**OECD GLOBAL SCIENCE FORUM**

# Report of the Workshop on Large Facilities for Studying the Structure and Dynamics of Matter

Copenhagen, 20 - 21 September, 2001

## I. PRINCIPAL FINDINGS AND CONCLUSIONS

### Background

During the next 10-15 years, the governments of the OECD countries will make large investments in facilities for research into the structure and dynamics of matter: neutron sources, photon sources (X-ray sources, lasers, etc.) and nuclear magnetic resonance spectrometers. As funding agency officials consider new projects (as well as the maintenance and upgrading of existing facilities) they will take into account the concerns and needs of the scientific communities. They will need information on scientific priorities and promising future lines of research, as well as information on the utility, feasibility, time-scale, and cost of various types of research facilities and related infrastructures. Delegates to the OECD Global Science Forum agreed on the need to consider these facility-related issues in a comprehensive and coherent way, and they authorised the convening of an international workshop, based on a proposal from the delegations of Denmark and the United Kingdom.

The workshop was held in Copenhagen on September 20/21, 2001, under the chairmanship of Professor Arthur Bienenstock of Stanford University. It was attended by fifty-five government-appointed participants representing eighteen countries (plus the European Commission), invited scientific experts, and representatives of three scientific organisations. The principal findings and conclusions of the workshop are as follows:

## The Evolving Role of Large Facilities

Findings:

Condensed matter science is flourishing, thanks to an increasing ability to analyse and manipulate matter (including biological matter) on the atomic and molecular levels. Using powerful theoretical, computational, and experimental methods, scientists are able to study, design, and create materials whose properties (mechanical, chemical, optical, electrical, magnetic, etc.) make them suitable for a wide range of applications, such as nanostructures, "high-temperature" superconductors, and advanced semiconductors. The study of genome-related proteins and protein complexes has already produced enormous benefits to society, for example, new drugs and therapies. An increasingly important trend is the study of dynamic, functional states of matter, and short-lived phenomena such as catalysis.

To an ever-larger extent, the study of condensed matter requires the availability of sophisticated instrumentation, and a supply of probing particles and radiation with high intensities and other characteristics that can only be produced at large facilities. The process of planning, financing, and building these facilities takes many years, which puts them in the "megascience" category, but much of the research performed at these facilities is "small science". That is, it is done by numerous small groups that use the facilities for relatively short periods (days or weeks), as part of research that is carried out, for the most part, in laboratories not directly linked to the facility.

Conclusions:

Given the growing importance of large facilities and the long time needed for their implementation, there is a corresponding need for long-term, strategic national and international planning and priority-setting, taking into account the anticipated needs of scientists and technologists in many diverse disciplines, and considering the relative benefits of the various probes. In the case of the biggest, most expensive facilities, regional[1] collaborative projects on the continental and sub-continental scale are favoured, including joint R&D on sources and instrumentation, sharing of instruments and software, and development of methods for remote operation. When policymakers anticipate the establishment of such international facilities, they should allow sufficient time (two years or more) for negotiating the needed formal agreements.

Long-term planning exercises should take into account the potential offered by upgrades to sources, instrumentation and detectors, as these can often provide great increases in effective intensities at relatively low costs. Policymakers should avoid under-instrumenting new facilities, and should anticipate an instrument upgrade/R&D fund as part of normal lab operating costs. Detector R&D can often be productively conducted via international collaboration.

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[1] In this report, the term "region" denotes several countries or an entire continent.

## Neutron Sources

Findings:

Neutron beams have numerous applications, among them studying magnetic structures and elementary excitations in condensed matter, and determining the structures and dynamics of amorphous materials as well as polymers and polymer melts.  The largest, most advanced neutron sources are increasingly based on nuclear spallation using proton accelerators, but small- and medium-scale reactor sorces will continue to be constructed for national/regional use.  Significant advances in source performance can be achieved through proposed and planned upgrades of existing spallation and reactor facilities.

Conclusions:

The principal conclusions of the 1998 OECD Megascience Forum Neutron Sources Working Group are still valid.  These are: (a) the desirability of advanced sources, providing 1-2 orders of magnitude increase in effective flux, in each of the three major scientific regions: Asia/Pacific, Europe, and North America; and (b) urgent attention to refurbishing or up-grading existing front-line facilities.  With the construction of powerful spallation sources being well under way in Japan and in the United States, the focus of attention has shifted to Europe, where a decision will have to be made about a proposed ten megawatt facility, the European Spallation Source.  In addition, decisions are expected on upgrades for ILL, a second target station for the existing ISIS source, and the AUSTRON proposal.

## Photon Sources

Findings:

High intensity photon beams across a wide range of wavelengths are critically important for determining the structure and dynamics of crystalline and amorphous materials, as well as their electronic states and vibrational excitations.  Hard X-ray synchrotron radiation facilities have become indispensable for studying the structures of large biomolecules and molecular complexes.  There is considerable enthusiasm in the scientific community regarding the potential applications of free-electron lasers (FELS) with intensities that could be many orders of magnitude higher than those of existing sources.  Planning for X-ray free-electron lasers (XFELs) has started in Europe, Japan and the United States, and experimental tests of feasibility show great promise for the successful implementation of future large facilities.  These lasers are expected to make possible structure determination of condensed matter in excited and transition states, as well as the study of individual molecules of the many proteins that cannot be crystallised.  There is an interesting synergy between some of these facilities and proposed electron-positron colliders for elementary particle physics research.

Conclusions:

The latest ("third") generation of synchrotron radiation sources (including the ones being built of planned) will accommodate the needs of researchers for the next few years, but the advent of XFELs poses interesting challenges and opportunities for policymakers.  Because of the vast increment in performance, it is very likely that entirely new types of scientific measurements and applications will be enabled.  Scientific interest  is high, and the following questions were identified at the OECD workshop: (1) how can planning and priority-setting exercises best incorporate the known and projected applications, the technical feasibility, and the cost of these highly innovative facilities? (2) to what extent should future XFELs be linked to high-energy electron-positron colliders for elementary particle physics? (3) what is the optimal global inventory for the first round of XFEL construction, for example, should one of these facilities be built in the United States, one in Japan, and one in Europe?

