discoveries must be confirmed where possible by what has been revealed so that we can further investigate creations in order to reinforce our faith with our rediscoveries. At the same time, we can disseminate the knowledge thus obtained with greater confidence, without any doubt of misleading our followers.

Science in itself is valueless. Its real value lies in its applications. It depends on the *niyya* or *niyyat* (intentions) at the start of our approach to discoveries.

From the fruits of the date palms and grapevines you derive intoxicants as well as fine nourishments ... An-Nahl, 67.

If our motive is right, it is for the sake of God, and then it is the most valuable undertaking that we can do. If it is otherwise, then it is *Shaitan's* (Satan's) way and that makes the knowledge that is gained useless as far as *ibadah* (worship) is concerned.

Science is the study of things and therefore it has limitations. Science cannot explain what has not been explored though the event is observable. Included in this are the miracles bestowed on His prophets. Science cannot explain matters related to the unseen world though some do believe in the sixth sense, occult and others. Science can predict the future only when collected data are available. Even then, science can do this only with approximation and uncertainty. Science can predict with exactness if the events were to follow a certain *Sunnah* of God discovered beforehand. According to Einstein, God does not play with dice in managing His creations.

The most important aspects of science are correct observation and reproducibility of measurements. Of course, we also recognize that reproducibility is the way of God. In their search for the truth, therefore, scientists must be able to repeat the events for others to observe. These two aspects of science enable it to help us preserve our faith. By itself, science cannot establish faith because it does not recognize the Prime Mover. The value of science is, therefore, to help in strengthening the faith that has been established by other means before: that is "*taqwa*."

It is the intention of this paper to highlight the difficulties faced by some of us in interpreting scientific findings such that these findings concur with the Revelations made to Muhammad (peace be upon him (pbuh)). Philosophising

on the meaning of the Revelation to suit present mathematics and physics is not good enough because this may lead to disagreement among Moslems. Worst still, in some respects philosophising Revelations is simply a way to avoid the issues.

Hence, our *taqwa* depends on our ability to face the mystery of Revelations squarely with the facts and figures of science, and not just philosophy.

3 THE CREATION OF THE UNIVERSE

3.1 The *Qur'anic* backdrop

The study of the universe is one of the most interesting and fascinating branches of science. The universe is full of mysteries that have led to the formulation of many theories and investigation protocols. It would certainly be wonderful to know about the universe from the *Qur'an* for, being the truth; such knowledge can guide us as well as complement our findings. There are a number of references made about the universe in the *Qur'an*. Application of such truth to cosmology and astronomy will give the latter added value.

When God refers to Heaven and Earth in the *Qur'an* we are not quite sure what He really means by heaven: is it just limited to the region of space containing the stars that we can see, or the Milky Way galaxy (about 100,000 light years in diameter) or is it even bigger: the whole universe itself? There are seven well-layered heavens (*Al-Talaq*, 12; *Al-Mulk*, 3; *Nuh* 15) but the meaning of each is still beyond our comprehension despite some efforts put by our *ulama* to philosophise about it.

When He mentioned six times in the *Qur'an* (e.g. *Yunus*, 12) that heavens and Earth were created in six days we cannot but believe it to be really six days. How do we interpret this so that our cosmological findings can be upheld? According to the modern cosmology, the age of the universe is in the range of 10 billion years or more with our sun, moon and Earth formed 4.6 billion years from primordial gas and dust clouds. According to this theory then, from zero time to the formation of our solar system it took more than 5.4 billion years for the photons and other nuclear particles to form atomic species and aggregate into matter in order to establish our solid mass, Earth: not six days.

A further complication is posed by the Revelation:

...who created the Earth in two days... And measured out its types of nourishment for it in four seasons. Then he soared up to the heaven while it was still a haze. He determined there should be seven heavens constructed within two days and inspired its own order in each heaven. We have beautified the lowest heaven with lamps and a safeguard. Ha-Mim (Fussilat), 9-12.

To simplify our understanding, some authors use philosophy to explain all these Revelations (e.g. Haeri, 1985). However, such treatment means that no

science can be involved in understanding this fascinating subject and to the men of science, the creation of the universe will forever remain a mystery.

Figure 1 roughly represents the time scale of the evolution and temperature progression of the universe as described in cosmology.

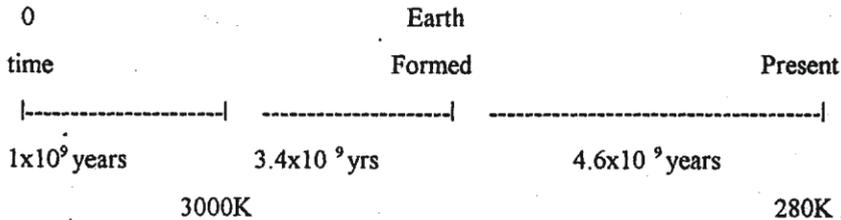


Figure 1. Evolution of the universe.

According to the Big Bang theory, just fractions after the big event took place, the universe was filled with very strongly interacting subatomic particles and radiation whose temperature exceeded 10^{12} K. These particles collided with each other and as time progressed and temperature lowered, heavier and heavier particles were formed. By the time the universe was 1 second old the temperature had already dropped to 10^{10} K. At this point nuclear particles such as protons, neutrons and positrons could exist in stable forms. One minute and 46 seconds later, when the temperature went down to 9×10^8 K, stable atomic nuclei were formed. It was only 7×10^5 years later that the stable atomic particles were formed when the temperature had cooled down to 3000 K. Even though things got easier after that, it was only one billion years later that stars and galaxies were beginning to form and even now, some are believed to be still forming.

*The sky We have built firmly and We are extending it. Az- Zariat,
47.*

If the Big Bang theory were true, then the period of six days and fractions thereof revealed for the creation of heaven and Earth must be according to the then Earth-day and not the present days that we are experiencing. We can try to make some simple calculations to show this by assuming that the angular momentum of the spinning Earth were conserved right from its gaseous state 4.6 billion years ago to the present state. Other characteristics, such as the volume, temperature and rotational velocity, all had changed. This is illustrated in Figure 2.

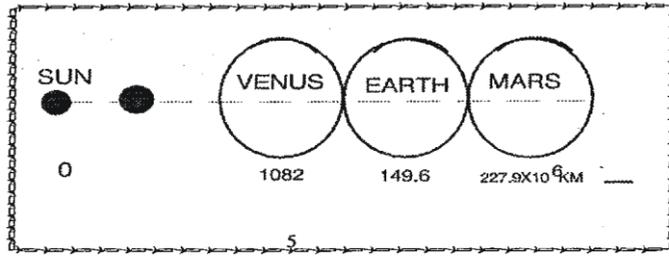


Figure 2. The Earth is born.

We can picture that one billion years after the Big Bang took place, the atomic particles, mostly hydrogen and helium, condensed together to form a big ball, which subsequently formed the sun as a star and the planets around it. Those particles that were not aggregated into the solar system were drawn away by local gravities to form other systems and galaxies. This was perhaps what God meant by "*ayahs*," *Ha-Mim (Fussilat)*, 9-12.

The gaseous Earth had a radius many magnitudes higher than that of present solid Earth. Assuming that its dust cloud occupied the space in between Venus and Mars, we can attempt to calculate the time for each spin of the gaseous Earth in terms of the present 24-hour day.

	VENUS	EARTH	MARS
1. Radius of planets, km	6052	6378	3397
2. Distance between planets, $\times 10^6$ km		41.4	78.3
3. Density g/cm^3	5.3	5.5	3.9
4. Euipartition of radius of the Earth	$\frac{41.4 \times 10^6 \times 5.5}{10.8}$	$\frac{78.3 \times 10^6 \times 5.5}{9.4}$	
	21.1	45.9	
5. Diameter of gaseous Earth at 280K		$67.0 \times 10^6 km.$	
6. Diameter of Earth at 3000K		$73.7 \times 10^6 km.$	
7. Conservation of angular momentum requires that mvr of the Earth in 2002 = its mvr 4 billion years ago.			

$$\frac{m \times 2\pi 6378 \times 6378}{\text{day now}} = \frac{m \times 2\pi 73.7 \times 10^6 \times 73.7 \times 10^6}{\text{day then}}$$

$$\therefore \text{day then} = \left(\frac{73.7}{6378}\right)^2 \times 10^{12} \text{ day - now}$$

$$= 1.16 \times 10^8 \text{ days-now}$$

8. Therefore 6 days required to make the heavens and Earth amounts to about 1 billion days now.

The number thus obtained is too small compared to that proposed by the Big Bang theory but the magnitude obtained from this very simple calculation indicates that it is probably the right approach towards the understanding of *Ha-Mim (Fussilat)*, 9-12.

The seemingly large discrepancy between the calculated rotational period and its corresponding cosmological value may be attributed totally to the inappropriateness of the approach itself. If, on the other hand, the approach were correct, then the discrepancy could have been due to other factors. Some possibilities are:

- (1) The effects arising out of the opposite spin of Venus, which indicates that its primordial gas cloud must have had opposite spin as well. The actual significance of this is not known but could have counter balanced the effect due to Mars;
- (2) The effects of giant impacts by other extraterrestrial bodies such as that which consequently formed the moon;
- (3) The formation of Earth by the aggregation of planetesimal meteor-like bodies and their accretions at later stages. This is very different from what was believed to happen to the giant planets when condensation of primordial gas was the principle stage of planet formation;
- (4) The effects arising out of the estimation of the size of the gas cloud (perhaps the most significant of all). The boundaries of the Earth-gas were taken to be somewhere in between the planets Venus and Mars as if the centre of these planets were situated on a line, Figure 2. In fact, this was not the case. The planets were randomly distributed around the sun in their respective orbits. Some physical parameters are given in Figure 3; and
- (5) The effect of the mass of the Earth, which was heavier then due to the presence of light gases, such as Hydrogen and Helium which have since escaped from the Earth's gravitational pull to outer space.

The results obtained for other planets calculated using a similar procedure are given in Table 1. Though none of them gives the expected result to unify *Ha-Mim (Fussilat)* 9-12 to cosmology, the general agreement within these values lends good support to the present technique of interpreting *Ha-Mim*

(*Fussilat*) 9-12. More importantly, however, the results seem to indicate that it is indeed true that the planets were formed roughly about the same time.

