Five-Year Scientific Vision for the Advanced Photon Source

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The Advanced Photon Source (APS) in 2005 is beginning its eleventh year since producing first light, and has seen its user base grow to nearly 3,000 individual scientists per year. Today, the APS has 46 instrumented beamlines occupying 30 sectors. Nonetheless, there remain four uncommitted sectors, opportunities to optimize existing insertion device beamlines or expand others with canted undulators, and over a dozen undeveloped bending magnet beamlines. Furthermore, the highest priority identified for the facility by the most recent University of Chicago Review Committee was the evolution of a greater number of dedicated, and fewer multipurpose, beamlines.

For these reasons, the APS and its Scientific Advisory Committee have developed plans that address priorities for new or improved beamlines over the next 5 to 10 years. To make choices that will have the most positive scientific impact, we have engaged the wider community in developing our plans. We recognize that powerful new instrumentation is needed, but that, in many cases, outreach to new user communities can be just as important. We commissioned a broad study on "Future Scientific Directions for the Advanced Photon Source," which looked at the scientific opportunities where synchrotron radiation could play new roles, and we connected these with instrumentation and community needs. The study chairs, Gopal Shenoy, of the APS, and Professor Sunil Sinha, of the University of California, San Diego, made use of extensive community input in organizing a series of nine workshops that were held in 2004 (see page 8). Each workshop focused on a compelling scientific area and brought together synchrotron experts with scientists who had not previously used synchrotron radiation. Every workshop provided an executive summary and aims to publish a full report in a scientific journal.

Following the conclusion of the workshops, that in total involved over 300 scientists, a summary strategic planning meeting was held at which the workshop highlights and other relevant input were presented and discussed with a broadly representative audience. This document is based on that summary meeting. It briefly summarizes the scientific opportunities in the fields identified through the study and categorizes the major needs for instrumentation and community activities to maximize APS scientific impact in the next decade. Our scientific vision, and its follow up, serves as a blueprint for the development of new instrumentation, including entire beamlines, and for APS management decisions on staffing, accelerator operations, and improvements. It also puts flesh on Phases I and II of the APS 20-year plan submitted to the Department of Energy in 2003 (http://www.aps.anl.gov/aps/downloads/20030223-roadmap.pdf). If the vision for new instrumentation and community support in this document is fulfilled, we have every confidence that the scientific impact of the APS will grow dramatically in the next decade.

This vision for the next five years at the APS has been reviewed by the APS Scientific Advisory Committee. Input was also sought from the two representative user bodies at the APS—the APS User Organization Steering Committee and the APS Partner User Council. Of course, this is not intended to be an all-encompassing, detailed plan. Instead, it identifies a menu of persuasive opportunities at the time of writing. As in the past, new beamline construction at the APS is expected to involve external partnerships and will remain proposal-driven. This document will provide a context in which existing and future proposals can be reviewed, and it is expected to stimulate successful proposals.

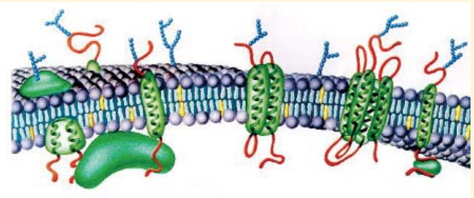
Because this is an executive summary, further details will be made available elsewhere. There are three sections here: a summary of fields in which new impacts from synchrotron radiation science are anticipated, a high-priority list of necessary major beamline-scale instrumentation, and a discussion of areas and approaches to build new APS user communities. Where major new instrumentation needs are identified, the APS has appointed technical liaisons for each instrument, who will co-ordinate the technical aspects of instrument design with internal and external teams, as appropriate. In recent beamline construction projects, partners (in the form of collaborative development teams) are involved in initial development and commissioning through close collaboration with the APS. During operation, the APS expects to take primary responsibility for beamlines in the physical sciences and operate them for open access through the general user and partner user programs.

New Scientific Opportunities for Synchrotron Radiation

Across the wide spectrum of scientific areas covered by the workshops, several general themes emerged. The need for simultaneous characterization with high spatial and temporal resolution was appreciated in diverse fields—from biology to condensed-matter physics. This frontier challenges the limits of third-generation sources, and exciting development opportunities will be built-upon by the next generation of ultra-fast ultra-brilliant x-ray laser sources. Second, in many fields, the unique capabilities of hard x-rays to perform *in situ* studies of materials in real environments will become increasingly important. Last, but by no means least, it is apparent that close juxtaposition, if not integration, of complementary tools is invaluable. For example juxtaposition of tools and expertise for electron, optical, and x-ray microscopy, or x-ray and neutron scattering, offers the

Membrane Science

Membrane technology has advanced the state of the art in water treatment and purification; in the electronics, semiconductor, chemical, petrochemical, and pharmaceutical industries; and in environmental applications, such as low-cost control of carbon dioxide absorption to combat greenhouses gases. New research opportunities include medical and biological processes (such as the hemo-dialysis used in artificial kidneys); essential components for fuel-cell and hydrogen-energy economy and technology; and separation of proteins in the food, beverage, pharmaceutical, and biotech industries. Biomembrane science takes this field back to its source: a better understanding of cell membranes themselves. These complex, heterogeneous systems are highly adaptable and are critical to a wide range of biological processes, including ion transport and signal transduction. The evolution of a wide range of synchrotron-radiation-based techniques is proving to be essential to gaining molecular-level structural information about membranes, membrane interfaces, and interacting supramolecules. Moreover, applying these varied techniques to real-time studies can provide information on the time evolution and molecular interactions in membranes. *(Image: A natural membrane. Courtesy of Garrett & Grisham)*



most compelling resource for users. Co-location of tools for materials synthesis and processing, such as in the new Center for Nanoscale Materials at Argonne, is an excellent example. This integration of capabilities should also extend to theory and modeling.

The pulsed structure of synchrotron x-ray sources offers access to **Time Domain Science** down to the tens-of-picosecond (ps) scale. Future x-ray lasers promise three orders of magnitude improvement. Stimulating scientific opportunities are found in atomic and molecular physics, chemistry, biology, and condensed matter physics—from the study of chemical reactions and excited states to the transport of carriers in semiconductors. This group of scientists can take much greater advantage of existing sources such as the APS and grow a community that will use x-ray lasers in a decade or more. There is great interest in pushing the capabilities from the current time structure of the APS toward shorter time scales, and in better utilizing experiments from the current limits up to much longer time scales. A novel approach to generating 1-ps pulses is under serious consideration within the APS. Developments in choppers and detectors are also very important to maximum utilization of the time structure of the beam.

Whereas high-energy machines like the APS are often associated with hard x-rays, the performance of the machine promises new **Frontier Science Using Soft X-rays**. At 0.5–3 kV x-ray energy, the APS ring (with a suitable undulator) can produce exceptionally brilliant beams that are very stable and can be controllably polarized. There are several exciting areas of science that this capability can impact, including nanomagnetism. Soft x-ray imaging was identified, in the APS 2003 cross-cut review of microbeam science, as an important frontier. A unique and interesting opportunity involves the use of angle-resolved photoemission spectroscopy (ARPES) and related spectroscopies at these energies. Such experiments would provide access to the momentum-resolved electronic structure that ARPES gives so well, while at the same time being less surface-sensitive. Applications include understanding electronic transport in exotic conductors and untangling the role of magnetic and charge transport in materials.

There are abundant **Emerging Scientific Opportunities Using X-ray Imaging** in fields including geology, paleontology, biology, engineering materials, and complex systems. In fact, the interest from new user communities in full-field x-ray imaging is probably the widest of any x-ray technique. The ability to study structure in materials on scales from nanometers to centimeters is very powerful. For example, it can be applied to understanding materials failure by crack propagation, to real-time imaging of physiological processes in insects and small animals, to understanding gene expression in plants, and to the study of micro-fossils to find clues to the origins of the earliest life in the solar system.

The excitement of producing new **Mesoscopic and Nanoscopic Materials** that are not found in nature, and that have unique properties, has driven the burgeoning field of nanoscience in the last decade. Such properties include improved catalysis through tailored nanoparticle surfaces, better information storage and computation, and self-organized structures for better drug encapsulation and delivery. Many of these materials are complex and hierarchical. Key frontiers to enable progress include the understanding and control of self-assembly, where x-ray techniques, especially, *in situ*, will play a major role. It is also becoming clear, in nanoscale systems, that knowledge not only of structure, but of dynamics, will be key, and so x-ray spectroscopy will be important.

The goal of research in **Nanomagnetism** is to build, from nanoscale building blocks, complex integrated systems with new functionalities. It is clear that the ability to characterize both the magnetic structure and the dynamics of individual and assembled nanostructures will enable progress, and that synchrotron radiation will offer important capabilities. Frontier science will juxtapose high spatial resolution (the ~5-nm scale of the exchange interaction) and ultrafast studies (the ~1-ps time scale of spin-orbit coupling and other intrinsic magnetic phenomena) to revolutionize our understanding of nanoscale magnetism. Areas of impact include magnetoresistive memory, spintronics, and tailored magnetic materials for energy applications.

Measurement of short- and medium-range atomic structure in nanomaterials is one powerful application of **High-Energy X-rays**, which provide a unique tool to study real materials in realistic conditions. The penetrating power rivals that of neutron sources, but adds a finer microfocusing capability for inhomogeneous materials and the higher Q-space range needed for disordered materials. Revolutions in the micromechanics of materials and improved disordered and nanophase materials can all be anticipated from increased synchrotron research with high-energy x-rays.

Membrane Science is a truly interdisciplinary emerging field, at the interfaces amongst chemistry, materials, physics, molecular biology, and medicine. There is synergy to be exploited between inorganic membranes—of importance for chemical separation such as hydrogen fuel—and organic membranes, including the vital cell wall. Techniques of particular value include small-angle x-ray scattering, reflectometry, and photon correlation spectroscopy. The major technical challenges are extending experiments to the time domain and enabling specialized *in situ* experiments.

Synchrotron radiation has had a stunning impact on **Biological Crystallography** in the last 20 years, to the extent that most structures are now solved on synchrotron sources. In particular, the tunability and intensity of insertion devices has permitted the development of anomalous dispersion techniques for structure solution. Given the great importance of this field to human health and biology, it is imperative that facilities such as the APS remain at the forefront, anticipating the scientific needs of the community. The scientific impact from expected developments will involve understanding molecular machines, the critical role played by membranes, and the dynamics of proteins. In all these areas, x-ray techniques will play a role, but it is increasingly apparent that integration of x-ray techniques with other methods (e.g., electron cryomicroscopy) will also be essential.

Environmental Science presents multidisciplinary challenges in complex systems that have tremendous societal importance. Synchrotron radiation is playing a large and growing role, especially through its ability to characterize on the molecular scale with high spatial resolution, for example to elucidate bioremediation in soils. Challenges include understanding and controlling the transport of contaminants in the ground, developing approaches to environmental remediation based on understanding at the molecular level, and ensuring the stability of environmental repositories.

New, Large-Scale Instrumentation Priorities

In almost all of the workshops, it was evident that the evolution of dedicated and well-supported beamlines is of paramount importance at the APS. Nonetheless, many science areas, such as nanosciences, will not rely on just a single x-ray technique, but will need access to many. Better technique-dedicated facilities are the most effective solution, except where a technique will be almost exclusively used by one community, in which case the advantage of staff and ancillary infrastructure specific to the science will be highly desirable.

The following prioritized list contains compelling new instrument capabilities, all of which are needed in the near term to realize the scientific promise of the APS. More details about each instrument can be found in the workshop reports and through the appropriate APS technical liaisons (page 6).

• ***Shorter Pulse Capabilities from the Storage Ring***

As a result of stimulating discussions at the time domain science workshop, the APS has investigated a scheme (due to Zholents et al.) for the creation of picosecond pulses by a transverse radio frequency kick and x-ray crystal optics compression. The initial study was just completed, and the results indicate that this is feasible. The capability can be applied to one or two sectors without disturbing the storage ring, and offers extremely exciting and unique possibilities to extend the capabilities for time-domain science by two orders of magnitude. This would be associated with dedicating either one or two adjacent sectors to ultrafast time-domain science and parallel efforts elsewhere to support such science at longer time scales.

• ***Long Beamline for Full-Field Imaging***

Phase-contrast imaging and tomography require coherent beams with large illuminated fields of view. At present, this is best achieved with a very long (~200 meters) beamline free of focusing optics. Options still remain at APS to construct a new beamline, or modify an existing beamline, for these purposes, and it is strongly believed that we need such a dedicated facility to foster the tremendous needs of the imaging community.

• ***Bio-Nanoprobe***

This tool is focused on the study of metals in cells, which is very important to biology and medicine. There is a large community of users who could take advantage of the unique and complementary aspects of x-ray spectromicroscopy. The APS could serve this community with a dedicated beamline offering high spatial resolution and spectroscopic sensitivity. This oppor-

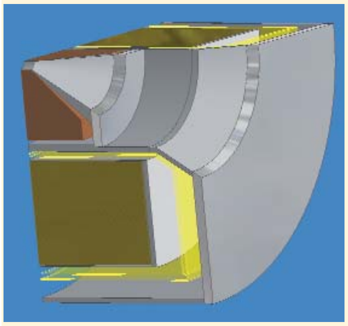
Environmental Science

The largest poisoning in history is believed to have occurred due to natural arsenic (As) contamination of the wells in Bangladesh. These deep wells, sunk in the 1970s, were introduced to avoid surface cholera contamination. Controversy still brews as to the origin of the arsenic contamination, but recent micro-x-ray absorption spectroscopy studies carried out at the APS suggest that cyclic changes in mineral hosts of arsenic are the culprits. Depth profiles of As concentration and oxidation state suggest As bearing sulfides account for a majority of arsenic at well depth and that arsenic is being liberated from this source during natural seasonal redox cycles.