## II. INTRODUCTION/RATIONALE

During the next 10-15 years, OECD countries will be making significant investments in facilities for research into the structure and dynamics of matter: laboratories based on neutron sources, photon sources (X-ray sources, lasers, etc.) and nuclear magnetic resonance spectrometers. Policymakers will be considering new projects, as well as the maintenance and upgrading of existing facilities. Their goal will be to ensure that the priorities and needs of the scientific communities are taken into account in projections and plans for major new research facilities. To achieve this goal, they will need information in the following areas:

- The scientific priorities and promising future lines of research that will require the use of various probes (photons, neutrons, electrons, etc.) to study the properties of matter, with emphasis on those techniques that require large new or upgraded facilities.
- The utility, feasibility, time-scale, and cost of various types of facilities, including incremental advances, and potential breakthroughs in performance. The advantages and limitations of each technique have to be evaluated in relation to scientific and technological goals.
- The optimal balance between investments in the sources themselves, and in the accompanying scientific instruments and software.

Information on the above topics has been developed in the course of specialised studies and workshops. Delegates to the OECD Global Science Forum agreed, however, on the need to consider the issues in a comprehensive and coherent way. Accordingly, they authorised the convening of a workshop, based on a proposal from the delegations of Denmark and the United Kingdom.

The study of the structure and dynamics of matter is an extensive scientific undertaking, and it was not the purpose of the workshop (or of this report) to review the totality of work in this area. Rather, the goal was to highlight those trends and challenges that deserve the special attention of policymakers as they consider investments in medium- and large-scale facilities during the next 10 to 15 years. The preparations were supervised by an international Steering Committee[2], with overall co-ordination being provided by Dr. Jørgen Kjems (Risø Laboratory, Denmark) and Dr. George Stirling (CCLRC, United Kingdom). The workshop was chaired by Prof. Arthur Bienenstock (Stanford University) and was attended by fifty-five government-appointed participants, plus invited experts, representatives of scientific organisations, and members of the OECD secretariat (the list of attendees and the agenda are appended to this report).

In authorising the workshop, the Global Science Forum was following up a series of inter-related activities that it had sponsored during the past several years, aimed at exploring policy issues surrounding large research facilities: the Working Group on Neutron Sources (1996 - 1998), the Working Group on Access to Large-Scale Facilities (1996 - 1998), the Working Group on Nuclear Physics (1996 - 1999), the Workshop on High-Intensity Proton Accelerators (2000), the Workshop on Structural Genomics (2000), and the Workshop on High-Intensity Short-Pulse

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[2] Bernard Frois (France), Lucia Incoccia-Hermes (Germany), Jørgen Kjems (Denmark), Stefan Michalowski (OECD), Masayuki Mori (Japan), Yukio Morii (Japan), Carlo Rizzuto (Italy), George Stirling (United Kingdom), Iran Thomas (United States) and Thomas Weber (United States)

Lasers (2001). The reports from these activities are available on the OECD website, www.oecd.org/sti/gsf.

The workshop covered medium- and large-scale facilities dedicated to the investigation of matter on the atomic and molecular levels, and/or on time scales that are typical of atomic and molecular processes. Smaller-scale facilities, instruments, and techniques that are often of major scientific value (for example, electron and atomic force microscopy) were not discussed at the workshop because they do not present the same type of policy-level challenges for the funding and organisation of research. For biological systems, the scope included molecular and structural biology but did not extend to other domains, such as functional imaging.

## II. PRINCIPAL PROBES AND TECHNIQUES FOR THE STUDY OF MATTER

Understanding condensed matter means knowing its atomic composition, the locations and motions of the nuclei and electrons, and the electron energies. These properties can be determined using probes like electrons, neutrons and photons, and nuclear magnetic resonance (NMR). In some cases specialised probing beams (for example, muons) are generated as secondary or auxiliary beams in the some large facilities. Other probes do not as yet require large facilities, for example, beams of atoms or positrons.

Most of these methods can be used to determine the motions of the atoms by noting the decrease or increase in the energy and/or momentum of the probing particles. Often, a combination of information is used, because each probe interacts differently with matter.

***Neutrons*** can be produced with energies in the range needed to study excitations in solids, and with wavelengths that are comparable to inter-atomic spacings. There are practically no laboratory-size (small) neutron sources, and all research activities of this kind are performed at medium- and large-scale facilities.

Since neutrons are uncharged, they can penetrate deep inside materials, which means that bulk properties and samples inside thick containers can be studied. Neutrons have a magnetic moment, which means that they can be used to probe the magnetic properties of materials. Neutrons interact with atomic nuclei, and their interactions are not directly dependent on the atomic number, so they can be used to locate lightweight elements, including hydrogen. Neutron scattering is important for studying both the structural and dynamical properties of soft condensed matter, with two special advantages: it probes the relevant length and time scales, and it allows the highlighting of specific components through selective deuteration.[3] Neutron scattering is the preferred tool for unravelling the molecular morphology and motions of soft matter systems, particularly when applied in combination with advanced chemistry techniques and molecular modelling. Experiments with neutrons permit the study of very dilute components, or of very small amounts of matter (for example, particular topological points at interfaces), as well as in-situ studies of time-dependent and transient phenomena, and non-equilibrium states.

***Photons*** are the quanta of electromagnetic radiation, ranging in wavelength and energy from radio waves to gamma rays. Radio waves are used in NMR experiments, while photons ranging

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[3] This method (dubbed “contrast variation”) is used for studying selected parts of large molecules that contain numerous hydrogen atoms (for example, nucleic acids or proteins). Scientists can study the regions of special interest by measuring samples in which the hydrogen is replaced by its heavier isotope deuterium. Because neutrons scatter differently from the two isotopes, this technique can yield the desired structural information.

from the infrared (IR) to X-rays are used directly as probes. IR is mainly used to probe molecular vibrations, ultraviolet (UV) and "soft" (low-energy) X-rays probe chiefly the electronic energies, while the "hard" (high-energy) X-rays probe mainly the arrangements of atoms in solids. All these measurements are needed to achieve an understanding of the increasingly sophisticated and complex materials of basic and applied research, ranging from basic physics, chemistry and materials studies, to the biological and environmental sciences. Typically, ever-higher intensities and brilliances[4] are required to explore subtle, detailed aspects of these new materials. High intensities are essential for phase contrast imaging, micro-tomography of soft matter, and studies of bulk properties. Resonance scattering provides element-specificity. Today's benchtop photon sources (chiefly lasers) already provide the highest intensities and brilliances in the IR and visible spectrum, but facility-based synchrotron radiation (and future free-electron laser) light sources extend the continuous wavelength range of high-intensity, high-brilliance sources into the UV and X-ray regions. Major increases of photon source intensity would be consistent with historical trends which, during the past four decades, have involved increases by three orders of magnitude every ten years.