Table 1. Rotational speed of planets (in units of 10^9 Earth-day) at 1 billion years after the Big Bang

Planets	Period of rotation (x 10^9 Earth-days)
Venus	30.4
Earth	0.116
Mars	0.768
Jupiter	0.184
Saturn	0.0598
Uranus	3.31
Neptune	21.6

Despite the hazy relationship just described, the general concept of the Big Bang seems to be valid and useful for Moslems believing that:

... Heaven and Earth were once one solid mass which We ripped apart. Al-Anbia', 30; and ...Nor how the sky has been lifted up. Al-Ghashiyah, 18; and

Then He soared up to up the Heaven while it was still a haze. Ha-Mim (Fussilat), 11.

As the world is round, the separation of the heavens from the Earth seemed to occur in all directions just as what has been proposed by the theory of expansion of the universe. By the time He (God) finished forming the Earth, heavens were still hazy, implying that the condensation of matters and nucleosynthesis in other stars and galaxies were still not complete. Until today, the scientists still observe these happening. In fact, if nucleosynthesis were complete the night-sky would be very dark, indeed starless.

Thus, it is clear that there is a lot more to be done by Moslem cosmologists in particular to have a better grasp at the meaning of those *ayahs* mentioned. One cannot imagine the degree of benefit given to such a work because it can push our *taqwa* to a greater height through their findings.

3.2 The sky

Present day cosmologists believe that the universe is still expanding. The rate of expansion is proportional to the distance of the object from the centre of the universe. It is not known what lies beyond the edge of the universe (or if there is any edge?), but certainly according to this theory, there is no such thing as the sky. Maybe not, but Moslems believe that there is such a limit beyond which no creation can surpass except the prophet Muhammad (pbuh). This limit is "*Sidratul Muntaha*." Even Jibril (peace be upon him) could not rise higher than this point.

God said;

*Nor how the sky has been lifted up. Al-Ghasiyah, 18;
We have placed the sky as a roof which is held up.... Al-Anbia', 32, as if
He meant that the sky is a physical reality. His further addition;
When the sky will split open. Al-Insyiqaaq, 1, indicates that sky is a real
thing.*

Scientists have sent spaceships beyond the edge of our solar system but these did not seem to bump into any sky. This should not be surprising because the nearest sky is indeed very far away, where stars are placed:

We have beautified the worldly sky with the splendour of stars. As-Saffat, 6.

Other than the planets, the bodies that we can see in the night sky are light years away: The nearest galaxy in our cluster, Andromeda, is over 2000 light years away. The nearest sky is well protected from *Shaitans* and the unbelievers amongst the *Jinns*, and it is far beyond the reach of humans. A new complication has recently been thrown in by the suggestion that the Earth today is spinning at a lower rate than yesterday so that in the very near future, we have to add a leap second to our calendar. While this does not have much effect on our faith, the following ayah tops them all:

He organizes the matter from heaven to Earth, then it will soar back up to Him on a day whose measure is a thousand years according to the way you count. As- Sajadah, 5.

This really means that God used a different solar system as His reference point for telling the time. This may indicate that there are other solar systems in the universe, which could perhaps support life.

3.3 Meteorites

We have placed constellations in the sky and embellished it for on-lookers. We have safeguarded them against every outcast Shaitan, except for such as may try to eavesdrop, so a blazing "meteor" follows him. Al-Hijr, 16-18.

We have beautified the worldly sky with the splendour of stars plus a safeguard against every stubborn devil so they may not listen to the supreme council and are hurled forth on every side. Driven away, they will have lingering torment except for someone who tries to eavesdrop so that a blazing "meteor" follows him. As-Saffat, 6-10.

There are two protective elements for the sky against *Shaitan*: the safeguard and blazing "meteor." If the blazing "meteor" is really the meteors that we know, then the safeguard could be an asteroid.

Meteors shower the Earth in hundreds every year. Meteors as we know them are heavenly bodies that revolve around the sun in elliptical orbits inclined at

certain angles to the Earth's orbit. In the path of their revolution, should they encounter the Earth's atmosphere and get captured by the Earth's gravity, they will burn giving a trail of light due to the evaporation of their volatile matter. That will happen at a distance of less than 200 km above the Earth's surface when they meet the Earth's atmosphere in their journey. Could the nearest sky be there? Impossible.

Could the blazing "meteor" then be a comet? A comet is now also considered as an interplanetary reject that belongs to our solar system. A comet can be seen at a greater distance than a meteor because its blazing tail is the result of an interaction between the solar wind with vaporizing matter from its body, as it gets nearer on its approach to the sun. This vaporizing matter can be water-ice, carbon dioxide, carbon monoxide, ammonia or methane. Comets have their own individual orbits and therefore may approach the Earth from any direction and periodically, even after several tens of years. Thus, a comet is also an unlikely candidate for the blazing "meteor." Hence blazing "meteors" must be something else such as exploding stars or supernovas.

There is another form of loose bodies in the sky. They are called the asteroids. Asteroids lie between the orbits of Mars and Jupiter. They are the remnants of primordial gas clouds, which failed to form a solid planet. They can collide with each other. They are hardly visible to the naked eyes as meteors are. Even then, perhaps they are also too close to be considered as at the edge of the nearest sky. Therefore, the interpretation for them to be the blazing meteor is questionable.

Could this asteroid belt be the safeguard of heaven then? Might be. Its hindering nature may be interpreted as the great challenge in travelling through it. Voyager II did it but that must have been with permission:

... if you can manage to penetrate beyond the realms of Heaven and Earth, then pass beyond them! Yet you will only penetrate them through with some authority. Ar-Rahman, 33.

Encountering such objects in the sky can be devastating. Haley's Comet that periodically appears in the Earth's atmosphere measures about 12 km by 8 km and travels at about 75km/s. An encounter with such a comet should be avoided because anything ejected out from it, even a grain of dust, could pierce an object like a bullet. Even at a distance of 8000 km away such an impact was found to be considerable, being able to destroy VEGA 1 and VEGA 2 solar cells and measuring instruments aboard them. Perhaps this is how the worldly heaven is protected from intruders.

Hence, similar to the case of creation of heaven and Earth in 6 days, which was associated with the origin of universe, the full interpretation of the blazing "meteor" for the protection of the sky is still not quite fully satisfactory. It is best to leave it to our scientists to find out more.

3.4 Creation of the Earth

He has placed headlands towering above it and blessed [whatever is] on it, and measured out its types of nourishment for it in four seasons, equally [within reach] for those who ask for it. Fussilat, 10.

When the solar nebula cooled down, it began to spin and was compressed into disc-shape. The planets started forming around the sun randomly. The sun itself by its own sheer weight started to kindle thermonuclear reactions producing radiation to warm the cooling planets around it. Those planet closest to the sun were rich in metal, followed by those with rocky materials and lastly by those that are mostly composed of ice and solidified gas such as methane and ammonia. Such differentiation was mainly due to their temperatures that in turn depended on their distance from the sun.

The age of the oldest rocks on the Earth has been found to be about 3.8×10^9 years, that of the moon about 4.2×10^9 years, and meteorites 4.5×10^9 years. All three bodies are thought to have been formed at about the same time from the same primordial gas cloud. As this gas cooled down, chemical reaction occurred, producing metal oxide, nickel-iron alloy, silicates, iron oxide and silicate, sulphides, hydrated minerals and water. These chemicals first formed droplets and grains that grew bigger by coalitions into planetesimal size bodies.

It is not difficult to picture that as the liquid Earth cooled down, its crust was first formed. The density of the Earth's crust is lower than its liquid core and therefore the crust floats and moves around; continental drift. This is a direct consequence of upswelling of the liquid mantle that pushes the plates apart at the rift zones. Some parts of the crust slide against another, some dive beneath the other and some collide frontally with the other to form mountain folds. Apparently, the extent of rock material beneath the mountains runs deep into the core of the Earth and acts as an anchor to the crust and stabilizes it.

Have We not made the Earth as a wide expanse, and the mountains as pegs. Al-Naba', 6-7.

A detailed discussion on the subject has been published (El Naggar, 1991).

3.5 The importance of water

Life as we know it cannot survive without water because water is required for the transport of nutrients to the vital organs both in plants and animals. Water is also important for the transportation of toxic by-products resulting from biochemical reaction in living tissues for disposal. Water has been mentioned many times in the *Qur'an*.

It is not known how water came to the Earth. It is believed that water-ice chunks of extraterrestrial origin were acquired through the process of accretion. Water accumulated over millions of year on Earth to form rivers and seas. In these bodies of water, all the necessary ingredients to support organic growth and life were present. The initial organic molecules that were to form primitive

life later on were believed to have been formed at the stage of primordial gas cloud. They came with rain and meteorite showers and dissolved in seawater. Hence, as soon as the first strand of DNA was formed duplication went wild. The aggregation of DNA led to the formation of the first primitive living organism. Subsequent to that, life forms that are more complex evolved and flourished. It was only much later that some of these water creatures ventured into land and evolved along many different lines ending up with the most advanced species, man.

Well before this theory was proposed, God already indicated that life begins in water:... *We have made every living thing out of water. Al-Anbia, 30; An-Nur, 45.*

Hence, water plays a more important role than a media of transportation for food and nutrients. It was where life originated. As water itself is important to life, it must have certain properties and characteristics that enable it to play the role effectively. The most well known properties are its density, including ice, at various temperatures. Water has its maximum density at 4°C.

In a tropical sea or lake, the warmer water underneath the surface floats to the top and is cooled by evaporation. The cooled water then swirls down pushing the hot layer to float. The cycle goes on indefinitely to ensure a conducive environment for life to flourish.

In cold climates, the reverse is true. When the surface temperature of the lake is at 4°C, the cooler water is pushed to the surface. Hence, on a freezing night the top layer of water will turn into ice leaving the deep water relatively warmer for the aquatic life to survive. The ice formed will float at the top, as its density is lower than that of water. This is His way of creation so that He does not have to create fish all the time after every winter to replenish the stocks. Not that it is a difficult job for Him (Ar Rum, 27). The density of water as a function of temperature is given in Figure 3 (CRC Handbook, 1971).