This study is only one example of the growing role to be played by synchrotrons in advancing environmental science. *(Photo: http://asp.grameen.com/annualreport/2001/arsenic.htm)*

Science with a High-Field Magnet

In the study of matter, going to extremes is often the path to startling and useful discoveries. Just as extremes in pressure and temperature have provided fruitful experimental environments, the use of high-field magnets to study the properties of matter remains a frontier. High magnetic fields interact with charge and spin in materials but, until now, any structural effects of the highest fields could not be measured with synchrotron radiation. The National High Field Magnet Laboratory, at the University of Florida, and the APS are proposing construction of the largest high-field magnet beamline facility in the world, to be located at the APS. To achieve the desired steady fields of up to 35 T, the magnet would marry resistive and superconducting technology to produce a hybrid "magnet within a magnet" that has demonstrated the world's highest fields to date. *(Image: Proposed "down-bore" magnet for APS beamline. Courtesy G. Boebinger, National High Field Magnet Laboratory)*



tunity emerged from a number of workshops held at the APS in recent years. The large demand justifies a dedicated facility and the advantage would be an expert staff to interact with novice users and a close connection with related facilities such as those for optical and electron cryomicroscopy. It is expected that the user base at the APS will sustain several nanoprobe instruments such as this. The nanoprobe, for the Center for Nanoscale Materials (under construction at sector 26), will focus on nanoscience in non-biological, or biologically inspired materials. The bio-nanoprobe would focus on biology itself. A third instrument for environmental sciences, for which the resolution demands are often less severe, could likely be accommodated at an existing or improved beamline.

• ***Dedicated Microfocusing Station for Structural Biology***

There is an important subset of structural biology problems which need a small-crystal (<10 μm) capability, where no such dedicated capability exists today at the APS. It makes sense that one of the structural biology sectors at the APS should offer such a dedicated capability. It is not anticipated that a new sector need be constructed. Other innovations in structural biology can be accommodated at existing sectors.

• ***High-Magnetic-Field Facility at the APS***

High magnetic fields offer a unique probe to understand, and ultimately control, the transport properties of materials. A recent National Research Council report emphasizes the need for *in situ* x-ray scattering tools at high magnetic fields. This could be accommodated at a new dedicated scattering sector for magnetism. We propose that one beamline should have a high-DC magnetic field capability (at least 20 T), with both horizontal and vertical field geometries, which would be unique in the world. Collaboration with the National High Magnetic Field Laboratory, and related plans to establish facilities at neutron sources, are being explored.

• ***Dedicated High-Energy X-ray Capabilities***

Particularly, there is a need for a high-energy undulator line dedicated to applications requiring high brilliance, especially microfocusing. In addition, dedicated beamlines with high flux will be needed for pair-distribution-function and other work (e.g., in solution). The latter could likely be accommodated by restructuring existing beamlines.

• ***Improved Soft X-ray Capabilities***

A dedicated soft x-ray beamline in the approximate energy range of 0.5–3 kV should be produced with a specially designed undulator to allow ARPES and related spectroscopies with sub-surface sensitivities. The brilliance from a specially designed source, combined with the stability and polarizibility of the beam, would lead to a unique capability for those experiments requiring illumination of small volumes. Additional soft x-ray capabilities for imaging, scattering, and magnetism should also be provided.

• ***Inelastic X-ray Scattering***

The Phase I design of the Inelastic X-ray Scattering beamline (APS sector 30) involves the co-existence of medium-energy-resolution (MERIX) and high-energy-resolution (HERIX) capabilities at one sector. Whilst we have investigated options for increasing the length of the straight section to accommodate more and longer insertion devices, it seems clear that a sector dedicated to HERIX and a sector dedicated to MERIX should be Phase II of this plan. The best choice would be to accommodate dedicated HERIX capabilities at sector 30, and to establish another insertion device sector with a dedicated MERIX beamline. The latter might be accommodated without constructing a completely new sector. Because of the brilliance needs of both techniques, the MERIX sector requires a longer straight section with multiple permanent magnet undulators, and the HERIX sector a dedicated superconducting undulator (now under design).

• ***Improved Detectors***

Optimized detector systems will be critical to fully realize the expected increase in productivity from dedicated beamlines and specialized insertion devices. We recognize that a sustained effort in detector development could have the most scientific leverage, and we aim to be aggressive in securing advanced detectors for our users. We will be preparing detailed plans in the near future for detector development in areas such as avalanche-photodiodes and pixel-array detectors. We will work in close collaboration with other facilities in the U.S. and abroad.

Note that this list neglects important capabilities already existing or under construction at the APS. For example, a need expressed by the materials science and structural biology communities for powder studies will be accommodated by the dedicated bending magnet powder diffraction beamline under construction at sector 11. Also, this list does not include many techniques that are very important yet do not yet exist in dedicated form at the APS, such as small-angle x-ray scattering, because we believe that such dedicated facilities will emerge from reorganizing our internal X-ray Operations and Research (XOR) beamlines. A strategic plan for the development of XOR sectors has recently been prepared.

While the list above focuses on large-scale instrumentation, there is strong support from the existing and potential user community for broader instrumentation development. This includes improving the x-ray source, which is a high priority for the APS, and x-ray optics and end station instrumentation, where responsibilities are shared with partner users.

Intrinsic to the success of all these plans is the need for the APS to develop insertion devices optimized for each of our dedicated beamline capabilities. For example, superconducting undulators are being developed for high-energy and inelastic scattering. Development of such devices represents Phase II of our 20-year strategic plan and goes hand-in-hand with creating dedicated beamlines which is the principal aspect of Phase I.

Outreach to New Scientific Communities

In this section, we discuss some important issues, which emerged from the workshops, related to nurturing and building new user communities. As a general observation, it is well-recognized that APS scientific staff or resident partner users, who are expert in the fields of the user, are best suited to maximizing the scientific impact of user research. Such resident scientists provide expert assistance and they reach out to the relevant scientific communities. Not only is this best for the users and the facility, but it is also very effective for career development of beamline research staff. Given the balance of time available for user support versus personal research, it is highly effective for a beamline scientist to collaborate with outsiders and to specialize in a particular field, at least for a period of time. Whilst the APS staff will strive to provide more expertise, the partner user program offers a vehicle to leverage this expertise by bringing in expert users who may choose to reside for extensive periods at the facility. In almost all the areas covered by the workshops, the need for this expertise is established, but particular needs stand out: in environmental molecular science, biology, imaging science, and membrane science. In addition, industrial partner users offer an important conduit from industry to general users and strengthen the coupling of science and technology.

Critical to the success of all our beamlines is adequate staffing; we are committed to using our resources in the best way possible to foster productive and well-supported beamlines.

A powerful method for preserving scientific specialization, as beamlines become optimized by technique, is the use of *virtual portals*. In this concept, a group (typically partner users) acts as a conduit for all experiments into a number of APS beamlines and provides the high-level scientific expertise and advice that is most effective. Although this model has not yet been tested, we are anxious to begin exploring it. An example could be in structural biology, where access to specialized beamlines—for systems under extreme conditions, for powder diffraction, and for small-angle scattering, to name a few workshop priorities—could be coordinated by an existing resource in cooperation with the APS and other partners.

Another vehicle recommended during several workshops was the establishment of advisory panels in strategic scientific areas to help guide the APS as programs and capabilities evolve.

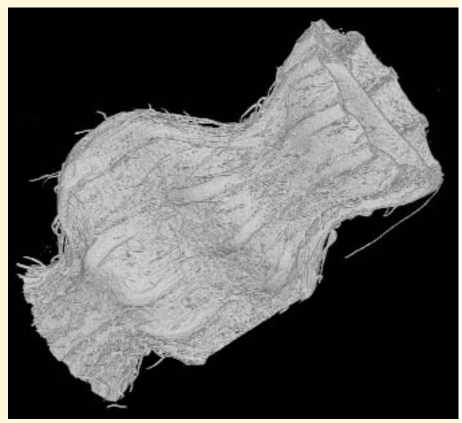
Joint appointments between the APS and other Argonne divisions, universities, and other institutions offer a special kind of partnership that can be very effective.

The need to facilitate *in situ* experiments, which may take a longer time than typical experiments and may often be effective in partnership, is clear in many areas. These experiments can be fostered through dedicated end stations. Frontiers of *in situ* experiments include time-resolved measurements at high spatial resolution.

As we bring in new communities of scientists requiring synchrotron methods, but with little synchrotron research experience, we recognize that they will need consistent help with the

X-ray Imaging for the Life Sciences

Many objects, from seeds (picture) to cracked concrete, exhibit complex hierarchical internal structures that cannot be properly preserved or studied by sectioning, and are thus not amenable to study with conventional microscopes. Many objects share a low density matrix and a low absorption cross section for x-rays. For such objects, x-ray phase-enhanced imaging is uniquely able to reveal complex internal structures on the submicron level in macroscopic objects without sectioning. A dedicated long-imaging beamline is necessary for sufficient coherence and field-of-view to study problems in food science, genetics, engineering materials, biology and a wide range of other subjects.



(Image: A mustard fruit rendered in three dimensions from tomographic data.. Diameter of the fruit is about 3 mm, length of image is 6 mm. Image taken at the European Synchrotron Radiation Facility, courtesy of W.-K. Lee [ANL] and K. Donohue [Harvard U.])

acquisition and processing of their data. This means that we will have to raise the level of APS staff support in terms of guiding researchers in synchrotron x-ray techniques, and increase the quantity and accessibility of robust data reduction and analysis packages. This implies a substantially higher level of APS involvement in data handling, but we see it as key to the realization of the promise in emerging areas of science.

Many enabling research areas that do not explicitly involve new instrumentation also became clear as priorities. One example is fundamental studies on radiation damage, both to understand the consequences of this limiting issue in biological crystallography and soft materials and possibly to use knowledge of the nature of damage for better structural insight. Details can be found in the workshop reports and summaries.

A Last Word

Strategic planning is essential, and for a national user facility, current and potential users must be fully engaged. We are delighted at the outcome of our series of vibrant planning workshops held in 2004. That outcome is embodied in this vision. The new directions identified here will undoubtedly pay off in high scientific impact, and we are committed to aggressively pursuing these opportunities with the help of our user community. Our plans for new scientific directions complement our equally strong commitment to improve the machine performance and productivity for our existing users.

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Future Scientific Directions for the Advanced Photon Source: *Workshop Summaries & Recommendations*

Introduction

Devising a menu of new possibilities for the APS experimental program defies the conventional wisdom about too many cooks. Workshops that brought together an abundance of experts from a wide range of scientific disciplines to consider "Future Scientific Directions for the Advanced Photon Source" have produced a bounty of ideas for expanding the already robust research at this national user facility.

The workshops, which were held in May, July, August, and September 2004, were organized and chaired by Gopal Shenoy (ANL-XFD) and Sunil Sinha (U. of C., San Diego). They brought APS users and personnel into contact with leaders from the broad scientific community who are both experts in their fields and newcomers to the use of x-ray techniques. The workshops had as a primary goal "the expansion of both the scientific leadership of APS users and the boundaries of science's frontiers in the next decade" by identifying new opportunities for scientific discovery and impact using synchrotron radiation sources during the next 5 to 10 years and seeking ways of bringing new scientific communities to the use of synchrotron x-ray beams. Speakers at the workshops also dealt with the (literally) nuts-and-bolts questions of new instrumentation and operational requirements needed for these programs. Also considered were evaluations of existing APS beamline capabilities in terms of the future beamline capabilities that would be needed for new programs.

A sampling of the topics presented at the workshops includes: a new source of x-ray beams that deliver pulses of light on the picosecond time scale; using x-rays to capture the detailed mechanisms of molecular functions as they occur; a wide range of new (or newly combined) synchrotron x-ray techniques to provide unprecedented insights about materials structures on the atomic scale; and the behavior of a wide range of biological functions on the molecular scale. Strategies for fabrication, characterization, and understanding of nanoscale materials, emphasizing new functionalities; and a beamline dedicated to the use of a 40-MW super magnet to be used for the study of materials under extreme magnetic forces were also discussed.