***Electron*** beams can be made fairly straightforwardly, and can readily be focused using magnetic lenses. Electron microscopes can be used to image objects directly like an optical microscope, but at much smaller length scales, down to atomic dimensions. Electrons can also be used to determine structure and composition.

In conjunction with the probes mentioned above, other techniques are often applied: high pressures, high magnetic fields, very high or very low temperatures. Sometimes these conditions are used in combination. Some of these extreme conditions are so difficult to achieve that they require expensive, specialised laboratories and experienced staff.

## III. SCIENTIFIC TRENDS, PROSPECTS, AND REQUIREMENTS

The study of condensed matter is a mature field with a long history. Research in this area has been driven by the desire to advance scientific knowledge, as well as the need for new materials and industrial applications. The properties of condensed matter are routinely examined and understood - both theoretically and experimentally - as expressions of the behaviour and spatial distribution of the constituent atoms and electrons. Scientists (and, increasingly, engineers) now think of the various properties of matter in terms of atomic and molecular arrangements rather than, as in the past, in terms of macroscopic aspects. Sometimes, experiments are even performed on single molecules (for example, directly measuring the force exerted on an individual strand of DNA) . Even at the macroscopic level, the mechanical, electronic, chemical, optical and biological properties of matter (even complex biological functions such as information transmission) are increasingly analysed in terms of molecular structure.

A distinguishing characteristic of modern condensed matter research is its increasing focus on dynamics, i.e., on the temporal dimension of physical, chemical and biological processes. The traditionally important measurements aimed at establishing atomic composition and the locations of constituent atoms have now been joined by experiments whose purpose is to understand the evolution in time of atomic motions and chemical reactions. For example, research being conducted at the most advanced photon sources is no longer confined to the observation of static ground-state phenomena, but is increasingly directed towards real-time observations of events

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[4] The brilliance of a light source is defined as the number of photons emitted per second, per unit source size, per unit space angle, for a bandwidth of 1/1000 of the mean photon energy.

such as catalysis, electrochemical processes, or magnetisation reversal in magnetic storage media. In studies of this kind, the relevant timescales are often very short and difficult to measure. Some of the advanced facilities and instruments discussed in this report are, or will be, particularly valuable for dynamics studies.

Scientists now know that a full understanding of many processes cannot be achieved by considering initial and final states alone, but must incorporate the role played by intermediate states (often extremely short-lived ones) and the transitions between them. Similarly, there is a growing emphasis on catalysts (for example, enzymes in living organisms) which make it possible for certain key reactions to take place in circumstances that are unfavourable from an energy balance point of view.

**Hard condensed matter.** Theoretical and experimental investigations of hard condensed matter (roughly speaking, solids) have produced some of the most spectacular successes derived from science in recent years. To appreciate this, one need only consider the examples of semiconductors (transistors, light emitters, sensors, microprocessor chips, etc.), magnetic memories, and advanced engineering materials (for example, composites and ceramics). Materials scientists have been able to create substances whose unique bulk properties (strength, electrical and thermal conductivity, etc.) can be designed and predicted by applying quantum theory at the atomic level. During the next 10-15 years, research in this area can be expected to continue to produce results with a major impact on society[5], and while exact predictions are not possible, the following scientific trends deserve special attention as they relate to the need for future large facilities:

- Researchers are focussing more and more on materials that are characterised by strong correlations among the constituent electrons, i.e., in which the electrons exhibit complex collective behaviour. The best known examples are “high temperature” superconductors.
- The ability to create and manipulate physical structures at the nano- and micro-metre scales is driving the nanotechnology revolution. Research funding in this field is increasing at rates that rival those of the life sciences. An extraordinary variety of applications is being proposed, among them devices that combine animate and inanimate components (for example, DNA computers). At the smallest size scales, researchers are studying and applying exotic atomic structures such as carbon nanotubes and fullerenes.
- Hard condensed matter often exhibits properties that are very difficult to comprehend theoretically, despite the increasing sophistication of the mathematical and physical models, and the impressive increases in computing resources available to theorists. In principle, the fundamental laws that govern condensed matter are known (they are those of quantum theory) but, in practice, the vast number of constituent atoms and molecules, and the complex interactions among them, make it difficult to predict and explain the bulk properties of the materials from first principles. These properties (expressed, for example, as phase diagrams or as the values of parameters such as the Curie point or the critical temperature for superconductivity) can vary radically as a function of small changes in the material (for instance, isotopic composition). As a consequence, the accumulation of large amounts of empirical data is of special importance, both for closing the gap between theory and experiment, and for increasing the chances of discovering useful materials such as room-temperature superconductors.

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[5] The impact of some potential discoveries could be very great indeed: for example, low-cost high-efficiency solar panels for large-scale commercial generation of electricity, or lightweight batteries for a new generation of electrically powered automobiles.

**Soft condensed matter.** The category of "soft" condensed matter includes colloids, gels, emulsions, micelles, foams, liquid crystals, polymer melts, and similar materials. In everyday life, it includes an enormous range of familiar and useful materials such as plastics, paints, surfactants, porous media, pharmaceuticals, coatings, foodstuffs and textiles. These systems are characterised by a large number of degrees of freedom, weak interactions between the constituents, and a delicate balance between disordered and ordered states. The dynamics of soft condensed matter are of great interest, for example, for optimising industrial processes.

Soft condensed matter research has many connections to biology, and it is widely regarded as a major growth area for the next decade. Biological physics, in turn, is closely linked to the study of macromolecules, notably nucleic acids (DNA, RNA) and proteins (which are discussed below). Chemical synthesis using biological methods will create new classes of materials amenable to physical measurements at atomic and molecular scales, with numerous applications.