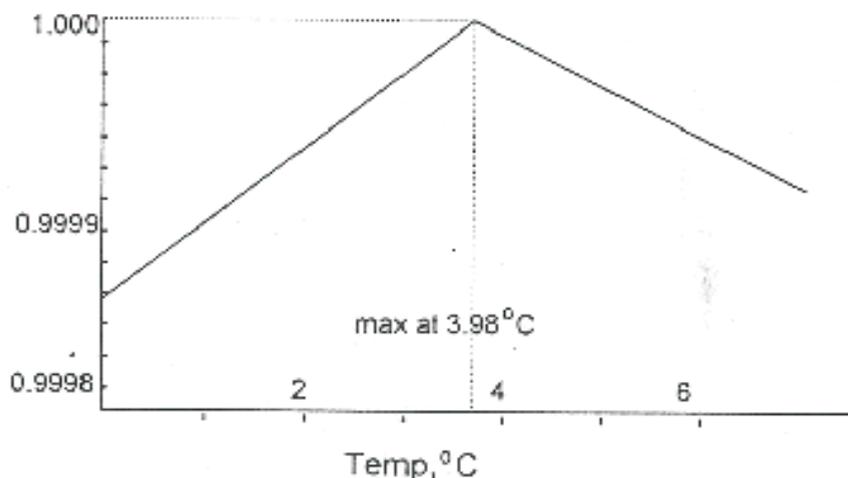


Figure 3. Variation of density of water with temperature.

Of course, there are many other verses cited in the *Qur'an* pertaining to water and well understood by all. The few examples mentioned here are for confidence building amongst us physical scientists in that our pursuance of science is not an exercise in futility. However, again, it depends on our *niyyat* (intentions).

4 WAS IT EVOLUTION?

Regardless of how the Earth was formed, the turmoil and harsh weather it had to go through, when Adam (peace be upon him) and Eve were sent to Earth, it was already made habitable. Through various chemical and biochemical reactions, the reducing atmosphere has been turned to be an oxidative one that suited Adam's physiological requirement.

According to the theory of evolution, human beings including Adam (pbuh) are descendants of ape-like creatures that appeared on Earth at about 2 million years ago. If direct intervention by God is excluded in the development of man then Adam could not have been very smart. On the contrary, Moslems believe that he was because he was a prophet. He had already been guided and taught about things in Jinnah (*Al-Baqarah*, 31). As a messenger, he prayed and preached, but it was limited to his children only.

A more fundamental difference between science and Islam lies in the creation of Adam himself and subsequently Eve. Adam was physically created in the Jinnah (*Al-Anfal*, 12; *Sad* 71-78) and it is clear that Jinnah was not on Earth (*At-Takwir*, 13). Therefore, it is quite wrong to say that Adam was descendant of an ape-like creature and developed through evolution.

Paleontologists also failed to indicate the age of their "Adam." They only suggested that man-like ape did exist at around 2 million years ago. The missing link between these creatures, and "Adam" has not been found yet. If the above literal translation of the events were correct, then the search for the missing link will definitely end up in a failure. That is how *Qur'an* can guide scientists.

One further point that can be understood from the *Qur'an* with regard to this subject is the creation of Eve (*Al-A'raf*, 189). Paleontologists had not indicated anything about this because presumably the female counterpart of their "Adam" was of similar origin and has reached a similar evolutionary status. The *Qur'an*, however, tells us that Eve was created after Adam and became his companion in the Jinnah (*Al-A'raf*, 189).

From Adam (pbuh) to Muhammad (pbuh), twenty-five Messengers were mentioned in the *Qur'an* but their life spans were not known except for Noah, 950 years (*Al-Ankabut*, 14), and Muhammad (pbuh), 63 years. Some of these Messengers were contemporaries, such as Moses and Aaron, Abraham and Lut. Christ was born in the days of Zacchariah. Therefore, it is reasonable to estimate that man as the descendant of Adam has only been on Earth for over 25,000 years and not in terms of millions or even hundreds of thousands of years, as a paleontologist may believe. The Moslem scientist should discover

the correctness of this fact so that it can help us to sharpen our faith and put the theory of evolution in its proper perspective.

Even before Adam was created, God and His angels knew that men would spoil the Earth (*Al Baqarah*, 30). We have been reminded not to do this (*Al A'araf*, 56; *As Shu'ara*, 83). We are told that we will suffer through our own recklessness (*Ar-Rum*, 41) and indeed, we are suffering now not only from pollution of water, land and air but also the global increase in temperature due to the greenhouse effect, (Hileman, 1995).

Something even worse is yet to come; the depletion of ozone layer and the subsequent penetration of strong UV-light to the surface of the Earth. We have been warned that we can be wiped out from the surface of the Earth through our own action either physically or spiritually:

Have they not travelled around the world and seen what the outcome was for those who preceded them? ...” Muhammad, 10. “Pollution has appeared on land and at sea because of what man’s hand has accomplished, so He may let them taste something of what they have earned.... Ar-Rum, 41.

Despite of our humble beginnings, we were created to be the best of all creations:

We have created man with the finest stature. At-Tin, 4.

God made us even better:

...and shaped you and even improved on your shapes.... At-Taghabun, 3.

Due to improved diets, men are believed to be healthier and bigger today than those in the dark and middle ages. However, there are indications in the *Qur'an* that older man were stronger.

They had confidently built houses out of the mountains. Al-Hijr, 82.

They were even stronger than they are. Ar-Rum, 9.

... and make you grow so very tall.... Al-Aaraf 69.

What could the reasons for this be?

All creations are perfectly created (*Al-Mulk*, 3) but man is specially favoured (*Bani Israel (Al- 'Isra')*, 70) over others. However all these creations celebrate God (e.g. *Al-Hasyr*, 1).

“... Nothing exists unless it hymns His praise.... “Bani Israel (Al- 'Isra'), 44.

Plants worship God (*Ar-Rahman*, 6) and birds glorify God (*An-Nur*, 41). Prophet Sulaiman (pbuh) understood the language of birds and ants (*An-Naml*) to the extent that he could talk to these animals. Maybe the abilities of Sulaiman (pbuh) were a part of the miracles bestowed upon him, but the other revelations

clearly indicate to us that all creations have their own languages and modes of communication (*Al-An'am*, 38).

If we were to know what their prayers are, it would be really wonderful because we will be constantly reminded of God's presence wherever we go. This will increase our *taqwa*. Hence, instead of trying to understand what the dolphins and whales talk about, perhaps if we should try to understand what they are saying about God, maybe our effort in trying to understand their languages will bear fruit faster.

5 FOOD

Food is important for humans to sustain life. God has specifically mentioned in the *Qur'an* that we should eat any wholesome food provided (*Al-Imran*, 4; *Al-Baqarah*, 168). There are only a few kinds of food that are not allowed because they bring more harm than good to human beings by the nature of their filth, dirtiness, and toxicity or simply killed for "*shirk*" purposes.

Pigs are filthy (*Al-An'am*, 145). It has been well documented through intensive scientific research that pork can contain many kinds of germs and worms that can sustain their lives in the human body. Even if these were to be cleaned, pork is still forbidden because pigs are a type of wild beast. A detailed account of this subject has been given by Ma, Hj. Ibrahim T. Y. (1991).

A more subtle danger that may come from eating pork is the escalation of tumour and cancer development in human body. Lard promotes tumour growth due to the presence of linoleic acid in a larger quantity than that found in beef. Furthermore, the position of the linoleic acid in the triglycerides of lard is different from that of tallow. This is believed to be a more serious factor in its cancer promoting properties, for it is more prone to lipid peroxidation due to single oxygen intake or production in the body. Table 3 shows the composition of lard, tallow and palm oil. Despite the similar composition of linoleic acid in lard and palm oil, palm oil is a non-promoter of tumours because of the presence of antioxidants mainly the carotenoids and vitamin E.

Liquor, including wine, also brings more harm than good to human body. All liquors contain ethanol which can react with biochemical components in vital organs. The cells die out. Worse is methanol that can cause almost instant blindness.

Ethanol as an intoxicant is very well known. It should be avoided.

...liquor and gambling, idols and raffles, are only the filthy work of Satan.... Al Ma'idah, 90.

In a limited quantity, ethanol can be a mild depressant by slowing down both physical and mental activities. However, consumption of 500 ml of pure ethanol at a single time can bring sudden death (Hill, 1988). Excessive consumption over a period can cause cirrhosis of the liver. This is further enhanced by

consumption of excessive linoleic acid- rich oils and fats (Nanji, 1985), e.g. lard and corn oil, without an accompanying intake of antioxidants.

Promotion of wine, if taken moderately, as health food apparently arises out of its vitamin E content. Regardless of this beneficial effect, we have been cautioned:

... In each of them there lies serious vice as well as some benefits for mankind. Yet their vice is greater than their usefulness. Al Baqarah, 219.

A recent controversial issue in Malaysia was the banning of cigarette smoking among Moslems. Nothing is mentioned specifically about smoking in the *Qur'an* but due to its health hazard, our "*ulama*" feel that some definite actions must be taken. Cigarettes contain well over 4000 chemicals, including threat posing formaldehyde, benzene, cyanide, phenol and arsenic. Tobacco smoke is a ubiquitous personal and environmental pollutant. The constituents that pose great health hazards are:

- (i) Nicotine: imparts many complex effects on cardiovascular, metabolic and coagulatory processes. Its lethal dose is only 50 mg. It can be addictive.
- (ii) Carbon monoxide: effects oxygen transport and utilization. It is a much stronger ligand compared to an oxygen molecule and hence can desorb the latter from the haemoglobin.
- (iii) PAH: tumours promoters and accelerators especially in oral cavity. Tobacco and alcohol can promote tumours synergistically.
- (iv) Smoke particles: pulmonary irritants and allergies as manifested by asthma.
- (v) Tar: covers the alveoli surfaces in the lung, causing slowed oxygen diffusion in the blood.

It is perplexing though why tallow from the belly of ruminants was a forbidden food to the Jews (*Al-An'am, 146*). Tallow is very much like palm oil in the triglyceride composition. They differ in the contents of minor components. In tallow, there is quite a bit more of cholesterol present which when oxidized can be deposited in the blood vessels. In palm oil, on the other hand, there is quite a bit of vitamin E which can help the human body fight heart disease, carotene, sterol and a host of other chemicals which can act as antioxidants.

Lauric and Myristic acids, the main components of coconut oil are considered as harmful to human body as well, especially those with high cholesterol concentration in their blood. However, there are populations that show no ill effect at all through consumption of coconut oil all throughout their lives. Breast milk contains medium chain triglycerides. These triglycerides can be absorbed by infants intestinal walls for nourishment and that is why mothers are encouraged to breastfeed their babies (*At Baqarah, 233*). It is for these reasons that baby's formulae should be as close to breast milk as possible.