The conclusions of each workshop are summarized as follows:

1) Emerging areas of biological crystallography will address the essence of living systems through the measurement of structural dynamics at the molecular level and the responsible chemical forces.
2) High-energy x-ray tools will focus on understanding the relationships between the structure and the properties of materials over several hierarchical length scales ranging from the atomic to the nanoscopic to the mesoscopic scale.
3) The emerging research topics in membrane science are truly interdisciplinary and represent the interfaces among materials chemistry, physics, molecular biology, and medicine. They will have the broadest industrial impact in areas ranging from gas-phase separation to the hydrogen economy to drug delivery.
4) Basic understanding of environmental materials and processes at the molecular scale will be provided by x-ray techniques. This knowledge is essential for risk assessment and management and for reduction of environmental pollutants at field, landscape, and global scales.
5) X-ray phase analysis lends itself to numerous emerging opportunities in x-ray imaging with ultra-high spatial resolution. The impact of both 2-D and 3-D x-ray imaging on many areas such as medical diagnostics, new materials discovery, paleontology, etc., is huge.
6) It is of paramount importance to understand the magnetic behavior of individual nanomagnetic building blocks, which are combined into more complex structures leading to the development of spintronics devices with new functionalities. The spin-sensitive x-rays techniques will have a major impact on the field of confined magnetism.
7) Rearrangement of atoms or electronic states or protein structures in response to various external stimuli takes place over 15 orders in time domain. The time-resolved x-ray techniques utilized at storage rings can be the most powerful probes of this important science, which has broad applications in astrophysics, atomic physics, chemical physics, materials science, and biology.
8) Understanding the behavior of confined matter when the length scales range from the mesoscopic to the nanoscopic has attracted recent attention because of the potential nanotechnology applications. The x-ray methods that offer atomic resolution will provide considerable understanding of nanomaterials and processes that occur at the nanoscale.The summaries of the workshops were presented at the second APS Strategic Planning Meeting (SPM), held on September 2–3, 2004, and co-chaired by Shenoy and Gabrielle Long (ANL-XFD). The SPM served to summarize all of the workshops in the series, highlighting scientific opportunities identified during each of the workshops and, ultimately, leading to a plan for the APS that stretches out over the next 5 to 10 years and that will fall into two broad categories: new instrumentation and techniques that must be developed on existing APS beamlines, and new scientific user communities that must be nurtured.

Workshop and SPM slides can be accessed on the Web at http://www.future.aps.anl.gov/Future/future.htm. The study is documented through the following reports, which are based on the summaries from each of the workshops. Detailed reports from each workshop are in preparation for publication in several scientific journals.

Summary of the Workshop on Time-Domain Science Using X-ray Techniques

The goal of the workshop on "Time Domain Science Using X-ray Techniques" was to identify future directions in scientific research using time-resolved x-ray techniques and to address possibilities to produce picosecond (ps) x-ray pulses at the APS. The workshop brought together internationally-renowned leaders in atomic, molecular, and optical physics, chemistry and biology, and condensed matter physics, as well as accelerator physics. The participants presented the frontiers in their fields—not limited to x-ray techniques—so that, in addition to the interdisciplinary format, there was also a balance of existing and potential synchrotron users.

Time-domain research has been a mainstay for the APS. Researchers at the APS have contributed greatly to our understanding of structural changes on the ~100 ps and longer time scale and on the atomic length scale. The workshop examined current research occurring on these and shorter time scales, including examples in isolated atoms and molecules, chemical and biological systems, and condensed matter. In order to ensure that APS remains a leader in these fields, specific recommendations to facilitate and enhance experiments on time scales >100 ps were made and will be detailed at the end of this summary. However, by far the most exciting element of the workshop was exploring the possibility of shorter time scales at the APS, i.e., the generation of ps x-ray pulses while retaining high flux. This important time domain—from 1 ps to 100 ps—will provide a unique bridge for hard x-ray science between capabilities at current storage rings and future x-ray free-electron lasers (FELs). This unique potential has generated substantial interest and technical activities, both during and subsequent to the workshop, and we believe, is of primary strategic importance for future scientific directions for the APS. Such a development has the potential to turn the APS into a Mecca for time-resolved x-ray work!

Current time-domain work in atomic and molecular physics in the hard x-ray regime focuses on the understanding of strong-field effects on inner-shell processes and monitoring Coulomb explosion dynamics. Strong AC fields of >3 V/Å are generated with standard ultrafast lasers and will be present at $t = 0$ of all laser-initiated dynamics. An understanding of accompanying perturbations to absorption and emission spectra is important for the interpretation of optical pump/x-ray probe experiments, particularly those planned for next-generation light sources. Looking forward to the 1 ps era, many new classes of experiments emerge. Among the most exciting is the ability to monitor coherently controlled molecular processes. An example is field-free molecular alignment, in which an impulsive kick is used to transiently align molecular axes with respect to laser polarization axes. Because the alignment lasts only for ~3 ps, x-ray pulses of ~1 ps duration are required for probing. Aligned molecules under field-free conditions would be of substantial interest for the proposed single-molecule imaging with ultrafast x-rays, but the alignment process still requires study, which could be done with ps x-ray probes at the APS.

Advances in chemical and biological sciences depend upon the development of correlated time-resolved structural, kinetic, and functional analyses. X-ray techniques provide the most powerful means to resolve molecular structures at the atomic level. X-rays with high photon flux in each pulse enable the extension of molecular dynamics studies by sophisticated ultrafast laser spectroscopy to structural dynamics studies at similar time scales. Therefore, the size of the community of chemists and biologists focused on time-resolved structural studies is growing fast. Increasing needs for time scales ranging from <1 ps to >100 ps were identified. On the time scale of >100 ps currently provided by synchrotron x-ray pulses, targeted scientific developments were: a) extension of time-resolved macromolecular crystallography, scattering, and spectroscopy to a broader range of chemical and biological systems (such as light-sensitive or artificially engineered light-sensitive systems, temperature- or pressure-triggered processes, and fast chemical mixing initiated reactions); b) time-resolved structural studies of molecular electronic excited states and reaction intermediate structures; and c) structural intermediates in biological enzymatic/protein, chemical catalytical processes, nanomolecular machines, and supermolecules. On the time scale of <1 ps, many more chemical and biological processes can be followed—such as coherent structural movements from a Franck-Condon state through vibrational relaxation to thermally equilibrated excited states, atomic rearrangements in isomerization, bond breaking/making, electron transfer coupled atomic movements, transition structures in catalysis, and enzymatic reactions. Moreover, the control of chemical dynamics through diverse structures of molecular surroundings can be investigated.

Dynamical studies in condensed matter physics span a wide range of time scales, from subpicosecond to millisecond and longer, and broad fields of science, from phase transitions to photoluminescence to nonequilibrium processes. In the workshop, we heard many examples of cutting-edge research in all of these areas including nonequilibrium electron and phonon dynamics, shock compression, self-trapped excitons in molecular solids, and domain reversals, as well as nucleation, growth and phase separation. For long-time dynamics, coherence studies using photon correlation spectroscopy access a unique area of spatial and temporal (wave vector and frequency) phase space. Faster detectors are required to close the gap between systems that can be studied by using these techniques and those that can be examined by means of inelastic neutron and x-ray scattering. Ultrasmall means ultrafast. The dynamics of nanoscale devices such as ferroelectric switching occur on subnanosecond time scales. The time domain aspects of nuclear coherent scattering and spin dynamics, both of which have world-leading programs at the APS, were covered in other workshops in this series. On the fastest time scales, photoinduced phase transitions, and coherent excitations have been primarily studied by using optical techniques. A few pioneering x-ray experiments show that there are interesting dynamics that remain unresolved due to the relatively long x-ray pulse duration. An example is the photoinduced insulator-to-metal transition in V02 in which it is known, from optical studies, that the band gap is lost in a few hundred femtoseconds. Heroic x-ray diffraction experiments using both low-brilliance (but short-pulse) laser-produced plasma and slicing sources provide evidence that this transition is of an inverse Peierls-type distortion accompanied by a change in valence.

Recommendations

The workshop was an unqualified success: the participants were unanimous in their recommendations and excitement. The recommendations are critical components if the APS is to maintain a leadership role in the rapidly growing field of time-resolved x-ray science.

1) The APS must maintain the successful environment that both enables and enhances experiments on the ~100 ps and longer time scale;
2) The APS should pursue the development of high-flux picosecond beamlines through the use of advanced accelerator techniques. Such beamlines could produce 1 ps x-ray pulses and would be complementary to future x-ray free electron laser facilities.

The first goal can be best achieved by forming a time-domain advisory panel to interface with the APS on detailed issues such as providing maximum beam time for time-resolved research through a suitable choice of standard operating fill pattern with maximal single-bunch current; optimizing insertion devices, x-ray optics and end stations (including a soft- x-ray beamline) on dedicated time-resolved beamlines; and performing necessary R&D to develop advanced chopper designs and time-resolved detectors (fast readout two-dimensional detectors, streak cameras, avalanche photodiodes, etc.). It was also recommended that time-domain science be well represented at the APS users' meetings.

For the second goal, we realized that the development of a high-rep-rate, high-flux, short-pulse beamline would be complementary (and in many cases preferable) to x-ray FEL and energy recovery linac sources. This goal can only be achieved through a high priority R&D program in both the accelerator and optics areas for short-pulse generation. The participants of the workshop proposed to seize this unique opportunity to implement the short pulse scheme on presently unused sectors of the APS. Significantly shorter pulses will enable fundamentally new science, as discussed above, while providing a unique capability to the APS, and will minimally impact other sectors.

These recommendations were designed to effectively utilize unique intrinsic capabilities of the APS for frontier time-domain science; develop infrastructure/technology to make the tools for time-resolved science more broadly available; and expand the capacity of time-resolved experimentation at the APS. Finally, the present and future scientific users of the time-domain science who participated in the workshop are eager to be fully involved in the implementation and success of both of these recommendations.

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Summary of the Workshop on Frontier Science Using Soft X-rays at the APS

Introduction

A workshop was held to explore the question of what frontier science might be carried out with a high-resolution, small-spot soft-x-ray beamline at the APS. The workshop covered the following areas:

1) Angle-resolved photoemission;
2) Soft x-ray inelastic scattering;
3) Coherent x-ray diffractive imaging; and
4) Soft x-ray diffuse scattering and spectromicroscopy of biological samples.

All of these are emerging areas in the natural sciences that have in common the exploitation of the soft x-ray region of the electromagnetic spectrum (~400 to 3 keV). The APS can become the leading source in the world in this endeavor. There are several technical reasons that make the APS an ideal source for the proposed work: a long straight section (10 m) available for an insertion device; small emittance; a high ring energy that allows the entire spectral region to be covered in first order emission from the undulator for maximum intensity; and a long distance (greater than 80 m) available for the beamline, a pre-requisite for high-resolution performance of reflective optics used in this energy range.

The Science Case

1) Angle-resolved photoemission

Angle-resolved photoemission (ARPES) is a powerful technique for the study of electronic states in solids. It allows the determination of all the quantum numbers of the electrons, as well as the spectral function. The spectral function is the probability of adding or removing a particle from a many-body interacting system, and together with the quantum numbers, it provides the most complete information that can be obtained regarding the electronic states. The significance of this information rests on the fact that all the physical properties of a material, such as the conductivity, color, transparency, thermal conductivity, magnetism, heat capacity, etc., are given by the electronic states close to the Fermi energy, the highest occupied electronic states. This is in contrast to most other x-ray techniques, which provide structural information.

But in order to take full advantage of the information provided by ARPES, the experiments must be carried out at high energy resolution (of order of a few to 20 meV), because the relevant electronic excitations that determine these properties are affected by the temperature, also in the energy scale of meV (300K, ~25 meV). The biggest drawback of ARPES as it is currently applied is its surface sensitivity. Electrons scatter very strongly at low kinetic energies, and therefore if probed with low-energy photons, most only escape the material within a small depth of order 10 Å.

In early ARPES studies on relatively simple systems, the contribution of the surface to the signal could usually be delineated. However, in today's complex systems of interest (high-temperature superconductors, manganites, etc.), having to disentangle the surface contributions to the spectrum is a serious obstacle. To make ARPES a truly generally applicable technique, higher photon energies must be used, a technique that has been pioneered in Japan, and is now being developed in Europe, but not currently in the U.S. Two talks explored the application of soft x-rays to ARPES, one in the photon energy range <1keV and the other in the range ~6 keV. Although it is clear that using 6-keV photons provides a bulk signal that is not contaminated by surface effects, using such a high photon energy completely precludes the use of ARPES. Only angle-integrated information is available, which only provides the density of states of the material and no momentum-dependent quantities. Also, the use of such high photon energies precludes high-resolution experiments, although these might become possible with an order of magnitude or more improvement in electron energy analysis techniques. On the other hand, the work at photon energies of <1 keV has shown that the information originating on the surface of the material is sufficiently reduced to allow the researcher to obtain more reliable bulk information.

"The biological applications of soft x-rays are quite exciting, in that they open up a range of length scales not currently available."

Several notable examples were presented in which standard ARPES has led to incorrect conclusions, mostly in the case of materials with large unit cells perpendicular to the surface and strong surface alteration caused by large alterations of the surface potential with respect to the bulk.

2) Soft x-ray inelastic scattering

Although inelastic x-ray scattering is in development, and a collaborative access team is being implemented at the APS in the hard x-ray range, using hard x-rays does not allow the tuning of the scattering process to a resonant level close to the valence electrons. These resonances greatly emphasize the low-energy excitations of interest in the study of the physical properties, as described in topic 1). This was vividly demonstrated in two talks at the workshop.