### Molecular and structural biology

**Protein structure.** Information on the structure and function of the proteins encoded in human (and other) genomes is in high demand. The availability of protein structures has scientific implications that are far-reaching. It is vital for drug design (witness, for example, the successful clinical use of small molecules that latch on to, and block, the active site of the HIV reverse transcriptase enzyme). In agricultural research, structural information is needed to study the genetic characteristics of crops and animals. In fundamental biology, knowing the structures of proteins and other large molecules is vital for understanding cell metabolism, gene function and, ultimately, the process of evolution itself. Several concerted action projects exist in structural genomics in Japan, the United States and Europe.

Extracting structural information is a complex and time-consuming process, due to the enormous complexity of the individual proteins and the subtle interactions of proteins and other biomolecules that form transient functional complexes. X-ray diffraction and NMR spectroscopy are currently the most widely applied techniques for structure determination, but the sensitivity to hydrogen and contrast to deuterium give neutrons a potential to be more extensively exploited at future high-intensity sources. The modern trend in macromolecular X-ray crystallography is towards high throughput as well as high resolution, but since many proteins do not readily crystallise there is also a need to refine solution-based methods, high-performance electron microscopy and, if possible, single-molecule X-ray imaging.

**Protein function.** Enzyme catalysis, ligand binding, receptor action, electron and proton transfer, and other protein functions are strongly linked to internal dynamics. But the dynamics of biological processes is poorly understood. It is known, for example, that structural information alone is not sufficient to explain specific drug binding effects, and that the dynamics dimension should be taken into account. While information on the dynamics of complexes or similarly organised systems is still scarce, initial experiments on the dynamics of CO bonding to proteins have been performed using photons. Such information could be enhanced by combining structural data from X-ray studies with dynamic data from neutron scattering, NMR, and optical spectroscopy.

Studies on the molecular scale are crucial for the understanding of the self-organisation processes that underlie many functional aspects of the cell membrane, in particular membrane transport, molecular recognition on surfaces, and adhesion between cells and substrates. While these phenomena have been studied in the past, largely in model systems, there is now a tendency towards studying the far more complex natural membranes. New preparation techniques allow such membranes to be deposited onto solid substrates while maintaining their functional integrity, and hence open the avenue for *in situ* studies.

## IV. FACILITIES

### General findings about large facilities for studying matter

The cost of large- and medium-scale sources and instruments has increased to an extent that in most cases they must be shared by many scientists. Often, facility costs are a significant fraction of the total expenditures for the research fields that utilise them, and large organisations have to be established to build and operate the facilities. As a consequence of this change of scale, the working style of researchers has changed significantly since the days, not so long ago, when most experiments on condensed matter were conducted in individual laboratories, each equipped with the necessary equipment such as magnets, X-ray tubes, lasers, etc. Today, experimenters working at large facilities prefer to not be overly involved in the technical details of the large, complex, and expensive equipment that they use. For example, dedicated facilities now provide beams of neutrons or photons that are focused, monochromatised and/or polarised according to the needs of the researchers. Typically one or more instruments are used simultaneously on each beamline. A facility may have 10 or more beamlines and a total of 15 to 60 instruments[6], and it may host from several hundred to two thousand users per year. Individual measurement campaigns are normally carried out over a period of days by a few investigators, with students or other colleagues, working in shifts around the clock.

A typical experiment conducted at a large facility may simply constitute one stage of a larger programme of research involving many heterogeneous steps (for example, theoretical, computational, and experimental, using a variety of probes and techniques). Thus, for example, the determination, using X-ray crystallography, of the structure of an enzyme molecule could be just one step in a drug development programme that may include other phases such as theoretical molecular modelling and clinical trials. From a policy perspective, the overall challenge is to assure an adequate supply of user-oriented facilities that will serve the needs of researchers in the highly diverse set of disciplines that make up the modern scientific enterprise, whether it be medical research, advanced materials studies, or fundamental atomic physics. At the OECD Global Science Forum workshop, the following dimensions of the overall policy were identified and discussed:

**Investing in new facilities.** When pressure builds up from the scientific communities, governments are faced with the necessity of deciding on the construction of new facilities. Scientists may have a variety of motivations for promoting new facilities:

- The development of a consensus on a major research need (for example, the desirability of pursuing high-throughput structural studies of large numbers of proteins).
- The emergence of a major technological breakthrough or innovation that makes new sources and experiments possible (for example, the application of the “chirped pulse amplification” technique for generating ultra-high intensity laser pulses).
- The prospect of a scarcity of scientific resources (for example, the potential global shortage of neutrons caused by shutdowns of ageing research reactors).

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[6] At the European Synchrotron Radiation Facility (ESRF), one of the world’s premier photon sources, approximately 1000 separate experiments are performed annually using the facility’s 38 beamlines.

Often, there are overlapping and competing requests from the scientific community for major new facilities. Choosing is not easy, since it is difficult to evaluate and compare dissimilar probes (neutrons, photons, electrons, etc.) and there are strong vested interests among the highly diverse communities. There have not been, to date, any systematic attempts to set strategic, long-term priorities for facilities across all of condensed matter research at the regional or global levels. The undertaking of such exercises would require a strong mandate from the concerned political and funding authorities, as well as a credible organisational structure that would enjoy the confidence of the scientific community. There are some precedents in other, narrower, fields (for example, the "decadal" astronomy surveys conducted in the United States by the National Research Council).

Condensed matter research is characterised by an overlap between basic, applied and industrial activities. Clearly, policymakers are strongly motivated to promote the commercial use of facilities, since the potential users represent high technology and high-value economic sectors that are seen as vital for promoting competitiveness and employment. However, there are important organisational challenges involved in combining academic and industrial uses of government-funded facilities.