6 THE FIFTH DIMENSION

Many of us believe in ghosts, sixth sense, premonitions and so on. These are not part of mainstream science despite some efforts that have been made to communicate with the people of the past, ghosts, and to explain the sixth sense and premonitions. Of course, the soul is something that we are told not to discuss because it is beyond our comprehension. The scientists who carry out studies of sleep, dreams and the subconscious mind, should realize that in Islam the soul of a sleeping man is with God.

God needs souls at the time of their death, and those who have not died, during their sleep.... Az-Zumar, 42.

In fact, if one is close enough to God, one is able to interpret dreams (*Yusof, 46-49*).

More pertinent to us Moslems are the Shaitans and Jinns who were created from smokeless fire (*Al-Hijr, 27, Ar-Rahman, 15*). Some of the Jinns listened to the recital of *Qur'an* (*Al-Jinn, 1*) and understood it (*Al-Ahqaf, 29-32*). Consequently, Jinn can be either Moslem or non-Moslem just like a human. These two creations interact with humans. Shaitans, for example, are the cause of our forgetfulness (*Yusof, 42, Al-Kahf, 62*) and therefore deserve more of our attention.

7 THE QIYAMAH (DOOMSDAY)

7.1 The event

Just as we do not exactly know when the Earth was formed, neither do we know when it will end. According to the *Qur'an*, it is a certainty, and according to science, the probability that it will end is high. In fact, the end may come at an earlier date than we think. We have been reminded, however, not to discuss it (*Al-Ma'idah, 101*) and when the date will be (*Al-Mulk, 25-26*). It will happen all of a sudden (*Yusof, 105-107, Al-Anbia, 40*) and it will give the feeling to those who will be present that day that they have been living in this world for only a short while (*An-Nazi'at, 46*).

The signs for the impending event will be clearly seen, however. Things will seem heavy in the sky and on Earth (*Al-A'raf, 187*) perhaps because the sky will be filled with smoke (*Ad-Dukhan, 10*) and thus blacken out the moon (*Al-Qiamah, 8*). Except for the coming together of the moon and the sun (eclipse?) (*Al-Qiamah, 9*) those signs remind us of the effects of pollution or nuclear winter or even something worse.

On the day itself, the first thing that will be noticed is the sounding of the trumpet (*Al-Haqqah, 13-17*). With that, Earth will be jolted and the mountains will crumble into dust (*Al-Waqi'ah, 4-6*). The surface of the Earth will be flattened (*Al-Fajr, 21; Ta-Ha, 105-107*) with gushes of lava (*Al-Inshqaq, 1-5*) and big waves ploughing the seas (*At-Takwir, 6*). All these seem very much like

the events occurring during a severe Earthquake. In fact, there will be two big rumbles (*An-Nazi'at*, 6-7) at the starting of the chain reactions that follow.

In the sky, the stars will move and get shifted very quickly (*An-Nazi'at*, 1-3) and fade away (*Al-Mursalat*, 8-9) probably due to the same smoky atmosphere affecting the moon. The sky will also split open (*Al-Infitar*, 1). These special events cannot be due to an Earthquake on Earth. It could be due to something greater, such as a universal failure of gravity.

At this point two great meteoritic impacts on Earth should be recalled. The more recent one took place about 65 million years ago, the KIT event. The impact was believed to cause the end of the dinosaur age on Earth. The meteor has been estimated to measure about 10 km in diameter with a mass of more than a trillion tones. The energy released was equivalent to 5 billion of the atom bomb dropped on Hiroshima, lifting about 100 trillion tons of dust into space causing cold and darkness to envelope the world by blocking sunlight from reaching the Earth's surface. No seismic activities were described and thus it is difficult to correlate its similarities to the events of the Doomsday.

A more devastating impact took place just about the time when the Earth was formed. It was the giant impact that entailed the formation of the moon. It is believed that a large extraterrestrial body, about the size of Mars, hit the Earth with such great force that it rocked the Earth to its very core. Molten mantle was spewed out by the Earth's interior into space together with parts of the foreign body to form the moon. If these events truly happened, history can repeat itself in the future causing the end of the world. At the same time, as a result of such an encounter, the rotation axis of the world could be tilted at an unspecified angle in the same manner as is believed to have happened to Uranus and Pluto. The sudden change in its axis will be a good reason for observing a sudden shift in star formation (*An-Nazi'at*, 1-3).

On that day, sinners will suffer the most with torments coming both from above and below (*Al-Ankabut*, 55). They will behave like drunks (*Al-Hajj*, 2). The pictures just described, invoke the feeling that on the promised day, disturbances will occur everywhere in the sky and on Earth in unison. However, science has yet to explain the final events: *Hell looms for all to see...* (*An-Nazi'at*, 36), *...the Earth and the sky will be replaced with new ones...* (*Ibrahim*, 48) and *...a Garden broader than the sky and the Earth...* (*Al Hadid*, 25). Perhaps science will never be able to explain these because these happenings belong to dimensions beyond us.

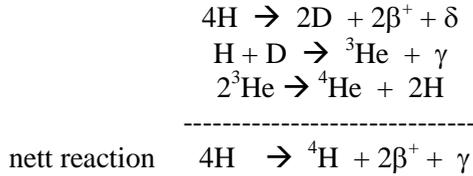
7.2 Sun as an indicator of Doomsday

The main gravitational interactions of the Earth are with the sun and the moon. The former controlling its orbital motion and hence the seasonal variations that we observe. If the events on the promised day were due to universal gravitational failure, perhaps we can look at the sun as the provider of the initial reaction.

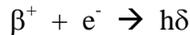
The sun is a star weighing about 2×10^{30} kg situated at 1 Au (1.496×10^8 km) away from the Earth. It provides energy to the entire solar system that it derives

from thermonuclear reactions deep in its interior where temperatures exceed 14×10^6 K. About 75% of matter making up the sun is proton and 23% helium nuclei. The rest are the heavier elements.

One of the several thermonuclear chain reactions that have been suggested to take place in the sun is as follows:



The positrons will react with electrons to produce energy via:



In this chain reaction, the final product ${}^4\text{He}$ is lighter than 4H , where it is derived from. The differential weight loss is termed as mass defect, Δm . For the reactions above:

$$\begin{array}{l}
 \text{the weight of the starting material } 4\text{H, is} \\
 4 \times 1.00728 \text{ amu} = 4.02912 \text{ amu} \\
 \text{the weight of the product, } {}^4\text{He,} = 4.00260 \text{ amu} \\
 \therefore \Delta m = 0.02652 \text{ amu}
 \end{array}$$

Δm appears as energy, which can be calculated by applying the Einstein equation

$$\begin{array}{l}
 E = mc^2 \\
 \therefore \text{energy released from 1 g H} = 0.006582\text{g} \\
 = 5.924 \times 10^{18} \text{ ergs} \\
 \therefore \text{total energy available in the sun is} \\
 75/100 \times 110^{33} \times 5.924 \times 10^{18} = 8.886 \times 10^{51} \text{ ergs.}
 \end{array}$$

The amount of the sun's energy received at the surface of the Earth, solar constant is 1.37×166 ergs per every sq. cm per second. This 1 cm^2 of area is a part of the total surface of a sphere that can receive the sunlight (Figure 4). The radius of this sphere is 1 Au (Earth-sun distance) and therefore its total surface area, $4\pi^2$, is $28.13 \times 10^{26} \text{ cm}^2$.

$$\begin{array}{l}
 = 8.886 \times 10^{51} / 38.26 \times 10^{32} \text{ sec.} \\
 = 7.36 \times 10^{19} \text{ years.} \\
 \therefore \text{sun's total radiation} = 38.26 \times 10^{32} \text{ ergs/s} \\
 \therefore \text{the time that the sun will last} = \text{total energy/energy out/s} \\
 = 8.886 \times 10^{51} / 38.26 \times 10^{32} \text{ sec} \\
 = 7.36 \times 10^{19} \text{ years}
 \end{array}$$

This is almost 100 billion years.

Many of us will be happy to know the result of this calculation. However, this is a question that poses a great challenge because we have been informed by Muhammad (pbuh) that:

In reality, the time lapse for you and the last day, in comparison to the prayer times for nations before you, is like Asr to sunset.

7.3 What makes us turn away?

Several passages of the *Qur'an* that involve technology development have been mentioned. There are still others that we can investigate further and perhaps in doing so not only will we receive proper guidance in our scientific research but we may also discover a technology that is useful for mankind.

One long-standing fact among these is the nutritional and therapeutic value of honey (*An-Nahl*). Instead of looking seriously into this we have passed it as a folk cure. We encounter passages on glass technology (*An-Naml*, 44), transparent silver (*Al-Insan*, 16), where God is (*Al-Ma'arij*, 4) and so on. Unfortunately, we have yet to follow his guidance to pursue them further in seeking the truth. Why? Simply because we are so concerned about our own material gains (Rahman, 1981), and... *Competition has distracted you until you visit graveyards. At-Takathur*, 1.

There is a host of other scientific based *Sunnah* (teachings, actions and sayings of the prophet peace be upon him), that are still left to be explained and not touched upon in this communication. These *Sunnah* involve human character and physiology directly and therefore need a lot of science-based investigation to reveal their true meaning. Furthermore, the signs of Allah's greatness and sovereignty can be discovered in each experience, phenomenon and experimentation (Hussaini, 1989) that can help us to raise our *taqwa*. It is worth noting that;

Those truly fear God, among his servants, who have knowledge. Fatir, 28.

They reflect, think and understand the parables of the *Qur'an* and His manifestation all around them and draw right and beneficial conclusion from them as the whole material structure is full of His signs (Rahman, 1981).

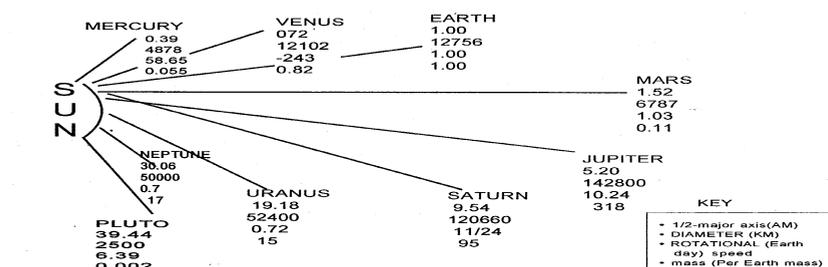


Figure 4. The planetary system.