One presentation showed how charge ordering in ladder compounds cannot be determined from hard x-ray scattering, but shows up dramatically when the relevant excitation channel corresponding to charge carriers in the ladder part of the compound is accessed at 528.6 eV. More significantly, any vestige of scattering disappears even when the photon energy is changed by a few hundred meV, to that of the chain part of the structure. This phenomenon permits the observation not only of charge ordering, but of the particular places in the structure where the charge is depleted and piled up. The main reason that this phenomenon, of great interest to the study of new materials with competing interactions, is not accessible by hard x-ray scattering is that no lattice distortion is involved. One measures charge ordering by hard x-rays only indirectly, by finding the structural distortions caused by the charge order.

Another area in which soft x-rays are invaluable is the determination of order in the nanometer scale, because soft x-rays (in the range 280 to 3,000 eV) cover the wavelengths in the ranges 4 nm to 0.4 nm. Examples of these types of order, such as in orbital ordering and in biological structures, were presented. The capability of studying order at such nanometer-scale distances is important in the understanding of electronic phase separation, nanoscale magnetism, lens-less imaging of nanostructures, magnetic x-ray dichroism, etc. Several of these examples were shown. The importance of lens-less imaging was dramatically demonstrated by showing the image of a three-dimensional disordered arrangement of nanoparticles. Such an image would not be possible with more conventional imaging employing lenses, due to the extremely narrow depth of field of lenses of large numerical apertures, such as the zone plate microscopes currently proposed.

3) Biological applications

The biological applications of soft x-rays are quite exciting, in that they open up a range of length scales not currently available. Most biological information has been obtained either with visible light or with x-rays and electron microscopes. This leaves open precisely the nanoscale range, which covers most of the functional units of the cell! A presentation in the workshop discussed a particularly important example, that of the structure of mitotic chromosomes. There are many levels of folding of the DNA in cells until they acquire a microscopic structure that can be seen by the light microscope. When the cell is about to divide, the DNA, which was floating as loose chains, folds itself as mitotic chromosomes (meaning chromosome structures present only during cell division) in several structural levels. Although some drawings exist in biology books about the structure of this folding, very little is known about it, even at the second structural level. There are several other aspects of biological structure that are also unknown, where soft x-ray scattering can contribute information of obviously great importance in the understanding of the fundamental processes of life.

Recommendations

The workshop members strongly urged that funding be sought for a new high-resolution soft x-ray beamline. Although the exact design of the facility requires in-depth study, its primary mission would be for studies using photoemission and scattering. We are currently in the process of forming an advisory committee to aid in the conceptual design of this facility.

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Summary of the Workshop on Emerging Scientific Opportunities Using X-ray Imaging

Introduction

The three goals for the Workshop on Emerging Scientific Opportunities Using X-ray Imaging were: 1) to identify the grand scientific challenges that can be addressed by full-field, hard x-ray (> 4 keV) imaging, including challenges from areas of science that had not benefited from x-ray imaging in the past; 2) to specify synchrotron-based techniques that address critical needs; and 3) to develop recommendations for instrumentation and facilities at the APS that respond to the scientific challenges.

The workshop participants included researchers from disparate fields, many of whom had never used x-ray imaging. They included scientific leaders in the fields of geology, paleontology, biology, medicine, engineering materials (structural, electronic, magnetic), complex systems (foams, fluid flow, fuel cells, real-time processes) and x-ray imaging. The participants were balanced between current and potential users of synchrotron radiation, and they included representatives of imaging efforts at the European Synchrotron Radiation Facility, SPring-8, the Canadian Light Source, and the Australian synchrotron, who also offered their perspectives and recommendations.

The participants presented results at the frontiers of their respective fields and also speculated on the challenges beyond. They discussed the potential of quantitative full-field imaging and tomography, coherent scattering, and holographic techniques to address the grand scientific challenges that were identified. Discussions included requirements regarding resolution, three-dimensional imaging, coherent diffraction, microfocusing, *in situ* and real-time imaging, and combinations of techniques. Finally, the participants recommended instrumentation and facilities that are needed at the APS for these new proposals/programs to be successful. It was repeatedly emphasized that, as one of the brightest hard x-ray sources in the world today, the APS can and should play a leading role in x-ray imaging science.

The participants in the workshop explored the broad applications of full-field hard x-ray imaging. Scanning micro- and nanoprobe imaging were not considered because they were beyond the scope of this workshop. The broad diversity of biological and physical sciences/engineering dictated two parallel tracks for presentations and discussion, and this summary integrates the imaging requirements common to both as well as discipline-specific needs. A strong focus for both the life sciences and the materials science/complex systems discussions was the dependence of function on a hierarchy of structural length scales from nanometers to centimeters, and the requirements for nondestructive 3D investigations, down to scales below 100 nm, of the critical structures responsible for biological functionality and for the properties and performance of next-generation materials.

Science

Presentations and discussions at the workshop centered on the investigation of structures on scales from nanometers to centimeters. Included were fracture mechanics of composites and biological materials; materials microstructure/properties research including deformation and sintering, bone and cartilage growth and formation; small animal and soft tissue research on vascular networks and pulmonary ventilation; the internal structures of microdevices, electronic components and packaging; characterization of geological structures and microfossils; cement and concrete research; structure and development of foams; and granular packing of non-equilibrium systems. Additional areas where x-ray imaging is expected to have significant impact in the future include small-animal physiology and biomechanics, porosity distribution in foods, structure and development of seeds, subcellular organelle structures in frozen-hydrated biological cells, self-orientation on nanotemplates or in molecular beams, three-dimensional nanocrystallites, nanoclusters, and other nanostructures, and complex fluidics. A listing of grand challenges developed by the attendees follows.

Materials deformation, fatigue, and fracture

This topic included service-related deformation, texture development during processing, crack initiation, and crack opening and closing phenomena during crack propagation. In all of these areas, current models are seriously inadequate for predicting behavior across the hierarchy of structural scales. Modeling efforts lack the critical correlated experimental data across multiple size scales that are needed to build the required models. In response to this, one of the grand challenges in materials science is the development of physically based constitutive equations for deformation processes. Without the necessary information, fundamental solutions remain beyond our reach.

X-ray facilities are needed to combine imaging and diffraction, precipitate imaging and phase identification, spatial resolution of 100 nm, and *in situ* measurements during straining and annealing.

Failure mechanisms within engineered structures

The two paradigms that were presented were multilayer semiconductor structures and environmental attack of cement in concrete structures. Complex layered semiconductor structures (features <1 μm and spread over millimeters) experience large thermal expansion mismatches plus “gale-force” electron winds; failures cannot be investigated without destroying the information of interest, and subtle effects separate marginal, failure-prone, ultra-large-scale integration manufacturing processes from robust ones. Cement manufacture is very energy intensive, producing large amounts of greenhouse gases, and extending the lifetime of cement-based structures is a major challenge with enormous environmental and economic consequences.

Capabilities for following environmental attack *in situ* and noninvasively with 1-μm resolution in centimeter-sized samples are required, as is 100-nm resolution in smaller samples.

Dynamic processes in extreme environments

X-ray imaging of dynamic processes such as fuel sprays and high-definition ink jet prototyping processes is essential to improving design of the systems. The "spray" is the direct link between "nozzle" and product, and understanding how delivery system design affects the "spray" is key to improving performance. Spray measurements are highly successful at APS 1-BM and real-time phase-contrast pink-beam measurements are being successfully implemented at APS 7-ID.

Experimental capability is needed to image the fuel spray together with the functioning nozzle to enable a comprehensive understanding of the dependence of the pattern of spray on nozzle structure and function.

Developing a digital morphology library

This challenge is analogous to the National Library of Medicine's "Visible Human Project" and the National Science Foundation's "Digital Morphology Project." The goal is to map three-dimensional branching structures in small organisms, such as plant root hairs, insect tracheal systems, neural networks and microcirculation networks. Currently, such 3D maps with 1- to 10-μm resolution do not exist. A library for small organisms will be an invaluable resource to biologists. Experimental requirements are centimeter-scale beam size; high throughput; possibly contrast agents; and data storage, distribution, and dispersion.

Real-time microscopic imaging of physiological processes

The physiological (chemical, mechanical, and transport) dynamics of small organisms related to breathing, feeding, and reproduction are largely unknown. What is required is a probe (further developing successful techniques now in use at the APS) that provides micrometer-level resolution real-time images of the internal workings of small organisms. Success in addressing this grand challenge is expected to lead to major revisions of textbooks as real-time, micrometer-resolution x-ray imaging opens a totally new window for physiologists.

Requirements are high speed, phase contrast, near-real-time tomography, simultaneous physiological measurements (such as gas exchange analysis and microstrain measurements), multiview radiography, and perhaps animal care facilities.

Imaging gene expression for discovery of gene function

Discovering when and where a gene is expressed is central to understanding developmental processes (e.g., definition of body axis in an embryo, knock-out models of various signaling pathways), but also to processes such as limb regeneration in some amphibians. This requires *in vivo* high-resolution tomography. X-ray image tags, analogous to luciferase, need to be developed.

Comparative characterization of evolutionary transitions underlying the diversity of life

Large numbers of samples from closely related populations must be examined in order to infer the types of transitions present and the mechanisms for diversification, especially in rapidly changing environments. Specific questions include: How does fruit morphology evolve as a function of geographic distribution? How is insect tracheal pumping related to insect flight or the absence of giant insects? How does the lock-and-key design of insect genitalia contribute to rapid speciation?

High-resolution x-ray tomography will make it possible to answer these questions. Key requirements include high throughput, simultaneous physiological measurements, development of new contrast agents, and environmental control.

Discovery and description of early terrestrial (extraterrestrial?) life (micro-fossils)

In its earliest stages, life was microscopic. Today, microfossils are difficult to find and, once they are found, they are difficult to isolate from the surrounding rock for study. Many samples are required to build an accurate view of the distribution of early life forms, and high-throughput, high-resolution synchrotron x-ray tomography can open a new frontier for paleontologists to study smaller and older fossils.

Requirements are phase-enhanced sensitivity, high throughput, and (possibly) elemental identification.

Imaging nanostructures via coherent x-ray scattering

Two talks at the workshop illustrated the exciting potential of this emerging technique for materials science and biological applications. Many materials at their functional levels are not crystalline. Coherent diffractive imaging using synchrotron radiation is an emerging technique that has the potential to image such structures, providing a practical alternative to electron microscopy for thicker specimens in their natural environments. The method has the potential to do "crystallography" without crystals and to allow x-ray imaging beyond the resolution limit by x-ray optics (~20 nm for intermediate-energy x-rays and ~60 nm for hard x-rays). Objects ranging from three-dimensional electronic devices, to magnetic films, to biological cells are already being imaged via the inversion of coherent x-ray scattering patterns.

Recommendations

The potential user community of synchrotron x-ray imaging is much broader than those of other synchrotron techniques, and addressing the grand challenges that they present requires quality dedicated facilities for a broad range of x-ray imaging techniques including:

- High-speed (phase-contrast and absorption contrast) x-ray tomography,
- Phase contrast x-ray microscopy,
- Coherent x-ray topography,
- Coherent imaging,
- Holography,
- Holotomography, and
- Diffraction enhanced imaging.

Excellent x-ray imaging research has been done at the APS. However, there are no facilities there dedicated to full field imaging and, as a result, there are important areas of x-ray imaging science that remain undeveloped. Furthermore, there is a serious loss of efficiency among the capabilities that exist because they are not dedicated. A focused effort and dedicated facilities are needed to create the premier x-ray imaging facilities at the APS that this brilliant x-ray source should have. The workshop participants concluded the following.

First, the APS needs a dedicated beamline to support the x-ray imaging techniques listed above. Second, along with the development of x-ray optics, the implementation of improved next-generation detectors, imaging theory, and robust image analysis software are critical elements in the development of dedicated facilities. Third, attention should be given to enabling multimodal investigations, along with the appropriate scientific and technical support, to ensure that the facility is second to none in imaging capabilities and productivity.

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Summary of the Workshop on Mesoscopic and Nanoscopic Materials

The goal of the "Workshop on Mesoscopic and Nanoscopic Materials" was to identify future directions in scientific research in the field of mesoscopic and nanoscopic materials that could benefit from the APS. The workshop brought together internationally renowned specialists in synthesis, characterization, and application of nanophase materials. The participants presented the frontier problems in their fields from experimental and theoretical perspectives.

Over the past decade, materials with nanoscopic to mesoscopic dimensions have been the subject of enormous interest because of the possibility of artificially creating materials not found in nature with completely new properties. These materials have the potential for wide-ranging industrial, biomedical, and electronic applications. Such materials can be metals, ceramics, polymeric materials, biomaterials or composite materials, and they are being assembled, layer-by- layer or even atom-by-atom, to generate new atomic arrangements with completely new properties. The interplay of confinement, proximity, and organization of the atomic and molecular constituents is the key to realizing materials with novel and unpredicted behavior. Understanding, characterizing, controlling, and tailoring materials with a view to harnessing materials properties on the nanometer to micrometer length scales and on femtosecond to second time scales are key strategies for materials research. For instance, the surface chemistry of nanoparticles affects their reactivity behavior in catalysts or in wear- and corrosion-resistant materials. The self-organization of nanostructured biomaterials could lead to broad applications in drug encapsulation and delivery.