Decision-making for new facilities is especially challenging when there is a potential for a very large increase in performance (for example, the increase by a factor of between $10^7$ and $10^{10}$ in photon beam brilliance at proposed UV and X-ray free-electron laser facilities). While there is a strong desire to base major funding decisions on accurate predictions of exactly how a new facility will be used, the inherent difficulty of predicting breakthroughs in science, and the conservatism of some scientific communities, can make it very difficult to provide such a prospective accounting. Thus, a decision on a new facility may require a "leap of faith" and an assumption that a vastly increased source capability will lead to new, exciting advances in scientific measurements and applications. Proponents of new high-performance sources (photons, neutrons, etc.) often cite historical evidence: for example, the initial reluctance of many biologists to take advantage of accelerator-based synchrotron radiation sources, whose photon beams are many orders of magnitude brighter than those generated by traditional X-ray tubes[7].

Upgrading can be an attractive alternative to building a new facility. Even a major upgrade (such as installing a new nuclear reactor core) can be more efficient if it occurs at a site that is already in use, and takes advantage of an installed infrastructure and existing human resources. Upgrading of detectors and other instruments can be an especially cost-effective strategy. Some of the considerations are described below.

While the number of probes for studying matter is limited, there is a considerable diversity in the types of facilities that can generate these probes. For example, neutron beams can be produced via fission of uranium in nuclear reactors, or via the spallation process using proton beams in the 1 GeV energy range. For choosing the best technology, extensive discussions among experts are needed, but these may have to be accompanied by consultations with members of civil society on matters such as safety, licensing and environmental impact.

**Choosing between central and distributed facilities.** While some facilities are built around a single source (for example, a nuclear reactor or a particle accelerator), others are a collection of smaller systems (for instance, nuclear magnetic resonance spectrometers, or high-field magnets). In the latter case, an interesting question arises regarding the merits and demerits of concentrating

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[7] Today, cutting-edge protein crystallography (which accounts for some 90% of solved protein structures) is mainly performed at storage ring-based facilities.

the systems at the single central facility, versus distributing them over several institutions such as university laboratories. The following potential advantages of a centralised facility were enumerated at the workshop:

- Exploitation of economies of scale for purchasing, installing and operating multiple components, as well as cost savings through sharing of infrastructures: buildings, electrical systems, cooling, etc.
- Opportunity for researchers to select the most appropriate source and instrumentation from a large variety of systems available at the single facility.
- Optimisation of the utilisation of expensive equipment by instituting a systematic procedure for evaluating research proposals and scheduling the use of equipment for maximum efficiency.
- Cost-effectiveness of co-locating large support facilities (for example, sample preparation), which is of special value for long-term, high-throughput programmes.
- Creation of a localised community of international researchers who can share experiences, ideas, equipment and software, including the development of advanced instruments and applications with the participation and guidance of resident experts.

**Implementing institutional, national or regional facilities.** As the size, cost and complexity of facilities have evolved, there has been a shift in their organisational structure as well. Fewer facilities are associated directly with university departments, while the number of large national and regional installations is increasing. When a facility is attached to a university, it is used primarily by the local researchers, and the assignment of “beam time” and other resources is relatively straightforward. National and international facilities, on the other hand, operate in “user mode” which requires them to put in place procedures for soliciting and reviewing proposals, and for welcoming users who may only spend a short amount of time at the facility. Indeed, steps are under way at some installations to allow purely remote access to the facility - for instance, by sending samples to the local staff and obtaining the raw data via Internet. In all cases, special attention must be devoted to ensuring that members of the scientific community perceive the allocation procedures to be fair and reasonable.

The implementation of an international facility must include decisions about the policies and rules that govern access to its resources, including the tricky question of whether users are charged for operating costs (with special attention to the case of users from countries that do not contribute to the construction or operation of the facility). There are no universal answers in this area, but some useful findings and guidelines were developed by the OECD Megascience Forum Working Group on Access to Large-Scale Research Facilities (http://www.oecd.org/pdf/M00004000/M00004537.pdf).

Planning and priority-setting for international facilities, and negotiating the needed formal agreements, can be a long and complex process. In this regard, the European region is presented with the greatest challenges and opportunities, since many of the smaller countries do not have the resources or numbers of researchers needed to support national facilities. While there are well-known European successes with multinational facilities (ESRF[8] and ILL[9] being the most

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[8] Eurpean Synchrotron Radiation Facility in Grenoble, built around a 6 GeV “third-generation” electron storage ring.

[9] Institut Laue-Langevin in Grenoble, built around the 58 megawatt High Flux Reactor neutron source.

prominent), policymakers will be hard-pressed in the future to maintain scientific competitiveness with the United States and Japan. In the near term, decisions will have to be made about a number of very ambitious projects that have been proposed, among them the European Spallation Source, and the TESLA free-electron laser.

**Providing instrumentation and other infrastructures.** The science policymaker's goal is to maximise the scientific output of research facilities. The upgrading of existing sources, and the construction of new ones, are essential steps towards achieving this goal. Participants at the OECD workshop repeatedly emphasised the critical importance of ensuring a correct balance between investments in the two major categories: sources (reactors, storage rings, lasers, etc.) and instrumentation plus other infrastructural elements. The latter category includes detectors, analysis tools (hardware and software) as well as sample preparation and handling equipment. Advanced instruments (especially those at high-power synchrotrons and neutron sources) need a dedicated staff of scientists and technicians to operate and maintain each instrument at peak levels of capability and performance. The operation of stand-alone instruments such as electron microscopes and NMR spectrometers is in many ways analogous to the operation of instruments at large facilities. These instruments need to be operated and maintained by professional staff if they are also to be used by an increasing number of non-expert users.

When a new facility is planned, the selection and distribution of instruments should be considered well in advance. Some instruments are highly specialised and are used by only a few researchers, so only a small number of these will be needed. Other state-of-the-art instruments can only be used effectively if they are backed up by a network of less advanced instruments at smaller facilities: these provide the training ground and backup for the community of users who can transfer their research to the more advanced facility at an appropriate time. Some instruments are vital to multiple areas of research and are used by many researchers, and several complementary instruments of this same kind need to be provided. In some cases the instruments are part of a network which supports a large campaign of measurements, for example the global effort to determine the structures of proteins. Such an effort might involve co-operation across several similar or complementary facilities, and across international boundaries.