Table 3a. Fatty Acid composition of Palm Oil, Palm Kernel Oil and Coconut Oil (% of Total Fatty Acids)

Fatty Acid	RBD Palm Oil ^a	Palm Kernel Oil ^b	Coconut Oil ^c
6:0	-	0.3	0.2
8:0	-	4.4	7.9
10:0	-	3.7	7.2
12:0	0.2	48.3	48.0
14:0	1.1	15.6	17.5
16:0	44.0	7.8	9.0
18:0	4.5	2.0	2.1
18:1	39.2	15.1	5.7
18:2	10.1	2.7	2.4
Others	0.9	0.2	Tr

tr indicates trace amounts

Source: a. PORIM Technology No. 3(1981); b. PORIM Technology No. 6(1981); c. *The Lipid Handbook (1986) – ed. F. D. Gunstone.*

Table 3b: Fatty Acid composition of some common edible oils and fats (% of total Fatty Acids)

	Saturated	Monounsaturated	Poly-unsaturated
Coconut ¹	94	4.5	1.4
Palm kernel ⁴	88	10	1.5
Butter ¹	66	30	4
Beef tallow ¹	52	44	4
Lard tallow ¹	41	47	12
Palm oil ²	50	39	10
Palm olein ³	46	43	11
Cotton seed olein ¹	30	19	51
Peanut ¹	19	39	41
Olive ¹	13	79	8
Corn ¹	16	30	53
Soyabean ¹	14	25	60

Source: 1. *The Lipid Handbook (1986) – ed. F. D. Gunstone*; 2. PORIM Technology No. 3 (1981); 3. PORIM Technology No. 4 (1981); 4 PORIM Technology No. 6 (1981).

Table 3c: Cholesterol content of edible oils and fats

OIL	Range (ppm)	Average (ppm)
Coconut ¹	5-24	14
Cocoa butter ²	n.a.	59
Palm kernel oil ¹	9-40	17
Palm ¹	13-19	16
Sunflower ¹	8-44	17
Soyabean ¹	20-35	28
Cottonseed ¹	28-108	44
Rapseed ¹	25 – 80	53
Maize ¹	18 – 95	50
Lard ²	3000 – 4000	3500
Butter ²	2200 – 4100	3150
Beef fat ²	800 – 1400	1100

Source: 1. *M J Downes (1982, 1983, 1985)*; 2. *The Lipid Handbook (1986) – ed. F.D. Gunstone.*

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Nurturing a Culture of Science

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1 SUMMARY

The gap between the science culture that exists in the Muslim world and that in the developed world may increase substantially in the future unless steps are taken to promote an awareness of the benefits of science together with drastic improvements in the teaching of science in an integrated curriculum.

A recent report detailing the situation in the Arab world cites the lack of translations of scientific works, impediments to education and creative opportunities for women, a culture in which scientific inquiry is considered harmful to religious development, and lack of intellectual freedom; as the major causes for the lack of scientific advancement.

This is a sad state of affairs for the Islamic world - a world with the richest pre-renaissance scientific culture in the history of human progress. There was a time when we led the world in scientific inquiry and development in a culture that valued the scientific method involving reasoning and experimentation. It was a culture in which learned men and women pursued scientific learning with the belief that they were in fact following the divine directive from the Holy *Qur'an* and the guidance of the prophet (peace be upon him) by studying and trying to understand creation and utilizing this knowledge for the benefit of humankind.

How will we re-energize the spirit of scientific progress and nurture a culture that values science? This paper makes some suggestions.

First is re-establishing our connection to our glorious past by teaching in detail at the school level the accomplishments of the great scholars of the golden age. This curriculum should focus on the following:

- (1) That pursuing science is not only not opposed to the religion but it is actually an act of *Ibadah* (worship) (when done with the proper intention of

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increasing faith and bringing benefit to humanity), as it is encouraged by the teachings of the Holy *Qur'an* and the guidance of the prophet Muhammad (pbuh);

- (2) That scientific endeavour was carried out as part of an integrated scholarly career in which the scholars studied in depth the Holy *Qur'an*, the *hadith* (prophetic guidance), the *shari'ah* (Islamic law) in addition to mathematics, physics, chemistry, biology, medicine, astronomy and other disciplines and made significant contributions to multiple disciplines; and
- (3) That today's budding scholars are encouraged to develop scientific inquiry within the bounds of what is permissible and encouraged in the *shari'ah*.

There needs to be a mechanism to determine the permissibility of scientific innovations in Islamic society. Some major benefits of scientific advancement are being better equipped to counter the media bias against Muslims.

The progress made in some Muslim countries in the area of science and technology is also discussed. Malaysia is chosen as a model for other Muslim countries to emulate.

Finally, we conclude with some recommendations to aid in strengthening the science culture in Muslim nations.

2 INTRODUCTION

The new millennium has caught the world with outstanding scientific breakthroughs such as the unravelling of base sequences of the human and rice genomes. Innovative technological tools and new appliances in the field of informatics have made these landmark advancements possible. Unless these incredible changes are viewed with seriousness and the challenge is met fairly and squarely, the economic conditions of Islamic countries will not improve. The worst fear is that on the one hand there will be more and more brain drain of scientists and technologists from the Muslim world to the developed countries. On the other, the economy of the majority of the Islamic countries will be controlled by multinational companies for the personal gain of an unscrupulous section of the rich of those countries whose only motive is profit.

An article entitled, "The Arab Human Development Report 2002" published in the July 2nd 2002 edition of the "New York Times," describes the findings of a report prepared by well-known Arab intellectuals from a variety of disciplines. The team was appointed by the United Nations. The co-sponsor was the Arab Fund for Economic and Social Development, a development finance institution set up by members of the Arab League.

The team consisted of Thoraya Obaid, a Saudi who is the executive director of the United Nations Population Fund; Mervat Tallawy, an Egyptian diplomat who heads the Economic and Social Commission for West Asia; and Clovis Maksoud, director of the Centre for the Global South at the American University in Washington, who served earlier as the Arab League's

representative at the United Nations. The report covered 280 million people in the 22 Arab countries.

The task of the team was to study the existing conditions prevailing in the Arab world in the field of science education, status of women and the extent of political freedom enjoyed by its citizens. There was something exceptional about this team in that instead of “finding fault with others,” it tried to study in depth “the deficits in contemporary Arab culture.” Its approach was to determine the major factors that stand in the way of progress of Arab countries in the field of science education and whether the lack of political freedom and obstacles that women encounter constitute a deterrent force resulting in the slow pace of progress in science and technology. According to the statistics provided in the article, the number of Arabs is expected to grow to between 410 million and 459 million by 2020. Unless the power of science and technology is harnessed to the full, these countries will face chronic shortage of food, housing, medical and health facilities. This will in turn create political instability because food shortage is one of the major contributory factors to fratricidal wars and power struggles.

In their report, the team pointed out that there is a severe shortage of new writings and a dearth of translations of works from outside. According to the report, the number of books translated annually in the Arab world is only a little over 325 compared to over 1600 done in Greece over the same period of time. The shortage, according to this report is due to “Islamic pressures.” The report says that creativity among Arabs centres around religious themes and as a result, only books on such themes are “best sellers.”

The report quotes Fouad Ajami, Director of Middle East Studies at Johns Hopkins University about what he said recently in an interview. He said, “There is a pervasive sense that life in the Arab world is repressed by both the state and religious vigilantes. Women are the worst sufferers.” About Arab women, the report said, “They are almost universally denied advancement” and that “sadly, the Arab world is largely depriving itself of the creativity and productivity of half its citizens,” denoting women. In the report there are a few more glaring revelations such as “Arabs today feel monitored,” as a result of the growing power of a lower middle class whose members are literate but not broadly educated,” trying to deny “intellectual freedom” to scientifically advanced scholars. This reactionary group shows its lack of “hospitality to anyone of free spirit, anyone who is a dissident, anyone who is different.” As a result, “research and development are weak or nonexistent. Science and technology are dormant.” The report presents its analysis, “rulers, even elected, stay in power for life and create dynasties. People feel powerless to bring about meaningful change in order to be able to pursue their intellectual goals for advancing themselves and their nations.”

In our opinion, the situation is not as dismal as it has been painted above. Even the adversaries of Islam admit that Muslim scientists laid the foundation of modern science. Our heritage in science culture is very rich, and we can capitalize on history to revive science culture to the full. However, before we

take upon this stupendous task, let us face some basic facts. For instance, no concerted effort has so far been made anywhere in Muslim countries to teach pupils the valuable contributions made by Muslim scientists. As far as we know, the history of Muslim scientists is not a part of school curricula. A few individuals may be familiar with some names such as Ibn Sina and Muhammad ibn Musa al-Khwarizmi, but hardly anyone knows about their great contributions in detail - something that may inspire them to follow suit. Their ignorance is certainly not their fault; the students are hardly exposed to the glorious past of Muslim scientists because such chapters do not feature in the syllabi in their entire career. As a result, they suffer from a sense of frustration and either move to the West to improve their career or suffer from “the inferiority complex of the generation before them.”

3 MUSLIM CONTRIBUTIONS TO SCIENCE IN MEDIEVAL AGES

3.1 General

Against the above backdrop, let us examine the situation as it existed during the period following the establishment of the Islamic state beginning in the late seventh century until the end of the twelfth century. This may motivate the policy makers to have a critical look at the current science syllabi and modify them in light of what present day Muslims can do, given the opportunity and facility now enjoyed by the scientists of the West and even by those in the newly developed and developing countries such as Taiwan, Singapore and India. It must be pointed out also to the policymakers that those who memorize the holy *Qur'an* have every right to know about every day science and be able to log onto the Internet to satiate their curiosity about the Creator and the world *Allah* has created.

Below is a description of the kind of intellectual environment and facility created by the Arabs at the dawn of “the Golden Period.” The Arabs encouraged learning of all kinds. Schools, colleges, libraries, observatories, and hospitals were built throughout the whole Islamic state from the Arab Peninsula to the East of Asia and to many parts of Europe and Africa. These educational institutions recruited highly qualified instructors and high quality research was initiated in these institutions.