It is a well-known paradigm for both biological and inorganic materials that structure determines function. There is also an emerging understanding that structure alone is not sufficient to determine function, but that dynamics play a critical role. Progress in the field of nanoscale materials is intimately related to the development of dedicated synthetic and analytical techniques that enable us to produce and examine the atomic and electronic structure of new nanoscale materials. These include optical methods, electron microscopy techniques, as well as x-ray microscopy, imaging, and scattering techniques. It is well known that x-rays are unrivaled in their ability to determine structure in the nanoscale range, particularly in the bulk of the material, at buried interfaces, *in situ* under a wide range of conditions, etc., and to study many properties not accessible via other probes, such as global statistical properties. X-rays can also be used to monitor the dynamic response over a wide range of time scales, including ultra-fast structural relaxation or dynamic and dissipative phenomena at surfaces and interfaces under extreme conditions. As the new hard x-ray tools deliver these types of capabilities, it is expected that the traditional boundaries between x-ray scattering, imaging, microscopy, interferometry, and spectroscopy will disappear. This new paradigm will provide unprecedented opportunities for progress in nanoscience.

The focus of this workshop was to identify the frontier problems in understanding interfacial structures, nanosystems, confinement, and self-assembly of hard materials, soft materials, and biomaterials, as well as nanofluidic phenomena. There was also a major effort during the workshop to assess the applicability of a variety of hard x-ray tools available at the third-generation synchrotron radiation sources, such as the Center for Nanoscale Material's hard x-ray nanoprobe and other probes such as electron diffraction and microscopy, which will become available at the new nanocenters at various DOE national laboratories.

The workshop plenary sessions consisted of science overviews on materials, phenomena, and characterization tools and techniques. Time was allotted in each session for discussions. Care was taken to ensure representation at the workshop by experts in the various fields of nanoscience and not solely synchrotron experts. It was clear from the excitement and enthusiastic participation in the discussions and recommendations that there is a great deal of enthusiasm for the potential inherent in synchrotron radiation for nanoscience.

The charge given to the workshop attendees was as follows:

1) Identify grand-challenge mesoscopic and nanoscopic science that should be addressed during the next 5–10 years using x-ray techniques at a third-generation synchrotron radiation source.
2) Identify and justify the technical requirements to meet the grand-challenge problems:
   - New instrumentation and techniques to be developed on existing beamlines to perform new kinds of science, and
   - Need for new dedicated beamlines and instrumentation for this community.
3) Identify both short- and long-term R&D needs in areas such as x-ray techniques, sample environment, optics, and data analysis that will prepare the community to address grand-challenge problems.

The workshop focused on three broad areas: controlled synthesis, directed assembly, and the study of new or collective properties. The main challenges in nanoparticle synthesis consist of controlling the physical properties of the core, developing facile and effective coatings that allow introduction of one or more functions, and determining the factors that determine the toxicity of the nanoparticles (e.g., shape, size, chemical composition, coating).

There was a discussion of how to calculate (and therefore predict and even design) the various hierarchies of structures formed as molecules self assemble, based on techniques such as steric and electrostatic models, Monte Carlo calculations, simulating the assembly using molecular dynamics, or using other agent-based algorithms, etc. It was pointed out that it would be extremely useful to use synchrotron-based methods for studying the details of the self-assembly of nanoparticle systems as a way of testing the validity of such calculations. There were presentations on methods and problems associated with nanoparticle synthesis, including the synthesis of functionalized nanoparticles with magnetic or other properties (such as iron oxides) and of the synthesis of inorganic-organic composite and inorganic-bio materials (e.g., DNA grafted onto inorganic nanoparticles).

There were discussions of granular particle assemblies and their flow patterns and jamming transitions and how these could be studied by the complementary techniques of nuclear magnetic resonance, light scattering, and x-ray microtomography; patterned assembly of nanoparticles on patterned substrates created by micro-phase separated block copolymers; assemblies of nanoparticles at air-liquid interfaces and the production of ultrathin membranes of controllable porosity, and wetting layers and nanodroplets at interfaces.

Participants also heard about techniques for characterizing systems ranging from coherent x-ray ("lens-less") imaging of single nanocrystals, to microdiffraction using microfocused synchrotron x-ray beams, x-ray diffraction of assemblies of nanoparticles, small-angle x-ray scattering, grazing incidence small-angle x-ray scattering, x-ray reflectivity, x-ray standing-wave-induced fluorescence, x-ray photon correlation spectroscopy, and the complementary but non-synchrotron techniques of electron microscopy and atomic force microscopy.

Finally, there were presentations that focused on the study of nanomaterials with new properties, such as molecular junctions used as transistors, composite magnetic films with exchange bias, spring magnets, magnetic/semiconductor composites for spin injection, quantum fluids and quantum well heterostructures, and nano/bio systems for medical applications. Also presented as examples of self-assembled nanosystems for study with synchrotron methods were purely biological systems such as the extracellular matrix and its response to external stimuli.

Findings and Recommendations

The following findings and recommendations are seen as critical components for APS to maintain a leadership role in the rapidly growing field of mesoscopic and nanoscopic science.

Finding

The APS already supports and develops many tools important for characterization of materials at the nanoscale (microprobe, coherent diffraction [proof of principle, so far], GISAXS, SAXS). Many of these tools are available in a non-dedicated mode at various beamlines around the ring. In general, setup of these experiments is timely. The hard x-ray nanoprobe being built for the Center for Nanoscale Materials will be an important component of the APS nanoscience tool set. The APS should continue to explore and support development of other new techniques as they become possible and to nurture the evolution of demonstration experiments to routine application, e.g., coherent lens-less imaging.

Recommendation

The APS must make every effort to support users without synchrotron radiation experience by providing user-friendly beamline and instrumentation support. The workshop participants expect a big demand for GISAXS, SAXS, and x-ray reflectivity measurements at the APS, and new and modern dedicated capabilities for these techniques should be developed to perform such studies in different sample environments. In the spirit of continued expansion of this field, APS staff should be provided with adequate R&D support to jointly plan new and high-risk experiments with the new user groups and for developing new tools to perform such experiments.

Finding

It is clear that there is a critical need for a complete characterization of nanomaterials as they are synthesized at both the individual nanoparticle level and at the collective, ensemble level—both of which can be studied by complementary x-ray techniques. These studies require *in situ* and real-time experiments, which in turn require extended setup and characterization time, substantial support, and adequate hutch space.

Recommendations

1) Provide maximum beam time for dedicated programs requiring *in situ* studies.
2) Optimize insertion devices, x-ray optics, and end stations on dedicated nanoscience beamlines (including a new soft x-ray beamline).
3) Assure that the end stations on these beamlines contain hardware that resides in-place for extended periods.
4) Support necessary R&D to develop advanced nanofocusing optics, scanning stages with sub-nanometer resolution, and image extraction software.

Finding

To optimize the benefit for nanoscience from the advanced characterization tools available at the APS, it will also be necessary to have a critical mass of world-class resident scientists, including experimentalists, technical innovators, and theorists.

Recommendations

1) The APS should provide funding on a long-term basis with dedicated beam time for experimental staff. In order to retain and attract the best talent, the APS should consider allowing its best and most productive scientists to dedicate some

fraction of their time to their own research programs, perhaps leveraging by raising their own research money.

2) Implement a theoretical program, perhaps in collaboration with the Center for Nanoscale Materials virtual fab-lab, for a theoretical modeling effort. Modeling tools developed in this program should be made available to the APS users.

These recommendations are designed to effectively utilize unique intrinsic capabilities of the APS and Center for Nanoscale Materials for frontier mesoscopic and nanoscopic science; develop infrastructure/technology to make the tools for this field more broadly available; and expand the capacity of nanoscience experimentation at the APS. Finally, the present and future scientific users in the nanoscience area who participated in the workshop were eager to be fully involved in the implementation and success of all of these recommendations.

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Summary of the Workshop on Nanomagnetism Using X-ray Techniques

Introduction

The goal of the Workshop on Nanomagnetism Using X-ray Techniques was threefold. First, we worked to identify the scientific grand challenges in nanomagnetism that we can foresee from today's vantage point. Second, we worked to identify the contributions that synchrotron-based techniques could make within the next decade to address these challenges. Third, we specifically discussed recommendations concerning the instrumentation needed at the APS to enhance its status as a premier facility in the field of nanomagnetism. In this summary, the prevalent common themes throughout the workshop are discussed. A comprehensive review of the workshop is in preparation and will be presented in a separate document.

Science

Because nanomagnetism covers a wide range of topics, three major themes were identified prior to the workshop for the purpose of facilitating scientific presentations. The themes were:

- Confined magnetism: Layered and artificially structured systems;
- Cluster magnetism: Molecule-based magnets, spin ice, and spin glasses; and
- Phase separated systems/complex oxides.

The unifying idea throughout the workshop was to understand the magnetic behavior of individual building blocks of matter and explore strategies to combine them into more complex structures, leading to integrated systems with new functionalities. For example, multiferroics—the complex property of simultaneous ferromagnetism, ferroelectricity and ferroelasticity—is one example in the category of new, emerging functionalities. Another common theme that permeated the workshop was the central role played by inhomogeneities in determining the collective magnetic response. Inhomogeneities can be driven by competing interactions at the nanoscale, as demonstrated in colossal magnetoresistive (CMR) materials and high-T_C superconductors, or they may be artificially introduced through tailored synthesis, as in the case of magnetic nanocomposites. Characterization of inhomogeneous systems requires measurements of the chemical, structural, and magnetic properties in a phase-specific way. Because x-ray diffraction can isolate coexisting phases by coupling to their different crystal structures, it is desirable to combine resonant x-ray diffraction with nanometer-sized beams to image inhomogeneities in real-space by diffraction contrast imaging. Adding circularly polarized x-rays allows for diffraction-contrast, real-space imaging of structure and magnetic phases to be done simultaneously (by adding and subtracting scattered intensities for opposite helicities of light). The application of very high magnetic fields (above 20 T) during spectroscopic and diffraction examination is an important capability to separate competing states in highly correlated electron systems (i.e., CMR materials). The ability to probe chemical, structural, and magnetic correlations in a phase-specific way, and simultaneously in the same measurement, is a key asset of synchrotron-based techniques. Resonances add invaluable element-specific information that is particularly useful in multi-element, heterogeneous systems.

In addition to fundamental science interest, there are a number of existing and emerging technologies that are driving today's nanomagnetism research. Fundamental scientific questions common to the technological pursuits include the origin of magnetic coupling; spin transport across interfaces; spin-lattice interactions in complex materials; and the magnetic domain configuration and dynamics arising from contact between different kind of magnets, for example antiferromagnets and ferromagnets. Among these focus technologies are magnetic information storage, advanced sensors, ultra-strong permanent magnets, and nanostructured alloys for transformer applications. Of interest in the field of magnetic information technology are sandwiched magnetic sensors, spin valves, spin transistors and magnetic media consisting of ferromagnetic thin films and multilayers that can store information in nanometer-sized bits. The phenomena of current-driven magnetic switching and the multiferroic response are integral to new sensor development, and self-assembled nanocomposite particle systems are envisioned to enable both ultra-hard permanent magnets and ultra-soft transformer alloys. In today's nanocomposite structures, magnetic switching times are about 1 ns. The future of magnetic technologies is guided by “smaller and faster.” Technology is dependent on the researcher’s ability to synthesize new materials that are patterned or can self assemble on the nanoscale. These materials must to be magnetically stable at room temperature, and methods are needed to manipulate the magnetization on the sub-nanosecond time scale.

Such challenges coincide with forefront questions in basic magnetism research—namely, the static or dynamic properties of small magnetic elements on very short time scales. This situation is illustrated in Fig. 1, which shows that, especially on the time scale below 1 ns, our understanding of the relevant processes in magnets is still very limited. Spin-orbit coupling, precessional switching, and magnetic anisotropy are correlated with time scales between 100 fs and 100 ps, which are rather difficult to access experimentally. However, by using the time structure of the synchrotron and fast detectors like streak cameras, researchers can address these fundamental questions to be addressed with high spatial resolution and sufficient elemental and magnetic sensitivity that will cover the relevant spatial

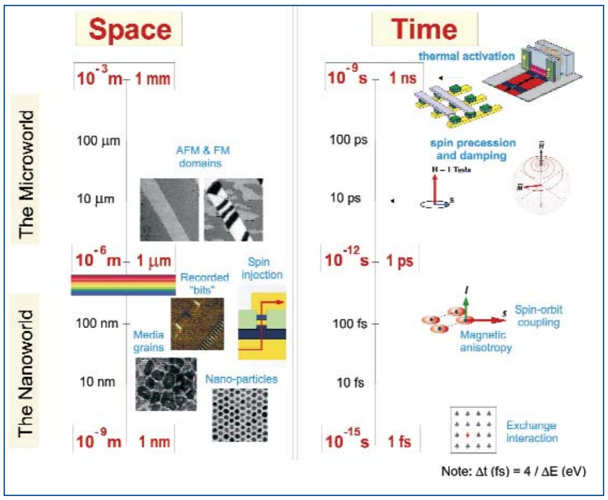

Fig. 1. Examples of magnetic structures relevant to computer technologies (left) and summary of state-of-the-art ultrafast time scales relevant to the scientific exploration of magnetic phenomena needed for tomorrow's technologies. (Courtesy H Ohldag)

scale of interest (5–50 nm). As a final comment, theoretical studies and modeling are ideally carried out concurrently to support the experimental scientific and technological efforts.