Increasing the efficiency of detectors (or the speed of sample-handling) can be a highly cost-effective "source multiplier", i.e., it can have the same effect as increasing the intensity of the source. The correct investment balance is not always easy to achieve, and instances can be cited of under-instrumented new facilities, and older facilities whose instrumentation has not been maintained at the state of the art (either because insufficient funds were provided for instrumentation R&D, or facility managers were reluctant to use facility funds for this purpose). Workshop participants agreed that more attention should be paid to instrumentation issues when priorities are set and funds are allocated for condensed matter research. Particular attention should be devoted to detector development, which is under-funded globally.

### Synchrotron radiation sources and free-electron lasers

Photons are emitted by high-energy electrons when their trajectories are deflected, for example in a synchrotron or storage ring. Particle accelerator physicists regard this phenomenon as a nuisance, but for material scientists it constitutes an extremely valuable source of radiation. The advantages and the availability of dedicated synchrotron sources led to increases in their use, and a constant demand for higher intensities. The latest ("third") generation of light sources and instruments, built in the 1980s and 1990s, are very large and very expensive. The ones built to produce the higher-energy X-rays cost around a billion dollars. The major sources are the European Synchrotron Radiation Facility (ESRF) in Grenoble (6 GeV), SPring-8 in Harima, Japan (8 GeV) and the Advanced Photon Source at the Argonne National Laboratory, USA (7 GeV). In recent years, almost similar levels of performance have been achieved through the use of innovative techniques at smaller, lower-energy (2-3 GeV) installations. These smaller facilities offer the additional advantage of being ideally suited for investigations of electronic structure by means of spectroscopic methods. Topmost in the world in this class of facilities are the ALS in Berkeley, BESSY in Berlin, ELETTRA in Trieste, MAXLab in Lund, Sweden, and the newly commissioned SLS in Villigen. The cost of instruments has increased along with the power of the sources. It is common for a single beamline and related instruments at high-intensity synchrotrons to cost over five million dollars.

Depending on the energy of the circulating electrons, and the details of construction of the magnetic devices that stimulate emission by the electrons, a wide range of photon energies can be produced, from the far infrared to hard X-rays. Beamlines at existing facilities are usually oversubscribed by potential users, but it appears that the current ensemble of facilities world-wide will be sufficient for accommodating the needs of condensed matter researchers, including biologists, for the foreseeable future. This estimate includes facilities that are planned and scheduled for construction (such as Diamond in the U.K., Soleil in France, as well as Australian and Canadian facilities) and those that will be modernised or replaced (for example, SSRL at Stanford University and DORIS in Hamburg). It is likely that no new major storage ring-based sources will be built beyond those being planned at this time.

The next generation of advanced photon sources will likely be free-electron lasers[10]. They offer the prospect of polarised, laterally fully coherent beams with vastly increased intensities and extremely short pulses in the femtosecond range (1 fs = $10^{-15}$ seconds). The fundamental principle - “self-amplified stimulated emission (SASE)” - has already been successfully demonstrated at wavelengths below 100 nanometres, opening the way towards the generation of laser-quality, femtosecond-scale, coherent radiation in the VUV/soft X-ray regimes and, ultimately, hard X-rays. The principal role of the new sources will be not so much to replace existing ones, but rather to enable entirely new kinds of measurements and, hence, directions for condensed matter research: studies of non-linear phenomena, exotic states, and dynamics of matter due both to mechanical (phonon) and electronic excitations (for example, using the so-called pump-and-probe method).

Planning of large-scale free-electron lasers has started in Europe and in the United States. Device testing and scientific experiments can already be performed at the TESLA Test Facility in Hamburg. There is an interesting synergy between some of these facilities and proposed electron-positron colliders for elementary particle physics research. It should be noted, however, that the generation of very hard X-rays can be accomplished with electrons in the 10-50 GeV range, whereas electron energies of 200 GeV and higher are needed for particle physics experiments.

The scientific potential of FELs is generating considerable enthusiasm in the scientific community, and a number of documents are available that describe new applications. For example, many scientists believe that the use of free-electron lasers could revolutionise protein structure measurements. Currently, one of the more difficult steps is making single crystals of the protein, and some proteins (most notably, many of those that reside in the all-important cellular membrane) do not crystallise. A free-electron laser may make it possible to determine the structure without crystallising the protein - the enormous radiation intensity should produce sufficient diffraction from a single protein molecule, and the extremely short pulse duration

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[10] These could conceivably be implemented using re-circulating electron beams, thus incorporating elements of today’s storage-ring based synchrotron sources.

should permit the accumulation of a sufficient quantity of data before the molecule is destroyed by the radiation.

The advent of XFELs poses interesting challenges and opportunities for policymakers. Because of the vast increment in performance, it is very likely that entire new types of scientific measurements and applications will be enabled. While scientific interest - indeed, enthusiasm - is very evident, the following questions were identified at the OECD workshop: (1) how can planning and priority-setting exercises best incorporate the known and projected applications, the technical feasibility, and the cost[11] of these highly innovative facilities? (2) to what extent should future XFELs be linked to high-energy electron-positron colliders for elementary particle physics? (3) what is the optimal global inventory for the first round of XFEL construction, for example, should one of these facilities be built in the United States[12], one in Japan, and one in Europe?

**Neutron sources**

Starting in the early 1980s, many studies recommended the construction of new sources with higher usable neutron fluxes. The studies also called attention to a looming “neutron gap” - a potential shortage of neutrons for research caused by the anticipated shutting down of ageing research reactors and the global slow-down in the construction and licensing of new sources. The OECD Megascience Forum (the predecessor to the Global Science Forum) established a working group to develop findings and recommendations on how OECD governments could maintain supplies of research neutrons over the next 15-20 years. A key recommendation promoted the development of three large regional spallation sources.

Any decision regarding a new source must involve a choice between the two principal processes for producing research neutrons, fission and spallation. Nuclear fission produces continuous flows of neutrons, most of which are needed to sustain the nuclear chain reaction, but the remaining ones can be extracted from the reactor core and used for neutron scattering experiments. This technology was almost at its peak with the high-flux reactors built in the mid-1960s. It might have been possible to obtain a neutron flux 10 times higher, and the United States designed a reactor (the Advanced Neutron Source) that was close to the limit of the technology, but this reactor failed to get approval.