3.2 Intellectual environment

What was unique in the educational system was that regardless of nationality and creed, scholars were invited to participate in learned discourses held in Baghdad and Damascus. According to *Introduction to the History of Science* by George Sarton, the old learning was transformed as a result of the intellectual freedom enjoyed by men of learning at the great centres of learning epitomized by Baghdad that became the intellectual centre of the world.

Their approach to science was as modern as that of present day science. Investigators would not accept any phenomenon as true unless confirmed by experimental evidence or by experience.

3.3 The ‘Golden Era’

This period witnessed the great contributions made by many outstanding Muslim scholars such as (a) Jabir Ibn Hayyan (eighth century); (b) Al-Khawarizmi (ninth century); (c) Al-Razi (ninth century); (d) Al-Mas'udi (tenth century); (e) Abu-l-Wafa (tenth century); (f) Ibn Sina (tenth century); (g) Al-Biruni (eleventh century); (h) Omar Khayyam (eleventh century); (i) Abul Qasim al-Zahrawi (eleventh century); and (j) Abu Muhammad Ibn al-Baitar (eleventh century). There were many other brilliant Muslim scientists who enriched the realm of science in many disciplines. Names of some of these scholars are: al-Jahiz, al-Kindi, Abu Bakr Muhammad al-Razi, al-Idrisi, Ibn Bajja, Ibn Zuhr, Ibn Tufayl, Ibn Rushd, al-Suyuti. Some of the most important discoveries that led to the foundation of modern science and played a significant role in the European “scientific revolution” are:

Muhammad Ibn Musa al-Khawarizmi was the founder of modern Algebra. The name ‘algebra’ is derived from the title of his book, “Hisab al-Jabr wa al-Muqabalah.” He developed sine, cosine and trigonometric tables and the concept of the equation. The West readily accepted the mathematical innovations and included them in their syllabi. Al-Khawarizmi also helped introduce Arabic numerals, the decimal position system, and the concept of zero.

Ibn al-Haytham (d. 1039), discovered the basic laws of optics, and al-Biruni (d.1048), measured the circumference of the earth and discussed the rotation of the earth on its axis.

Omar Khayyam, better known as a famous poet in the Persian language was also a great mathematician. He recognized 13 different forms of cubic equations. He was the first to develop the binomial theorem and determine binomial coefficients. He also introduced a solar calendar that was remarkably accurate (error of only one day in 3770 years) and was named *Al-Tarikh-al-Jalali*.

Ibn Sina is known in the West by the name of Avicenna. He was the most famous physician of his time. His famous book, “al-Qanun fil-Tibb,” known as the ‘Canons of Medicine’ in the West, was a masterpiece in medical science and was a standard text in the West up to the eighteenth century with a general discussion on the theory of drugs.

Abul Qasim al-Zahrawi earned fame as an outstanding surgeon. The Encyclopaedia called *Al-Tasrif*, which he composed, comprised a part of the medical curriculum on surgery in European countries for many centuries.

Abu Muhammad Ibn al-Baitar (eleventh century) from Spain was a famous botanist who explored over several regions in Europe and North Africa and made an extensive collection of plants. In his book, Baitar not only gave an

illustrated account of the salient features of the plants he collected but he also gave their importance as herbal medicines.

3.4 What Carly Fiorina, the CEO of Hewlett Packard, had to say?

In a recent speech defining the relevance of leadership in today's world. Carly Fiorina, CEO of Hewlett Packard said:

There was once a civilization that was the greatest in the world. It was able to create a continental super-state that stretched from ocean to ocean, and from northern climes to tropics and deserts. Within its dominion lived hundreds of millions of people, of different creeds and ethnic origins.

One of its languages became the universal language of much of the world, the bridge between the peoples of a hundred lands. Its armies were made up of people of many nationalities, and its military protection allowed a degree of peace and prosperity that had never been known. The reach of this civilization's commerce extended from Latin America to China, and everywhere in between.

And this civilization was driven more than anything, by invention. Its architects designed buildings that defied gravity. Its mathematicians created the algebra and algorithms that would enable the building of computers, and the creation of encryption. Its doctors examined the human body, and found new cures for disease. Its astronomers looked into the heavens, named the stars, and paved the way for space travel and exploration. Its writers created thousands of stories. Stories of courage, romance and magic. Its poets wrote of love, when others before them were too steeped in fear to think of such things.

When other nations were afraid of ideas, this civilization thrived on them, and kept them alive. When censors threatened to wipe out knowledge from past civilizations, this civilization kept the knowledge alive, and passed it on to others.

While modern Western civilization shares many of these traits, the civilization I'm talking about was the Islamic world from the year 800 to 1600, which included the Ottoman Empire and the courts of Baghdad, Damascus and Cairo, and enlightened rulers like Suleiman the Magnificent.

Although we are often unaware of our indebtedness to this other civilization, its gifts are very much a part of our heritage. The technology industry would not exist without the contributions of Arab mathematicians. Sufi poet-philosophers like Rumi challenged our notions of self and truth. Leaders like Suleiman contributed to our notions of tolerance and civic leadership.

And perhaps we can learn a lesson from his example: It was leadership based on meritocracy, not inheritance. It was leadership that

harnessed the full capabilities of a very diverse population that included Christian, Islamic, and Jewish traditions.

This kind of enlightened leadership that nurtured culture, sustainability, diversity, and courage led to 800 years of invention and prosperity.

3.5 Synthetic approach by mediaeval Muslim scientists

One remarkable trend among the Muslim scientists was that they underscored the need of interdisciplinary investigations and use of a wide variety of methods to reach their conclusion. It is only in the recent past that the significance of this unique approach is being realized in the West.

In their lives, these past scientists showed, contrary to the present day belief, that learning the *Qur'an* and *Hadith* and pursuing of basic sciences can be done simultaneously. For instance, by the age of ten, Ibn Sina became not only well versed in the study of the *Qur'an* but also in basic sciences.

Let us now examine what the holy *Qur'an* says about acquiring knowledge and how the Muslim community in the wake of the establishment of the Islamic statehood acted in order to transform the Qur'anic message into reality.

4 THE REQUIRED APPROACH TO REJUVENATE SCIENCE AND TECHNOLOGY IN THE ISLAMIC WORLD

4.1 Interpretation of the word, "Iqra"

The first verse that was revealed to the prophet (pbuh) was, "Iqra bi-isme rabbeka ...," enjoining us to acquire knowledge. There are numerous verses in the *Qur'an*, where Allah (subhanahu wa ta'ala) praises the people of knowledge and highly encourages them to ponder on the creation of the heavens and the Earth. In spite of such clear directives by the *Qur'an*, some hard-line religious leaders interpret the word, "Iqra" as implying acquisition of knowledge only in the field of religion and not in areas related to science. Even among highly educated engineers, medical doctors and scientists, there is a sizeable portion that does not want their children to go in for science education, being carried away by the thought that such an education would deviate them from the true path of religion. For argument's sake, let us assume that studies other than those on an Islamic theme are not permissible in our religion. If that were so, how would the proponents of this belief explain the phenomenal discoveries/inventions made by Muslim scientists in the golden age of Islam? Do they imply that these outstanding scientists were divested of religion? Moreover, how would the people of this group explain the above mentioned directive of Allah (SWT) for pondering on creation and also one of our prophet's great sayings, "Exploring mysteries of creation for a short period is more than praying for a long while?"

4.2 Necessity to evaluate new technologies

Another critical point to think about in this context is the ever-increasing dependence of the present day Muslims on technology. This dependence is creating complex problems in their lives. To solve the problems experienced by the Muslims, especially those living in industrialized countries, the scholars need to do intensive research in order to understand the various aspects of modern society. Their findings would give the Muslims a sense of direction about what is right and what is wrong. A case in point is the use of public address systems in the holy cities of Makkah and Medina. There was an uproar when the question came up whether to use it. But then, after considering the pros and cons of the issue, the scholars decided in favour of using this system. What a tremendous benefit it has generated! Those who have been in Makkah and Medina, either to perform ‘Hajj’ or ‘Umrah,’ hear each and every word uttered by ‘imams,’ regardless of the space he/she occupies for prayer inside the huge mosques. Another burning topic confronting the Muslim society is whether the technology for human cloning is acceptable; if so, to what extent! To take the right decision requires intensive study and research.

4.3 Insufficient influence over the media

In the absence of satellites of their own, Muslims have insufficient influence over the media. As a result, the only voices the Muslim youth and children hear is from non-Muslim newscasters and producers and those who are prejudiced against the Muslims to varying degrees and having no inherent sympathy for this community. To remedy this situation, an arrangement needs to be made; (a) to create a cadre of Muslim scientists who would acquire knowledge par excellence in modern science and technology; and (b) give their interpretation through a satellite-aided powerful media.

4.4 An S&T base in Islamic countries is necessary to stop persecution of Muslims

A strong science and technology base is a must for the safety and survival of Muslim countries. No country would have the courage to attack an Islamic country if it knew that force would be met with a well-educated and resourceful populace. There would have been no attack on Chechnya, Yugoslavia or on Kosovo, if we were advanced in S&T. Indeed, Pakistan’s possession of nuclear warheads acted as a deterrent to her neighbours’ wish to attack.

4.5 Promoting a science culture in Muslim countries

Since the mid-nineties, some Muslim states have been making genuine effort to initiate a science culture and apply it for the development. Malaysia is one such state. This is not say that there has been no progress of science in Islamic countries other than Malaysia. Indonesia, Iran, Egypt, Pakistan, Tunisia and Turkey have made considerable advancement in the field of science but yet the

impact of S&T is not perceived by common man and the vast majority of those who run the country. It is true that Pakistan has developed an atom bomb and long range missiles; but that outstanding feat was accomplished out of dire necessity. Science culture has not been established and the old environment still exists where common man is practically ignorant of the benefits that science and technology can bring about to combat poverty. Unless science is established at the ground roots level, the poverty level will continue to dominate in the Islamic countries.

4.6 The case of Malaysia

In Malaysia, the effort is directed to develop S & T to the level where it may be perceived by the common man as an important and 'integral' part of daily life. The first step to achieving this is to gauge whether the people recognize S&T's contributions to their present standard of living and what the future relationship between science, technology, and economic prosperity would be and what impact S&T would bring to their lives and well-being. Some specific questions that the government would like to pose and get feedback on from the public are: (a) How many of them have sufficient understanding of S&T to participate meaningfully in public policy debates, involving scientific and technological issues? (b) How do they view S&T compared with those in developed countries like the US, Europe and Japan? (c) What subjects of science and mathematics in school prepare the students for a lifetime learning process to deal with the new developments? (d) What capacity is required to test the reliability of information sources as being indicative of Malaysians' ability to prepare for the future?