An exciting emerging application is engineered nanomagnets for biomedical applications that provide opportunities for diagnostics and therapeutics in both *in vivo* and *in vitro* applications in biomedicine. The size of nanoparticles—similar to common biomolecules (<50 nm)—makes them interesting for a wide range of biomedical applications that includes intracellular tagging, contrast agents, targeted cancer treatment, antibody targeting, and hyperthermia. Key challenges include the modification of nanoparticles for enhanced aqueous solubility; biocompatibility or biorecognition; and optimization of their magnetic properties, including their relaxation dynamics over a broad range of frequencies and applied fields. In addition to surface functionalization, nanoengineering of particle surfaces to optimize both their magnetic and optical response is important for diagnostic and therapeutic applications. The APS is poised to play a critical role in realizing these advances by providing tools for structural identification and chemical and magnetic characterization of these magnetic nanoparticles and core-shells structures, with specific emphasis on the evolution of these properties as a function of their size and surface function.

To summarize the science drivers, nanomagnetism plays a vital role in:

- New paradigms for condensed matter science, specifically where competing interactions lead to phase separation.
- Sustaining progress in information technologies, specifically in the following areas:
  - MRAM: Magneto-resistive random access memory
  - Novel magnetic structures
  - Spin-based quantum computing
  - Magnetic semiconductors and spin transport
  - Molecule-based magnets and organic spintronics
  - Switching characteristics of nanomagnets
- Contributing to energy independence:
  - Ultra-strong permanent magnets via nanocomposites for motor applications
  - Highly-responsive magnetic nanocomposites for transformer applications
  - Efficient, multi-functional sensors
- Nanomagnets in biomedical applications

Frontier Technical Requirements

The important length scale in nanomagnetism is ~5 nm, which is the length scale of the exchange interaction. Developing synchrotron-based instrumentation and techniques to probe structural and magnetic properties with nanometer resolution is a major technical requirement. Furthermore, the ability to study magnetization dynamics at time resolutions greater than 1 ps would provide an opportunity to study spin dynamics. Finally, a combination of spatial (~5 nm) and temporal (~1 ps) probes would enable forefront studies of new phenomena in nanomagnetism. Extreme sample environments such as high magnetic field (>20 T) and low temperatures (~mK) are essential in the study of competing phases in complex magnetic materials.

Recommendations

Currently, the APS has two superb, but oversubscribed, beamlines dedicated to magnetism studies. One beamline is in the high-energy range (2.6–45 keV) and the other is in the intermediate energy range (500–3000 eV). Because requests for beam time exceed the available shifts by a factor of three, the present facilities are insufficient to provide adequate tools to a growing synchrotron user community. Also, the number of techniques (magnetic scattering, spectroscopy, and imaging) presently employed at each of the beamlines are too numerous to optimize each one in order to meet frontier technical requirements. However, by separating scattering and spectroscopy techniques, the APS can provide competitive tools for nanomagnetism studies. One can envision building two new beamlines; one in the hard-energy range and the other in the intermediate-energy range. The new hard x-ray beamline should be optimized for resonant magnetic diffraction studies in high magnetic fields. The new intermediate-energy beamline should be optimized for resonant inelastic scattering, diffraction, and imaging. The presently existing beamlines would then be optimized for spectroscopy techniques.

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Summary of the Workshop on Science with High-Energy X-rays

The goal of the “Workshop on Science with High-Energy X-rays" was to identify the emerging scientific areas that could benefit from the use of high-energy x-rays at the APS.

The 49 participants in the workshop included both experienced users of high-energy x-rays and scientists who have never used synchrotron radiation. Academia, national laboratories, and industry were all well represented. Topics for the 28 presentations ranged over a large variety of scientific areas, including materials science, condensed matter physics, chemistry, geology, and atomic physics. Several speakers spoke on experimental methods that are complementary to high-energy x-ray experiments (e.g., electron microscopy, neutron scattering), and there were several talks by theorists.

The first day of the workshop consisted of a series of plenary talks that highlighted major areas of high-energy x-ray research (three-dimensional x-ray microscopy, micromechanics of materials, rapid pair distribution function measurements) and several other talks that showed the breadth of high-energy x-ray experiments (atomic physics, x-ray absorption spectroscopy, small-angle scattering).

On the second day, the workshop was split into two parallel sessions, one on "Materials Engineering" and the second on "Structural Science." The first of these sessions focused primarily on studies of mechanics of materials and included several talks on theory. The second session was mostly concerned with various aspects of crystal structure determination. In both sessions, the emerging theme was the use of high-energy x-rays for *in situ* study of materials undergoing some sort of change.

At the end of the second day, a lengthy discussion session was held in both parallel sessions to identify the "Grand Challenges" in mechanics of materials and structural science, respectively, that could be addressed by the use of high-energy x-rays. Ersan Üstündag (Iowa State/Ames Lab.) led the discussion on materials engineering, and Angus Wilkinson (Georgia Tech.) led the discussion on structural science. A combined session was held with all attendees to discuss the grand challenges identified by each group before adjourning the workshop.

The grand challenges from the mechanics of materials session were found to be the need to collect rigorous *in situ* data at multiple length scales, and the need to integrate experimental results with mechanics modeling.

Related to this, the following were identified as scientific problems that especially benefit from the use of high-energy x-ray diffraction:

- Deformation mechanisms in complex materials (composites, ferroelectrics, etc.),
- Intra- and intergranular mechanics,
- Microstructure characterization (dislocation structures, etc.),
- Kinetics studies,
- Coatings,
- Buried interfaces,
- Residual stresses (in small structures, components, welds, etc.), and
- High-rate deformation (with seconds resolution needed).

In the area of structural science, the grand challenges were found to be:

- Fast, *in situ* studies of reaction dynamics (especially in realistic processing conditions),
- Determination of structures in extreme environments (e.g., high temperature, high pressure), and
- Obtaining structural information from buried interfaces.

Scientific areas that were identified as particularly important were:

- Accurate determination of structures for materials containing heavy elements due to low absorption, extinction, and polarization corrections (also possibly using high-Z K edges for contrast),
- Structures of nanophase materials with rapid PDF techniques, and
- Studies of bulk materials (e.g., defects using diffuse scattering, and variation in chemistry/structure for the bulk versus the surface in concrete).

Recommendations

Jointly, the attendees of both sessions agreed that the grand challenges could be reduced to one phrase: ”Real materials studied in realistic conditions.”

The following items were identified as technical issues that need to be addressed in order to help meet the grand challenges:

- Dedicated facilities (i.e., need for increased specialization at APS),
- Faster detectors,
- Multiple simultaneous experimental capabilities (imaging, SAXS, texture, etc.),
- Experiment simulation,
- Integration of mechanics modeling with experimental results,
- Software for fast and easy data analysis,
- Versatile ancillary equipment,
- Detailed instrument studies (for improved data integrity),
- Reduced sampling volumes,
- White beam capabilities,
- High-energy bend magnet station, and
- User education.

Generally, there was a consensus opinion among the workshop participants that many exciting and important opportunities exist for science with high-energy x-rays at the APS and that the use of high-energy x-rays at the APS will have a very bright future.

Dean Haeffner (ANL)

Summary of the Workshop on Membrane Science at the APS

The focus of the "Workshop on Membrane Science at the APS" was on emerging research topics in membrane science. These topics are truly interdisciplinary and represent the interfaces among chemistry, materials physics, molecular biology, and medicine. For example, inorganic membranes, owing to their thermal, mechanical, and chemical stability, have been used in many industrial separation processes. Organic membranes are used for a variety of liquid and gas-phase separations and for the extraction of trace organic pollutants from water. The supramolecular architecture of biological systems is based on ultrathin and highly flexible biomembranes. Most biomembranes exhibit a universal construction principle: a self-assembled bilayer of lipid molecules with many anchored macromolecules. The need to understand chemical ordering, pattern formation, kinetics, and dynamics in organic and inorganic membrane structures, as well as the physical interactions between biomembranes and supramolecules, their dynamics under stimuli, and the formation and structure of ion channels in these biomembranes, formed the basis for discussion at this workshop.

The workshop emphasized the need for fundamental structural understanding to control the formation of membranes on all length scales (molecular, nano, micro, and macro), whether the membranes are fabricated or self-assembled. It is even more challenging to create new types of so-called "bio-inspired" membranes without utilizing the insights obtained by studying biological structures. The new synthesis processes are driven by potential applications where the membrane properties and function are to be integrated from the molecular scale to the macro-scale, spanning 7-8 orders of magnitude in length and time scales. The workshop identified key problems where the application of x-ray analytical tools will enable significant progress in relating structure and function. Toward this goal, it is necessary to determine high-resolution membrane structures in one, two, and three dimensions in the molecular, nano, micro, and macro scales, and to perform element-specific mapping of real-time information on the kinetics and dynamics of the membranes on multiple scales.

The growing application of membrane technology in modem industrial processes has made it an integral part of many corporate and national (e.g., DOE, NSF, NIH) R&D programs. Membrane-based technologies have advanced the state of the art in such areas as water treatment and production; niche applications in the electronics, semiconductor, chemical, petrochemical and pharmaceutical industries; and environmental control. New research opportunities range from controlling medical and biological processes, such as hemodialysis for artificial kidneys or the separation of proteins and microorganisms, to providing essential components for fuel cell and hydrogen energy economy and technology. All these examples were well represented by the leaders in these areas at the workshop.

A successful hydrogen economy based on fuel cells to power cars, trucks, homes and businesses will require advances in key technology areas. Among different types of fuel cells, the most useful for vehicle transportation will be proton exchange membranes (PEMs) because they operate at relatively low temperatures. It was clear from workshop discussions that further research is needed in identifying new membrane materials with better efficiency to make them cost effective; structural information is the key to reaching this goal.

Membrane filtration at the micro- and nanoscales is also used for the separation of proteins in the food, beverage, pharmaceutical, and biotech industries. Within pharmaceuticals and biotech, membrane filtration is increasingly the method of choice for separating amino acids, enzymes, yeast, insulin, ferritin, glycoproteins and biopesticides from proteins. Membranes will play a major role in the recovery, isolation, and concentration of these proteins.

Membranes have been prepared with increasing sophistication to meet newer challenging applications, and commensurately scientists have refocused on the fundamental questions regarding their properties and performance. Some of these questions have become more complex, having to address physical, chemical, and biological properties and interactions at microscopic, nanoscopic, and atomic scales. Detailed understanding of these questions has demanded new experimental tools and theoretical models. Many experimental probes and techniques, such as laser spectroscopy, electron spin resonance, nuclear magnetic resonance, neutron scattering, Raman spectroscopy, electron microscopy, and computational modeling, can currently provide information bearing on the questions of interest. However, the diversity of interactions among molecules with membranes discussed at the workshop requires probes that are sensitive to the local and extended atomic and electronic structure, as well as to the geometric structure in membrane interfaces with solids, liquids, and gases over a wide range of spatial and temporal dimensions. Both lateral and vertical (depth) dimensions must be probed. During the last decade, techniques based on synchrotron radiation, such as wide-angle x-ray scattering, small-angle x-ray scattering, ultra small-angle x-ray scattering, grazing-incidence small-angle x-ray scattering, x-ray reflectometry, diffuse x-ray scattering, x-ray photon correlation spectroscopy, grazing-incidence x-ray diffraction, and x-ray absorption spectroscopy, have been shown to provide unique structural information at the molecular level on membranes, their interfaces, and interacting supramolecules. These techniques in the real-time domain give further insight into time evolution and molecular interactions in these systems. Together, these capabilities have clear potential to impact the future scientific directions for this field and perhaps begin to address some of the unanswered questions.

Recommendations

The workshop participants were unanimous in their recommendations and excitement about the potential use of the APS in membrane science research. The workshop participants viewed the APS as one of the world leaders in this research and they made the following critical recommendations for the APS to maintain a leadership role in the rapidly growing field of membrane science:

I) The APS must maintain the successful scientific environment that both enables and enhances experiments using the various x-ray tools mentioned above.

2) Potentially ground-breaking future research (nucleation, growth, dynamic self-assembly, molecular interaction, etc.) requires *in situ* investigations in unusual experimental environments capable of concurrently performing x-ray scattering as well as other optical and thermodynamic measurements. APS should aggressively work with science leaders in this field to develop such capabilities and make them available at the beamlines dedicated to membrane science.

Both these goals can be best achieved by forming a membrane science advisory panel to interface with the APS and develop a plan to:

1) Optimize and refurbish existing beamline capabilities and infrastructure to support membrane science experiments at a select set of beamlines;
2) Hire resident scientific staff with experience and interest to provide leadership to the user community in the field of membrane science;
3) Provide a new, dedicated bending magnet beamline with suitable x-ray optics, end-station instruments, and two-dimensional detectors (including various experiment environments and auxiliary non-x-ray tools); and
4) Provide modeling and simulation capabilities to perform in-line data analysis. It was also recommended that since there is a potential for bringing many new users to the APS, a workshop on the use of x-ray tools for membrane science research, with hands-on training for the workshop participants, be held as early as possible.

Also, a Membrane Science Interest User Group will be formed at the APS, which will meet on its own regularly as well as at the APS users' meetings. The 'membrane science advisory panel' will receive its input at these meetings of membrane science users.