In the spallation process, neutrons are produced when energetic (typically, 1 GeV) protons strike a heavy metal target. Spallation neutron sources were pioneered in the early 1980s in the United States and Japan with low-power sources of a few kilowatts. The success of the first spallation sources led to the construction of a source in the 50 kilowatt range in the United States and one of 160 kilowatts in the United Kingdom. The intensity limit of spallation technology is not known. In the future, very powerful sources (tens of megawatts) could conceivably be built for specific technological or industrial applications (for instance, transmutation of nuclear wastes, or testing of materials for fusion-based power reactors). These sources would be optimised for the generation of a wide spectrum of neutron energies, and for irradiating large volumes. Sources intended for general condensed matter research will differ in design and operation, since their purpose is to create collimated, high-density beams with well defined properties, and to deliver

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[11] The costs are estimated to be comparable to those of high-performance storage ring-based facilities.

[12] The U.S. Department of Energy has intiated research and development and approved the preparation of a conceptual design for the construction of an XFEL at the SLAC laboratory, taking advantage of the existing 50 GeV linear accelerator.

these beams to a large number of individual experimental stations where the neutrons are scattered from small target samples. A multipurpose facility, built around a single high-intensity proton accelerator, can supply a variety of particle beams: neutrons, protons, neutrinos, muons, as well as exotic unstable particles (pions, kaons, etc.). An example is provided by the Japanese facility that is currently under construction. The planning and design of such a facility requires a careful analysis of the scientific goals, user communities, operating modes, timescales and costs. Some of these considerations were examined at a workshop organised by the OECD Global Science Forum, and are described in the report from that event (http://www.oecd.org/pdf/M00004000/M00004528.pdf).

From a policy perspective, the design and upgrading of facilities must take into account the requirements of researchers. For any given experimental project, the relative merits and disadvantages of continuous beams, short (microseconds) and long (milliseconds) pulses must be weighed. Thus, for example the proposed new European project ESS is based on an optimised two-target design, one of which will exploit the advantages of long pulses. As with synchrotron radiation sources, the cost of neutron beamlines and instruments has increased significantly over the years, primarily because of increased capability. The average cost of a modern instrumented beamline is approaching ten million dollars. As in the case of synchrotrons, facility administrators must be responsive to the requirements of non-expert external users, and must anticipate the need to constantly maintain and upgrade their beamlines and instruments.
An important difference between neutron sources and synchrotron sources is that potential users of synchrotrons have the option of performing some of their work (for, instance, preparatory phases of experiments, or calibrations) using relatively small and inexpensive laboratory-based sources (for example, rotating anode X-ray sources). Neutrons, on the other hand, are only available at medium- and large-scale facilities. For this reason, policymakers should acknowledge the importance of regional or national reactor sources, at which local research programs can flourish, innovative experiments and methodologies can be developed, students and other users can develop their skills, thus maximising the effectiveness of projects performed at very large facilities.

The findings and recommendations of the Megascience Forum’s Working Group on Neutron Sources continue to be valid. Indeed, the United States is currently building a 2 megawatt source at a cost of $1.4 billion, which will be completed in 2006 at the Oak Ridge National Laboratory. In Japan, JAERI and KEK are jointly building a multi-purpose facility at Tokai that will incorporate a high-intensity (1 megawatt, upgradable to 5 megawatts) proton accelerator. The facility will include a spallation neutron source and a muon source, and will be completed by 2007. Thus, the focus of attention has shifted to Europe, where a decision will have to be made about the proposed 10 megawatt facility, the European Spallation Source. In a lower power range, a UK decision on a second target station for the existing ISIS source is imminent, and Austria is looking for a decision on the 500 kilowatt AUSTRON facility. The European projects will benefit from the experience currently being accumulated in the United States and Japan.

### Transmission electron microscopes and nuclear magnetic resonance spectrometers

The transmission electron microscope (TEM) remains a vital tool for microstructural characterisation of both thin film and bulk materials because its images are not limited to the surface of a sample. Resolution at the sub-atomic scale has increased in the last decade, and further improvements are expected from aberration-correction techniques and an increased electron energy beyond 1 MeV. Another important development is the ability to extract reliable quantitative information from the images combined with improvements in the efficiency and resolution in spectroscopy using TEM. Hence it can be expected that even non-experts will use TEM as a quantitative structure analysis tool in the not too distant future.

Nuclear magnetic resonance (NMR) has a wide range of applicability, from materials studies to the life sciences. NMR can provide insight into molecular motions on time scales ranging from picoseconds to seconds, including chemical reactions and other dynamic processes. It is also possible to measure transport phenomena such as diffusion and flow. NMR plays a key role for the study of solid materials such as polymers, glasses, ceramics, catalysts, molecular sieves, gels, etc. Phase changes such as fusion, solidification and glassification can be studied in detail. At very high fields, quadrupolar nuclei such as aluminium-27 offer an attractive means to characterise a wide range of materials. The performance of NMR spectrometers is continually increasing and is the subject of vigorous industrial competition. At present, intense efforts are under way to develop machines that can consistently reach operating magnetic fields equivalent to a 1 gigahertz resonance frequency.

Recently developed NMR methodology has extended the range of masses of the examined molecules to proteins, nucleic acids, and supramolecular assemblies. The NMR technique is effective for molecules in solution or in disorder solids, and does not require crystallisation of the samples. Biomolecular NMR entails extensive labelling with isotopes such as nitrogen-15, carbon-13 and, for large systems, deuterium.

Most electron microscopes and NMR spectrometers are not based at large facilities, but the cost of the most high-performance instruments is in the $10 million range. The most sophisticated models need special buildings to isolate them from vibrations and other external disturbances. These instruments require a high level of sophistication in their operation, and the needed investment is often too large for a single group of investigators. They can be operated for external users very much like the instruments at the large-scale facilities. Often they are not operated in a formal user mode, but in an informal collaborative mode. In some cases, centres have been established with a large number of different kinds of electron microscopes or NMR instruments. These centres provide specialised support for users, very much like the large-scale neutron or photon facilities.