As a result of the Malaysian Government's new policy to derive maximum benefit out of S&T, the incidence of poverty in that country has already drastically fallen from 49.3% in 1970 to 7.5% in 1999. The hard core poor was small at only 1.4% in 1999. Through the implementation of this dynamic policy, Malaysia hopes to mobilize and capture the full benefits of S&T by 2020. Such measures in which the government will spend a substantial amount of GNP are expected to propel Malaysia as one of the most advanced and affluent countries in the world.

4.7 Tunisia

Another Muslim country, which is progressing fast in creating and nurturing science is Tunisia. The tenth IAS Conference in 2000, which was held in that country provided an opportunity for us to see what was happening there in the realm of science and technology.

It should be noted that development in Tunisia has been approached from a purely secular angle whereas the object of this paper is to propose an integrated approach to knowledge that includes religious as well as scientific and technical knowledge.

4.8 The revival!

What measures should the policy makers take to turn the tide from one of slow progress of science to that of dynamism and rapid evolution? If they choose the Malaysian model to be the best, how should the implementation process proceed, encompassing and adapting it to suit the environment of each country? Here are some ideas:

- Preparation of a working paper on the ways and means to establish science and technology education at all levels in the Islamic countries. Emphasis should be laid on Internet use and the facility needed to be created for exploitation of this extremely powerful source of media;
- A principal outcome of this should be suggested curricula at school, college and university levels encompassing Islamic knowledge, science and technology, languages, social sciences and mathematics. These curricula should stress that the study of science and mathematics stems from the divine directive (and is far from being opposed to it). They should also stress uses of S&T in accordance with the divine law for the benefit of mankind;
- Arrangement of regular dialogues between policymakers and religious leaders who have misgivings about introducing science courses at elementary levels where only religious teachings are imparted;
- Development of the fast Internet system in Islamic countries, allowing students to have an easy and fast access to science education and literature to scientific and technological research;
- Arrangement of rapid translation of selected science books in native languages that will differ from country to country. Collaboration of the IAS, ISESCO and the local science academies needs to be established to undertake this seemingly difficult but doable task;
- Rendering of outstanding achievements of the past Muslim scholars into videos, CDs in an attractive format to inspire the youth to follow their examples;
- Another method, which has successfully worked to create awareness among common man, is “house visits.” In Texas, an organization to create leadership at the grassroots level was started in 1964 and now within a span of 28 years, trained 10,000 men, and women in local leadership. Taking a cue from this kind of system, house visits may be arranged to create awareness among the public in our countries about science. If such public opinion is created, then policy makers would have no choice but to give due importance to the cultivation and nurturing of science and technology.

5 CONCLUSION

It would be an extremely difficult job to revive science culture unless we come to terms with religious leaders of diverse opinions. If nurturing of science culture means introducing educational reforms, there would be a lot of opposition as is being faced by some heads of states of some countries. If we approach this Herculean problem cautiously, having frequent dialogues with the religious leaders, it may not be as difficult a task as we may think, especially against the backdrop of our glorious past heritage and rich culture of science. This would be a conciliatory and powerful tool to win over the support of those who for various reasons oppose the nurturing of a science culture.

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Culture of Science and Sustainable Development

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Culture is a collection of cultivated ideas, beliefs, traditions, sentiments and all that which affects human behaviour and determines the social standing in relation to geography, race or belief and is modified by the environment. All of these dictate individual attitudes to new ideas and innovations and changes, which can affect and add to culture and behaviour in acquiring scientific knowledge and accepting change.

Different cultures vary in the degree of acceptance of “change” or “civilization.” This last term can have a range of meanings to different peoples and communities, so one witnesses much diversity in social, economic and political entities and cultures all over the world. Culture is a human virtue and activity, which can reflect positive or negative attitudes towards new advances in life. The development and scientific knowledge, which are collections of new discoveries, directed to improve the quality of human life, add accumulatively to culture when accepted. The culture of science cannot be separated from the culture of development as science is associated with development, and nowadays there is a universal call for the sustainable development to benefit humanity and subsequent generations.

The involvement of cultural and scientific knowledge in development has been recognized in the last twenty years or so, and the UNESCO contributed, through the different studies, meetings and researches, to the cultural aspects and its role in development and peace, as it is a base to any advancement in science and progress.

Cultural dimensions and scientific achievements are gaining ground in sustainable development which involves the different resources and is defined as the good management of resources through scientific and technical knowledge satisfying human requirements in a sustainable manner to benefit present and subsequent generations. This involves, as we mentioned, sound scientific knowledge in the conservation of water, soil, energy, plant and animal genetic resources, and diversity, as well as the conservation of the environment in the face of physical, climatic, economic, social and political changes.

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In spite of the vast resources in a number of Third world and Islamic countries, many such countries exhibit low rates of development, food insecurity due to the weak association between science, the environment and development. This is manifested by low productivity in plant, animal and other resources due to attitudes that question some technical packages and scientific applications. Muslim countries are contributing very little to science advances, progress and development although during the golden era of Islam, a great civilization grew up and produced great changes in the Islamic world and beyond, and no doubt affected humanity and still has fingerprints in different areas of scientific knowledge.

In discussing the relationship between culture, science and development, the religious culture and beliefs stand out as having strong impact and role on the life of the individual and the community. The Islamic ideology, which affects all aspects of a Muslim's life, advocates strongly the acquiring of scientific knowledge and knowledge in general to benefit humanity at large. This ideology was new in those days and led to great movement of scientific discoverers and progress at a time when other communities and cultures considered and looked down upon those who indulged in consulting books and writing.

Islam calls for the conservation of the environment and the balanced utilization of resources (every thing created by *Allah* is in good dimensions and balance) "قال تعالى: ولقد خلقنا كل شيء بقدر". This depicts the teachings and the logic of Islam. The Holy *Qur'an* indicated in many verses the components of the environment and its conservation. Our prophet (PBUH) in one (Hadeeth) says: "He who removes a tree which gives shade in an open area, without good reason, his face will be directed to hell). قال رسول الله (صلعم) "من قطع سدره في فلاة يستظل بها ابن السبيل عبثا أو ظلما بغير حق له فيها صوب الله وجهه في النار).

There is no doubt that the marriage between indigenous cultural and suitable scientific knowledge in Third world countries can benefit sustainable development, if the correct approach and sound knowledge of cultural heritage are appreciated. The cultural and social heritage of human settlements usually embraces great knowledge of their environments. That dictates the behaviour of the individual towards the components and events that surround him and affect his life. He is able to translate any chance in his surroundings in a manner which enables him to survive. This ability to adjust and adapt to change dictates the appreciation and grasp of human values and knowledge when one tackles resource management and sustainable development.

The improvement of economic life in most developing countries is related to good planning and sustainable development that ensures food security and poverty reduction. To achieve all this, there is a great cry for environment conservation to go hand in hand with sustainable development which cannot be achieved without taking into consideration the cultural, social, spiritual, political, customs and values dimensions. A lot of studies have been carried out involving the cultural impact and its effects on technical, economic and social changes. The cultural role comes out to be of vital importance for a successful,

economic and social development, which fulfils the aspiration, religious beliefs, and the feeling of security and peace for any country or nation.

One would like to point out the importance of cultural dimensions and attitudes in science and scientific aspects of developments. However, science should be streamlined and transformed into a marketable commodity to benefit humanity.

Combating Desertification in Countries of the Aral Sea Basin: An Overview

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1 THE BACKDROP

Desertification is one of the most serious social-environmental problems that mankind faces on the threshold of the twenty-first century.

Desertification processes have been widely spread on the arid territories occupying more than 30% of the world's land. 69% of arid territories, including 30% of irrigated, 50% of dry and 75% of grazing land are subject to the processes of desertification of varying degree. More than 100 countries with a population of more than 900 million suffer from the threat of desertification.

Mankind has known desertification for a long time. It is historically connected with the irrational land management in easily vulnerable hot and dry territories. Heavy consequences of desertification could be seen in regions where large-scale withdrawal of natural resources has occurred. An unfortunate example is the Sahel zone in North Africa, the Aral Sea zone in Central Asia, etc.

As could be seen from the data of the UN Committee to Combat Desertification (UNCCD), out of 2 billion ha of arid land in Asia more than half is subject to desertification: in Central Asia 69 %, in South Asia 55 % and in North-East Asia 30 %.

Currently, about 13 % of the whole land area of the Asian-Pacific region is subject to desertification (851 million ha).

Problems of desertification control were discussed for the first time at the UN Conference, which took place in Nairobi (Kenya) in 1977, where the retrospective estimation of this event was given and the world action plan was adopted, which was meant for a 20-year period.

International cooperation in this sphere allowed experts not only to significantly expand and deepen their knowledge about mechanisms and meanings of desertification but to evaluate existing techniques of desertification

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control and elaborate a number of unique technologies, and partially introduce them into the practice of desert development.

However, results of the work in this sphere were rather insufficient. New efforts of the world community were necessary, which were directed towards solving urgent tasks to combat the processes of desertification. In 1992 the International Conference on Nature Protection and Development in Rio-de-Janeiro made a decision on the necessity of elaborating the UN Convention to Combat Desertification and Drought Mitigation as a new tool for mobilization of political, people's, scientific and technical resources to achieve the projected goals.

The UN Convention to Combat Desertification adopted in 1994 is the first diverse legal document, in which the whole complex of the newest approaches for solving this extremely urgent problem are reflected. It is a long-term action programme for the world community to combat desertification and prevent the threat to the welfare of the population of arid zones.

The convention not only emphasises the necessity of bringing up the sense of direct involvement into all stages of its implementation in the ranks of the population suffering from desertification, but also stresses the necessity of the direct participation of the local population and local authorities in its implementation.

Scientists, government and international organizations recognize the importance of involving the local population in solving problems connected with desertification. In the majority of important documents on the subject, it is clearly outlined that environmental issues in general are more efficiently solved with the participation of interested citizens. It is well known that public organizations with the participation of the local population could make a considerable input into solving of environmental problems by sharing their information, opinions of independent expertise, proposing alternatives for solving the problem, and implementing solutions etc. Developing a partnership between governmental and public organizations, scientific and educational centres should be considered to be the key factor in reaching harmony in the "man-nature" system.