These recommendations were designed to effectively enhance existing capabilities of the APS and to build a new, dedicated beamline with unique capabilities for frontier membrane science; develop infrastructure/technology to make the auxiliary tools, along with the x-ray tools for performing *in situ* membrane science research, more broadly available; and expand the capacity of membrane science experimentation at APS to support anticipated new users who were present at the workshop. Finally, the present and future scientific users in the membrane science field who participated in the workshop were eager to be fully involved in the implementation and success of both of these recommendations.

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Jin Wang (ANL) presenting his talk at the Workshop on Membrane Science at the APS.

Summary of the Workshop on Emerging Areas in Biological Crystallography

Developments in synchrotron radiation sources over the past 20 years have revolutionized protein structure determination. The intense tunable undulator x-ray sources available at the third-generation synchrotron facilities have enhanced the multi- and single-wavelength anomalous dispersion (MAD/SAD) techniques for solving the phasing problem to obtain novel three-dimensional structures. This has enabled the collection of MAD/SAD data sets from favorable crystals in a few minutes. Much emphasis in recent years has been given to the effective use of synchrotron sources for protein structure studies. This consists of protein crystallization, storage, monitoring of crystal growth, harvesting and freezing crystals, robotic capabilities to mount and dismount the cryo-cooled crystals on a goniometer, improved two-dimensional detector systems, and data acquisition. In addition, the interpretation of the x-ray diffraction data, and graphics displays to enhance the quality of the molecular model, as well as integration of all these components into a comprehensive system for structure determination, have been given very high priority by the research community.

The "Workshop on Emerging Areas in Biological Crystallography" addressed topics well beyond these issues to cover future grand challenges. The workshop identified four grand challenge topics to define the emerging areas in the field of biological crystallography. They are identified below.

Molecular Machines

Proteins combine to form multiprotein complexes that function as "molecular machines." The molecular machines function inside cells performing a variety of key tasks, and are produced, assembled, and controlled by the genome and the associated sensing and regulatory networks. The workshop addressed the methodology of mapping the structure of molecular machines by combing the results from electron cryo-microscopy (CryoEM) and x-ray diffraction using synchrotron radiation. The speakers at the workshop also addressed the structural changes in molecular machines associated with the dynamic interactions responsible for signaling, transport, motility, cell division, and virtually all other cell activities. This is an essential step before one can progress toward a systematic understanding of cell function. It was clear from the workshop discussions that this is a leading area of research being vigorously pursued by many of the principal research groups, which were well represented at the workshop.

The workshop participants presented frontier work which showed the need for integration of tools, such as large-angle and small-angle x-ray scattering, electron cryomicroscopy, and circular dicroism (CD). One example is the work of Jack Johnson's group (Scripps Research Institute), which used small-angle x-ray scattering, optical fluorescence spectroscopy, far-UV CD, and CryoEM to study the acid-induced maturation dynamics in virus particles. Bacteriophage HK97 is an icosahedral virus capsid that has a massive size, a large number of subunits, and a highly symmetric architecture. It contains the primary machinery that packages, protects, and delivers the genome of icosahedral viruses. The changes in the virus due to acidification of the buffer are measured through various physical techniques and reveal large-scale structural changes involving reorganization in its gross morphology, surface charge, and hydrophobicity result. Understanding of the mechanisms and dynamics of these changes has provided considerable knowledge of virus function and insights into the function of macromolecular assemblies.

The trend of integrating various tools is a clear new direction that will help researchers to understand the structure of complex macromolecular assemblies which form the important functional molecular machines (W. Chiu, Baylor; T. Steitz, Yale).

Membrane Proteins

The membranes in the human body keep a cell separated from the outside environment so as to protect the proteins and other components of the cell from dissipating, and to safeguard against and control the entry of foreign molecules through the membrane structure. The membrane proteins are vital to many functions of human cellular control and growth; they act as gates, transporters and receptors. Crystallization of membrane proteins is a major stumbling block en route to elucidating their structure using x-ray crystallography and understanding their function. The novel concept of membrane protein crystallization from lipidic cubic phases has yielded well-ordered crystals and high-resolution structures of several membrane proteins, yet progress has been slow due to the lack of understanding of the molecular mechanisms of protein transport, crystal nucleation, growth, and defect formation. Much anticipation existed among the workshop participants in reaching a rational understanding of the membrane protein crystallization process and, as a result, in the development of new techniques to adequately improve the quality and purity of membrane proteins suitable for structural and dynamics studies.

Dynamics

The field of biological crystallography has been astoundingly successful in the past at determining the static, ensemble-averaged structure of a wide range of proteins. What is increasingly important to biological understanding, however, are the questions: How do proteins move to effect their function? What is the role of dynamics in the microscopic mechanisms of enzymes? How can time-dependent structural changes be measured? How good are molecular dynamics theoretical models of these dynamics? Fundamental biology will drive dynamics to the forefront of many research programs.

The third-generation synchrotron radiation sources have provided many time-domain tools, which will form the core of future research programs to study protein dynamics. They include large- and small-angle scattering, inelastic nuclear resonance scattering, x-ray microscopy, etc. For example, x-ray small-angle scattering has been successfully used to observe the unfolding of RNA (L. Pollack, Cornell). The classic work of Keith Moffat's group on photobiology has opened new doors to study of the reaction intermediates with sub-nanosecond resolution. The dynamics of select atoms such as iron in heme-proteins has been studied using inelastic nuclear resonance scattering, which complements Raman scattering investigations (S. Durbin, Purdue). In addition, all these dynamical measurements are now leading to a focused theoretical effort in performing molecular dynamics simulations. This new trend is robust, both in terms of growing interest in the area of dynamics and successful development of a plethora of x-ray and optical tools for their study (G. Rosenbaum, UGA/ANL).

Physics and Chemistry of Biological Processes

It became apparent from the workshop presentations that there is a growing community of scientists that uses the tools of physics, both experimental and theoretical, in an innovative way to study biological problems, as well as research aimed at providing a better understanding of the physical and chemical principles underlying biological processes. In the post-genomic era, biology gets increasingly quantitative, and it is necessary to understand the biological processes at the molecular level. In order to address such problems, a whole set of complementary physical tools will be needed that are capable of monitoring, in real time, the behavior of individual biological molecules and complexes, *in vitro* and in live cells. An awareness of the need to bring physical insight into solving problems in the entire field of biological crystallography existed among the workshop participants. Special focus was in the areas discussed below.

"A new infrastructure may be called for, both in terms of physical facilities and of interactions among organizations in the community."

Radiation damage

Currently, in almost all protein structure determination studies using synchrotron radiation, the samples are always cryo-cooled to reduce the secondary radiation damage. However, there are limitations on the optimum use of high-brilliance beams, although less intense beams inflict the same damage per absorbed photon as intense undulator beams. In her well-received presentation, Elspeth Garman (Oxford) strongly argued for a systematic study of the effects of radiation damage on a structure and emphasized that wrong conclusions will be drawn on structure from damage-induced data on biological mechanisms.

Future directions in this field should focus on investigating radical scavengers to slow down the rate of radiation damage in cryo-cooled crystals, theoretical calculations and Monte Carlo simulations on the x-ray absorption process in protein crystals as a function of x-ray wavelength and presence of heavy atoms (e.g., Se), and finally on a study of unit cell and structural changes (phase transitions) in crystals as a function of temperature and radiation burden.

The subject of radiation-damage-induced phasing (RIP), wherein the damage is used to facilitate the structure determination, was also discussed in the workshop. Further development of the RIP method is expected to benefit the more traditional phasing techniques like S-, Se-, or Br-SAD/MAD (Z. Dauter, NCI/NIH).

Biomolecules under high pressure

Investigating proteins subjected to extreme conditions is not only an important field of fundamental biology, but also addresses the behavior of life, from deep oceans to high mountains. A significant proportion of the global biosphere is exposed to pressures of up to 120 MPa. The question is what happens to organisms when they are compressed, and how does life originate and survive at and below the deep sea floor? It is expected that, in future, extreme conditions will become an important variable in microbiological and biochemical research, in particular to understand the structure/function relationship of proteins.

Early work by Richard Kahn (IBS Grenoble) and his collaborators, presented at the workshop, has paved the way to performing studies of biological structure under hydrostatic pressure using synchrotron radiation beams. They foresee growth in this area with the availability of high-energy x-rays with sub-Å wavelength to facilitate high-resolution studies.

Crystallography with microfocused x-ray beams

Progress in the field of protein crystallography is often hindered by the size, shape, and quality of the available crystal. For example, crystals that are only a few tens of microns in dimension, or display the growth habit of a thin needle or a platelet, or are highly mosaic or twinned, will not produce quality diffraction patterns. It has been demonstrated that each of these difficulties can be overcome by the use of a microfocused x-ray beam of the type routinely used in materials research at the third-generation synchrotron radiation facilities (G. Schertler, MRC Lab., Cambridge).

Microfocused x-ray beams also offer the possibility to study partially ordered systems, such as membrane protein arrays e.g., a class of membrane-bound proteins made up of microarrays of G-protein-coupled receptors). These have potential use in medical diagnostics, biomarker discovery, and proteomics. Liposomes offer another example of microfocused x-ray beam investigation. Liposomes are made up of natural, nontoxic phospholipids and cholesterol. They are used as drug carriers to cure conditions ranging from inflammation to cancer. The challenge will be to identify such systems and to address the potential and the limitations of the technique in structure determination.

From an experimental point of view, providing 10^{10} ph/s in a micron-size spot, and aligning the micron-size sample in front of the beam over the duration of the experiment are quite challenging. But these requirements are becoming a commonplace at synchrotron facilities engaged in nanoscience research.

Diffuse scattering from biomolecules

Diffuse scattering has been used to study the nature of disorder in protein crystals and has been shown to be a useful experimental technique for characterizing the dynamics in crystalline proteins. It provides information regarding the directions of motions, as well as the lengths and directions of correlations, in atomic displacements. Diffuse scattering is usually thrown away in most crystallographic studies, but the availability of synchrotron sources, advanced detectors, and sophisticated computing have made it easier to use it fruitfully.

Since the detailed work of Michael Wall (LANL) and his collaborators, not much attention has been paid to this important area of research. Measurement and analysis of diffuse features in scattering patterns would help to distinguish Bragg scattering from diffuse scattering, to improve models of dynamics for x-ray structures, and to improve the resolution of x-ray structures. Studies of x-ray diffraction from membrane phases, in which both the membrane structure and the bending and bulk elastic moduli were simultaneously modeled from diffuse scattering, hint at the major advance in development of protein structural models that might be achieved through integration of diffuse scattering data into crystallographic structure refinement.

It was pointed out by Richard Matyi (NIST) at the workshop that high-resolution x-ray scattering methods can yield valuable insights into the nature of physical defects generated by radiation damage in protein crystals. In the semiconductor community, it has taken several years for these high-resolution methods to be elevated from laboratory curiosity to their current status as an established and important analytical technique. Hopefully, with continued progress (particularly in the modeling of the diffuse intensity), a similar progression will occur to the benefit of the protein crystal growth community.

Powder diffraction from proteins

Although powder diffraction is a routine tool in materials science, not a lot of attention has been given to this technique in biological structure determination. The pioneering work of Robert Von Dreele (ANL) leads to a new direction in this area, with the potential for powder diffraction to become an important complementary tool.

The reason that powder diffraction data from proteins and protein complexes have a high potential is fourfold:

1) Powders are easily prepared under a wide range of conditions and are not limited by the need for suitable single crystals;
2) Protein powders are inherently "perfect" for diffraction, as they are of the right size (about 1 μm) and are almost completely strain free;
3) Only very small samples sizes (μg quantities) are required, and
4) Data can be collected rapidly, making the observation of many dynamic processes straightforward. For example, this method completely removes the problem of radiation damage in biological materials and allows study of *in situ* processes on minutes-to-hours time scales.

Recommendations

The workshop brought together internationally renowned specialists in their fields, not limited to x-ray expertise. To supplement the interdisciplinary format, there was a fruitful dialogue between biologists, chemists, and physicists to address the grand challenge topics in the field.

The workshop participants focused well beyond the current aggressive trend in protein structure determination. The emerging areas of biological crystallography were identified, as summarized above. The recommendations stated below support some of the identified grand challenges in the emerging areas of this field.

A new infrastructure may be called for, both in terms of physical facilities and of interactions among organizations in the community. Some of the desired features of this new infrastructure are:

- Dedicated resident R&D expertise/personnel within APS;
- Extended beam time availability for suggested new programs, such as radiation damage studies, diffuse scattering, microfocus studies, time-domain investigations, etc.;
- Stations with flexible configurations to perform *in situ* studies using complementary tools; and
- Local availability of complementary facilities to develop integrated research programs, such as:
    - Cryoelectron microscopy
    - Associated biochemistry labs
    - In-line optical spectroscopies in experiment stations
    - Microfocus beams for biological crystallography
    - Dedicated protein SAXS, diffuse scattering, and powder diffraction capabilities
    - Resident detector development expertise

Resident physicists with long-term interest in molecular dynamics theory to perform radiation damage studies, diffuse scattering and small-angle scattering modeling, etc.