### High-intensity lasers

Beginning in the early 1960s, lasers have found innumerable applications, based on the exploitation of Einstein's fundamental discovery of the "stimulated emission" of light. Scientists and engineers have been able to fully control the coherence properties of light, leading to an unprecedented ability to produce intense, collimated, monochromatic, short-duration, and coherent beams of photons. From the beginning, researchers have sought to increase the power of lasers since, invariably, each advance has led to useful applications. In 1985, an ingenious technique, dubbed "chirped pulse amplification" (CPA) was invented, which enabled ultra high-power, short-pulse lasers to be introduced. These lasers now reach peak power levels in the petawatt range, i.e. twelve orders of magnitude higher than the first pulsed lasers. Moreover, because the light pulses are very short and are emitted at modest repetition rates, the average power levels of CPA lasers are low, presently ranging up to tens of watts even for the systems with highest peak powers. Consequently, the devices can be relatively small and inexpensive.

In general, very short pulses, ultra-high electromagnetic fields and progress towards soft X-rays are opening up interesting new niches for table-top lasers. When a field of science surges forward in this manner, new challenges and opportunities are created for policymakers as well as for scientists. A recent workshop organised by the OECD Global Science Forum has documented the many applications in atomic and molecular physics, biology, neutron science, nuclear and high-energy physics, fusion energy research, high-field science, non-medical imaging, medical applications and environmental science (http://www.oecd.org/pdf/M00019000/M00019936.pdf). Recent advancement of high-power femtosecond laser technology could enable a new generation of photon sources": coherent ultrashort VUV/X-ray radiation (such as high-order harmonics and X-ray lasers) and incoherent ultrashort VUV/X-ray radiation (from laser-produced plasmas or from high-power laser-driven inner-shell transitions). These light sources are potentially very valuable for such research areas as molecular imaging, gas-phase chemical reactions, solid-state physics, and dynamic structural analysis of biological materials.

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## Appendix 2: Participants at the Workshop on Large Facilities for Studying the Structure and Dynamics of Matter

| | | |
|---|---|---|
| Chairman | Prof. Arthur Bienenstock | |
| Australia | Prof. Lawrence Cram | |
| Austria | Prof. Dipl. Ing. Dr. Gerald Badurek | Dr. Wolfgang Reiter |
| Canada | Dr. John Root | Dr. Rob Slinger |
| Czech Republic | Dr. Jana Bystricka | Ms. Marie Rohlickova |
| Denmark | Dr. Kurt Norgaard Clausen | Dr. Roger Garrett |
| | Dr. John Renner Hansen | Dr. Jørgen Kjems |
| | Mr. Hugo von Linstow | |
| EC | Dr. Christopher Lowry | |
| ESF | Dr. Hans Karow | |
| France | Dr. Robert Comès | Dr. Bernard Frois |
| | Dr. Danièle Hulin | Dr. Jean-Claude Thierry |
| Germany | Prof. W. Eberhardt | Prof. A. Haase |
| | Dr. Lucia Incoccia-Hermes | Prof. Dr. Eberhard Jaeschke |
| | Prof. Werner Press | Prof. Wolfgang Sandner |
| | Prof. Jochen Schneider | Prof. Eberhard Umbach |
| | Dr. Hermann-Friedrich Wagner | Prof. Dr. Dieter Richter |
| | Prof. Richard Wagner | |
| Invited Experts | Dr. Peter Tindemans | Prof. Carl-Ivar Brandén |
| Italy | Dr. Massimo Altarelli | Dr. Paolo Perfetti |
| | Dr. Carlo Rizzuto | |
| IUPAC | Prof. Tony Ledwith | |
| IUPAP | Dr. Hiroshi Yasuoka | |
| Japan | Prof. Yasuhiko Fujii | Dr. Yukio Morii |
| | Dr. Shigeyuki Yokoyama | |
| Korea | Dr. Jungil Lee | Prof. Ki-Bong Lee |
| | Prof. Je-Geun Park | |
| Netherlands | Dr. Hendrik van Vuren | |
| Norway | Prof. Aurora Martinez | |
| OECD | Dr. Stefan Michalowski | Mr. Kenji Sudo |
| South Africa | Dr. Hardus Greyling | |
| Spain | Dr. Jose L. Martinez | |
| Sweden | Prof. Lars Börjesson | Dr. Gunner Leman |
| Switzerland | Dr. Heinrich Neukomm | Prof. Hans Rudolf Ott |
| | Dr. Paul-Erich Zinsli | |
| United Kingdom | Prof. John Helliwell | Dr. George Stirling |
| | Prof. John Wood | |
| United States | Dr. Thom Mason | Dr. Iran Thomas |
| | Dr. Thomas A. Weber | |
| Scientific Secretary | Prof. Peter Hansen | |
| Secretary | Ms. Birgitte Høyer | |

## Appendix 3: Agenda of the Workshop on Large Facilities for Studying the Structure and Dynamics of Matter

Thursday, September 20

### Session 1: Introduction

| | |
|---|---|
| 1 | Welcome on behalf of Denmark. *Jørgen Kjems* |
| 2 | Welcome on behalf of the United Kingdom. *George Stirling* |
| 3 | Welcome on behalf of the OECD. *Stefan Michalowski* |
| 4 | Introduction: history and purpose of the workshop.<br>Presentation and adoption of the Agenda. *Arthur Bienenstock* |

### Session 2: Scientific Prospects and Needs

| | |
|---|---|
| 5 | "Hard" condensed matter. *Massimo Altarelli* |
| 6 | "Soft" condensed matter. *Dieter Richter* |
| 7 | Biological materials. *Carl-Ivar Brandén* |

### Session 3: Facility-Based Probes for Studying Matter

| | |
|---|---|
| 8 | X-ray sources. *Jochen Schneider* |
| 9 | Neutron sources. *Thom Mason* |
| 10 | Neutron sources II. *Yasuhiko Fujii* |
| 11 | High-power lasers. *Danièle Hulin* |
| 12 | NMR spectrometers. *Shigeyuki Yokoyama* |
| 13 | Electrons. |

Friday, September 21

### Session 4: Discussion and Conclusions

| | |
|---|---|
| 14 | Scientific community perspectives: IUPAP *Hiroshi Yasuoka* |
| 15 | Scientific community perspectives: IUPAC *Tony Ledwith* |
| 16 | National, regional, and laboratory perspectives. |
| 17 | General discussion. Conclusions. |