A strategy for mankind to preserve the natural environment in extreme conditions is clearly expressed in the UN Convention to Combat Desertification and Drought Mitigation. It is an extraordinarily important document that includes opinions and experience of authoritative scientists and specialists, as well as a considerable amount of scientific knowledge that has been stored up during the previous decades.

The main goal of the convention is to be the guiding principle of the long-term policy in controlling desertification for institutional and governmental structures as well as individuals. Because of great differences in environmental, socio-economic and political conditions in different countries, it is impossible to draw up and implement a universal technology to combat desertification. Therefore, the convention stipulated the development of national action programmes to combat desertification, which are to be the long-term policy of

each of the countries in controlling the environmental integrity and enhancing the resource potential as a basis for sustainable development. National action programmes are considered to be a continuous process aiming at organizing a new approach to the planning and formulation of a new policy in the sphere of controlling desertification in order to achieve the desired results.



Figure 1. Central Asian countries after the break-up of the Soviet Union.

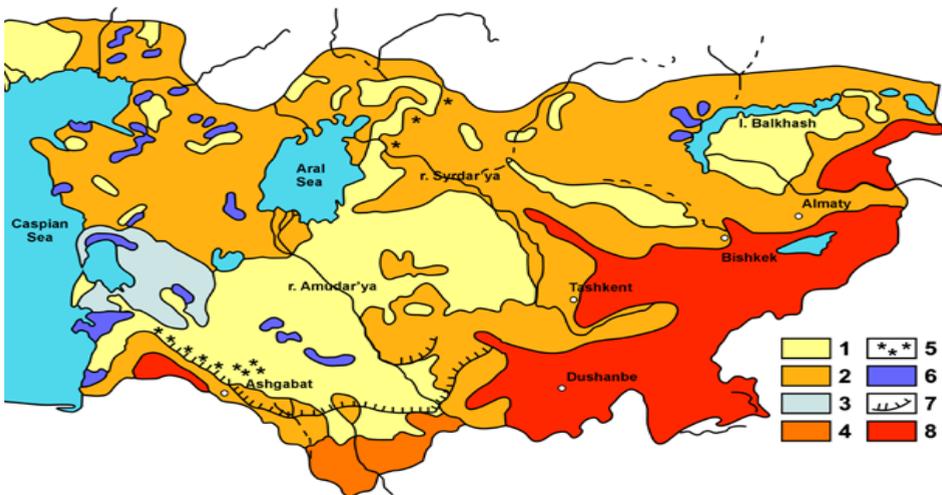


Figure 2. Desert types of Central Asia: 1 – Sandy; 2 - Clay; 3 - Gypseous; 4- Loess; 5 - Takyr; 6 - Solonchaks; 7 - Main Canals; 8 – Mountainous Region.

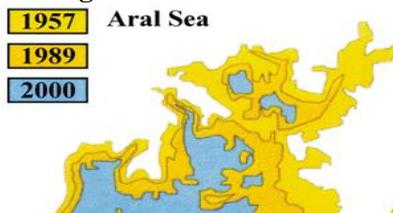


Figure 3. The demise of the Aral Sea over four decades.

2 TURKMENISTAN AND THE ARAL SEA

From a geographical point of view, the Aral Sea basin is situated in the internal part of the Eurasian continent, between latitude 35-55⁰ North and longitude 48-87⁰ East. Its total area is about 4 million square km, population is 55 million, with the average population density of 13.3 people per 1 square km.

After the collapse of the Soviet Union in 1991, five independent sovereign states appeared on the political map of Central Asia; Kazakhstan, Kyrgyzstan, Tajikistan, Turkmenistan and Uzbekistan (Figure 1). The natural conditions of the Aral Sea basin are extremely diverse. On the lowland part, which stretches for more than 3,000 km from the North to the South, the landscapes of the desert and semi-desert zones prevail. The climate here is sharply continental, with the extreme summer and winter air temperatures. The annual precipitation in the arid part of the region does not exceed 200 mm, while in the mountainous part, precipitation reaches more than 500-600 mm. The nature of Central Asia in general is considered to be a territory with arid landscapes.

The importance of active participation of states of the Aral Sea basin in the implementation of the UN Convention to Combat Desertification lies in the fact that more than 60 % of its territory is situated in the desert zone (Figures 2 and 3). Therefore, the sustainable social-economic development of the Aral Sea basin countries is inseparably linked to revealing and rationally using its mineral and raw material riches, and biological resources. Over the centuries, the local population has cultivated a unique experience of land use, water and vegetable resources, and for the last 25-30 years important technologies in this sphere have been worked out.

The main scientific centre for the development of new technologies to combat desertification is the Institute of Deserts, Flora and Fauna, of the Academy of Sciences of Turkmenistan, which was established in 1962. It took

an active part in the implementation of the action plan to combat desertification adopted at the first UN Conference on the subject, in 1977. During 1978-1990, international training courses were organised at the Institute of Deserts, Flora and Fauna, at which more than 600 scientists and specialists from 65 developing countries in Asia, Africa and Latin America raised their qualification. The international scientific-practical journal "Problems of Desert Development," published by the institute since 1967, with the English-language version being issued since 1979 in the USA, has considerably contributed to this matter. Many papers of different scientists in this sphere were published abroad. A number of methodological aids on estimation and mapping the desertification processes were prepared and issued. In 1998, the Institute of Deserts, Flora and Fauna prepared and transferred to the UNEP a package of project proposals to combat desertification in the Asian and Pacific region.

In 1999, the institute submitted a proposal on preparation of the "Map of Desertification in the Arid Land of Asia" to the UNEP with participation of scientists and specialists of Kazakhstan, Uzbekistan, China, India, Pakistan, Mongolia, Iran and other countries. Special English-Russian, Russian-Turkmen and French-Russian dictionaries of desertification terms were published.

In 1998, and based on space images, systemic observations at stations and stationary establishments, existing theme maps and statistical materials areas subject to desertification were verified, and a map of desertification processes on territories of the Aral Sea basin was compiled to 1:2,500,000 scale.

In countries of the Aral Sea basin, national action programmes to combat desertification have been worked out and are currently being implemented. In national programmes, the first part is devoted to peculiarities of natural conditions and resources, the second part to social-economic conditions, while the third to causes and criteria of desertification (degradation of pastures; forests and irrigated land; wind and water erosion; biodiversity conservation; economic damage and social consequences of desertification). In the fourth part, a strategy and an action plan are stated. In national action programmes, an important role is given to public organizations and local authorities in combating and improving the environment. Specialists and experts, NGOs and many other voluntary individuals and organizations considerably contribute to the implementation of national programmes.

In 1999, and in cooperation with the Springer Publishing House, a book entitled "Problems of Deserts and Desertification Control in Central Asia," was published in English. It contained the results of scientific and practical work of many years.

At present, a joint Turkmen-German project entitled, "Natural Resources Management in Central Karakums with the participation of the local population," is being implemented, as well as a broader pilot project, which is labelled, "Participation of the local population in the natural resources management in different bio-geological regions."

A new approach with active participation of the local population is being used in project implementation. It allows people to actively take part in planning and implementing measures undertaken to combat desertification. Within this

approach, meetings and workshops with the participation of veterans, young shepherds, schoolchildren and women, were organised and found to be very useful.

In 1999, work on the UNDP/UNSO project entitled “Implementation of the National Action Programme to Combat Desertification in Turkmenistan,” started.

A decree by the president of Turkmenistan in 1993 on the free use of natural gas, electricity and fresh water by the population of Turkmenistan played an important role in the protection of environment. At present, about 90 % of the country’s cities and populated areas are provided with gas, and 72 % with water supply. These measures considerably decreased the anthropogenic pressures on the environment and improved the ecological situation in the country.

The joint stock company “Gyok-Gushak” (Green Belt) established in 1999 placed the work on a broad footing for forest rehabilitation and forest growing around all the cities and large populated areas. In desert conditions, such greenery safely protects populated areas from hot and dusty winds and creates a favourable microclimate and improves the landscape.

In 2000, a new programme of the president of Turkmenistan was adopted. It was called the “Strategy of social-economic changes in Turkmenistan for the period up to the year 2010.” In this new programme, great of attention was paid to the issues of implementation of the national action programme to combat desertification.

The implementation of the new programme stipulated the improvement of the environmental legislation, support to the development of modern scientific-engineering techniques of estimation of the impact of the technogenic processes on the environment, introduction of modern technologies of rational land and water management, mastering of the world experience of desertification control, conservation of rare and vanishing species of flora and fauna, creation of information databases and electronic systems of their processing, monitoring and management of technogenesis processes.

The solving of problems of rational nature use and desertification control is a complicated task. The financial mechanism to provide measures to combat desertification includes such sources as the state budget, donors, international organizations, funds, etc. In the national action programmes to combat desertification, the necessity of cooperation with other national programmes and international conventions is highly stressed.

Heads of states of the Aral Sea basin have committed themselves to the implementation of national action programmes to combat desertification. These programmes are the main guiding principles in the rational use of nature, and the creation of the conditions of environmental safety.

National Action Programmes to Combat Desertification (NAPCD) in countries of the Aral Sea basin are being implemented phase by phase. In the first phase the state of the land subject to desertification was examined, surveys were prepared, the character and direction of processes was estimated, and a map of the desertification processes was compiled. The second phase envisages the implementation of pilot projects in separate standard farms; the third and last phase, stipulates preparation of the final document and recommendations for governments and decision-makers to implement.

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Prof. Djibril Fall	(1930-1992)	Senegal.
Prof. Salimuzzaman Siddiqui	(1897-1994)	Pakistan.
Prof. Abdus Salam Mia	(1925-1995)	Bangladesh/USA.
Prof. Suleiman Gabir Hamad	(1937-1996)	Sudan.
Prof. Mohammad R Siddiqi	(1908-1998)	Pakistan.
Prof. Abdullah M Sharafuddin	(1930-1998)	Bangladesh.
Prof. Achmad Baiquni	(1923-1998)	Indonesia.
Prof. Mumtaz Ali Kazi	(1928-1999)	Pakistan.
Prof. Faramaz G Maksudov	(1930-2000)	Azerbaijan.
Prof. Ali Kettani	(1941-2001)	Morocco.
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