Steve Durbin (Purdue U.), John Helliwell (Manchester U.), Wayne Hendrickson (Columbia U.), Andrzej Joachimiak (ANL), Gopal Shenoy (ANL)

Summary of the Workshop on Future Directions in Synchrotron Environmental Science

Our nation, and indeed the world, currently face the daunting task of characterizing, treating, and/or disposing of vast quantities of contaminated materials, including high-level nuclear wastes, mining and industrial wastes, atmospheric pollutants, and agricultural pollutants, all of which have major impacts on human health and welfare. To address these problems, both fundamental and targeted studies of complex environmental systems at the molecular level are needed. Synchrotron radiation studies provide the precise information needed to understand these complex systems at the molecular level, thereby advancing our knowledge of processes that cannot otherwise be directly studied. The increasingly significant role of synchrotron radiation in the study of environmental systems has led to a rapidly growing field that has become known as “molecular environmental science” (MES).

Adequate resources dedicated to MES research at the APS are required to meet current and future demands. The demand for beam time is of two kinds: users conducting individual experiments and established research programs requiring extended access. At the time of this summary, no dedicated stations for MES research existed at the APS, whereas such stations do exist at each of the other DOE-supported synchrotrons.

Planning for future MES research at the APS has taken four forms, as summarized below.

Workshops on Synchrotron Environmental Science

ANL has led the way in developing the synchrotron environmental science (SES) community through two workshops held at the APS in spring 1999 (SES-I), and a follow-up workshop (SES-II) held at the APS in spring 2002. The SES workshops, attended by up to 150 participants, brought synchrotron scientists together with environmental scientists to explore opportunities for using synchrotron radiation in environmental science research, including tutorials to help foster collaborations between the environmental and the synchrotron scientists. SES-III is planned to be held in New York during 2005. The large turnout at these workshops demonstrates the growing interest in MES research.

EnviroSync

EnviroSync (http://envirosync.org; S. Sutton, chair) is a national organization representing the growing community of MES synchrotron radiation users in the U.S. A 60-page report (http://www.slac.stanford.edu/cgi-wrap/getdoc/slac-r-704.pdf) entitled "Molecular Environmental Science: An Assessment of Research Accomplishments, Available Synchrotron Radiation Facilities, and Needs" includes the following recommendations for enhancing U.S. facilities: increased operations support for existing stations, increased station availability, and increased support for essential equipment. Station availability increases might be achieved by redirection of existing stations, new stations, and/or enhanced access to innovative instrumentation.

Workshop on Future Directions in Synchrotron Environmental Science

This workshop, held in conjunction with the 2004 APS users meeting, was the first in the series on “Future Scientific Directions for the Advanced Photon Source.” Invited speakers represented a variety of environmental science endeavors, including biogeochemistry, actinide speciation, mineral-water interface processes, contaminant transport, remediation technologies, and analytical instrumentation. Participants agreed that greater recognition of the specialized needs of the environmental science synchrotron user community is needed, in large part because environmental samples are among the most demanding of those brought to a synchrotron facility. Additionally, the nature of the samples can vary significantly, as do the requirements to handle these samples under carefully controlled environmental conditions. These specialized requirements suggest that science-focused facilities/beamlines should be considered for environmental science research in addition to more distributed resources. The synchrotron user community representing environmental sciences has experienced dramatic growth over the past decade, and it is likely that the user base could double over the next decade if dedicated and fully supported facilities are made available to the community.

EnviroCAT

A new sector dedicated to environmental science has been proposed to the APS (S. Sutton, EnviroCAT Acting Director). A Letter of Intent was approved by the Program Evaluation Board in 2002. In 2003, a “Proposal to the Advanced Photon Source Scientific Advisory Committee [SAC] for an Environmental Science Collaborative Access Team and Sector” was submitted. The SAC requested a revised proposal with a clearer definition of the biological component of the project and more details and expansion of the sector design. The proposed management plan calls for 50% beam time allocation to institutional members and 50% to general users. Thus, half of the project costs would be covered by institutional funds and the other half by a federal grant. EnviroCAT currently has three institutional members: Argonne National Laboratory-Environmental Research Division, Environmental Protection Agency-National Risk Management Research Laboratory, and the University of Notre Dame. The United States Department of Agriculture is another potential member as part of the recently approved multistate project entitled “The Chemical and Physical Nature of Particulate Matter Affecting Air, Water and Soil Quality.”

Recommendations

A compelling case exists for the development of additional experimental stations for MES at the APS, primarily focused on such microscale techniques as microXAFS. This expansion can be accomplished in several ways, as described below.

Development of a New Sector

This option, the preferred approach, would greatly increase the amount of dedicated beam time for MES research, maximize scientific productivity by giving control of the beamline operations to MES scientists, and allow optimization of instrumentation for MES experiments. This option is also the most expensive approach, and insufficient monetary support has been identified at this time by the EnviroCAT group. Partnering between EnviroCAT and the APS in the development of a new sector is an option.

Reassignment of an Existing Sector

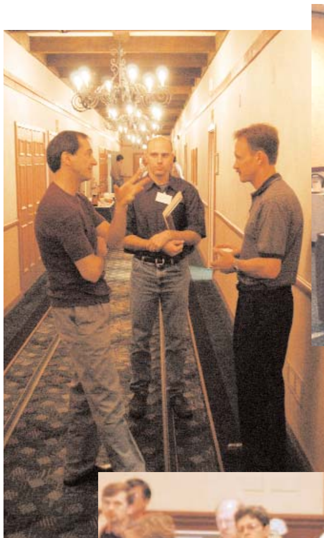
This approach will also greatly increase the available beam time dedicated to MES research, at a reduced cost compared to development of a new sector. The trade-off is that any existing sector will not be perfectly suited for MES experiments, so substantial upgrading should be anticipated. Existing EnviroCAT funding commitments are sufficient to support the operation of an existing sector. As above, partnering between EnviroCAT and the APS in the operation and upgrade of an existing sector is an option.

Augmentation of an Existing Sector

This option will increase the available beam time for MES research. It is the least expensive approach, but it will have limited effectiveness. Extensive undulator beam time (required for these brilliance limited experiments) is unavailable for this purpose at existing sectors. In addition, the merging of disparate management styles and scientific programs will lead to inefficiencies and reduced scientific productivity. It should be noted that two of the current EnviroCAT institutional members (ANL-ER and U. of Notre Dame) are currently members of MR-CAT (sector 10), a sector where such an augmentation might logically be pursued.

The APS has a tremendous opportunity to expand its impact on human welfare issues related to environmental challenges. Greatest impact will be realized through the dedication of a full sector operated by MES scientists. Augmentation of existing sectors with new MES programs will be less effective but valuable nonetheless. In all scenarios, the key to success will be the presence of beamline scientists knowledgeable in environmental science problems and willing to collaborate with users with broad differences in experience.

Steve Sutton (The U. of Chicago), Ken Kemner (ANL), Shelly Kelly (ANL), Paul Bertsch (U. of Georgia)






Clockwise from upper left: Hallway conversation during a workshop break. Gabrielle Long (ANL) at the Strategic Planning Meeting (SPM). The workshop secretariat: Bonnie Meyer, Noreen Czyz, Judy Walden, Rose Torres, Becky Forsythe, and Pam Dalman (all ANL). The Workshop on Science with High-Energy X-rays. Closing out the SPM: questions from the audience—foreground, left to right: Thomas Gog (ANL) Efim Gluskin (ANL), Keith Moffat (The Univ. of Chicago), Peter Ingram (Duke Univ. Medical Center). Akira Kira, director of SPring-8, and Bill Stirling, director of the European Synchrotron Radiation Facility, in the audience for the SPM.

APPENDIX: WORKSHOP PRESENTATIONS

Future Scientific Directions for the Advanced Photon Source

Gopal Shenoy, Argonne National Laboratory (Chair)
Sunil Sinha, University of California, San Diego (Co-chair)

Objective: The user community at the APS continues to contribute to the leadership across the frontiers of scientific knowledge in various fields of research. The objective of the study was to explore future science directions for APS users that will expand their scientific leadership and push the boundaries of the scientific frontiers in the next decade.

Approach: Through extensive survey of the national science community, an initial set of workshop topics was selected. These workshops included leaders of the scientific community who are both experts and newcomers to the use of the x-ray techniques. The general objectives for each of the workshops were:

1) Identify new opportunities for continued scientific discovery and impact using synchrotron radiation sources during the next 5 to 10 years.
2) Explore the breadth of science covered by the workshop topics, not limited to synchrotron techniques alone.
3) Discuss how the existing community can be grown by bringing scientific leaders to the workshops who will benefit from the addition of synchrotron techniques in their research arsenal.
4) Identify a few dozen new scientific programs that the participants will bring to the APS during next 5 to 10 years and evaluate the new instrumentation and operational requirements for these programs to succeed.
5) Examine existing beamline capabilities at the APS and define what future beamline capabilities would be desirable.
6) Prepare a summary document for the archival literature to serve as a roadmap for the future of the workshop topic utilizing the capabilities of the APS.

Report: The study will be documented through a report based on the summaries from each of the workshops.

Workshop on Future Directions in Synchrotron Environmental Science

May 4, 2004, APS, Argonne, Illinois

Chairs: Steve Sutton (The U. of Chicago), Ken Kemner (ANL), and Shelly Kelly (ANL)

Workshop Presentations

The purpose of the workshop is to evaluate future directions in environmental science amenable to experimentation with synchrotron radiation. The intent is to focus on frontier science and to evaluate the science-driven requirements for future instrumentation. Although the focus will be on research opportunities at the APS, this will not be a strict limitation. The outcome will be a summary to be submitted to the committee on "Future Scientific Directions for the Advanced Photon Source" chaired by G. Shenoy and S. Sinha.

Tuesday, May 4, 2004

Ken Kemner (ANL) - Overview of Synchrotron Environmental Science

Jim Frederickson (PNNL) - How do Metal-Reducing Bacteria Deal with Solid Phases?

Jeremy Fein (U. of Notre Dame) - Surface Complexation Models of Metal Cation Adsorption onto Bacterial Surfaces

Shelly Kelly (ANL) - Bioremediation of U-Contaminated Subsurface Environments and the Role of Synchrotron Based X-ray Absorption Measurements

Sam Webb (Stanford U.) - Application of Synchrotron Radiation Based Techniques to the Biogenic Oxidation of Manganese

Steve Heald (PNNL) - Environmental Science using the PNC-CAT Microprobes and Possible Future Directions

Tom Trainor (U. of Alaska) - Mineral-Water Interface Studies

Paul Fenter (ANL) - Elemental, Chemical and Structural Characterization of Mineral-Water Interfaces with X-ray Scattering Techniques

Kirk Scheckel (Environmental Protection Agency-Cincinnati) - Correlating Metal Speciation in Soils to Risk

Robert Ford (Environmental Protection Agency-Oklahoma) - Impact of Redox Disequilibria on Contaminant Transport and Remediation in Subsurface Systems

Scott Fendorf (Stanford U.) - Resolving Biogeochemical Processes of Metals within Physically and Chemical Heterogeneous Media

Workshop Summary - Paul Bertsch (U. of Georgia/SREL)

Workshop on Emerging Areas in Biological Crystallography

July 27-28, 2004, APS, Argonne, Illinois

Chairs: Wayne Hendrickson (Columbia U.), John Helliwell (Manchester U.)

Workshop Presentations

The workshop program includes plenary presentations that highlight overviews of the field and potential future in emerging areas.

Tuesday July 27, 2004

Welcoming and Opening Remarks - Wayne Hendrickson (Columbia U.)

Plenary Session I: Molecular Machines

Jack Johnson (Scripps) - Bringing Molecules to Life: Novel Blends of Crystallography and Electron Cryomicroscopy (Cryoem) t Study Virus Particle Dynamics

Wah Chiu (Baylor College of Medicine) - Electron Cryomicroscopy of Biological Assembly

Tom Steitz (Yale U.) - Structural Insights Into The Peptidyl-Transferase Reaction ad Antibiotic Resistance in the 50S Subunit

Plenary Session II: New Approaches

Zbigniew Dauter (BNL) - Locating Weak Scatterer Substructures

Richard Kahn (Institut de Biologie Structurale, Grenoble) - Fully Fledged Macromolecular Crystallography Under High Pressure and Lessons: Plea For Ultrashort-Wavelength Beamlines

Bob Von Dreele (ANL) - Biological Structures from Powder Diffraction

Plenary Session III: Radiation Damage

Elspeth Garman (Oxford) - Kill Or Cure: Radiation Damage in Cryo-Cooled Macromolecular Crystals

Max Nanao (EMBL, Grenoble) - Radiation Damage Induced Phasing

Richard Matyi (NIST) - High-Resolution Diffuse X-ray Scattering by Structurally-Defective Protein Crystals

Plenary Session IV: Dynamics

Vukica Srajer (The U. of Chicago) - Watching Proteins Function with Time-Resolved X-ray Crystallography

Lois Pollack (Cornell U.) -Time-Resolved Small-Angle X-ray Scattering Studies o Macromolecular Dynamics

Wednesday July 28, 2004

Plenary Session V: Dynamics

Gerd Rosenbaum (UGA / ANL) - Dynamics of Molecular Complexes from Small-Medium-Angle X-ry Scattering/Diffraction

Steve Durbin, (Purdue U.) - Dynamics from Nuclear Resonance Inelastic Scattering

Plenary Session VI: Microfocusing and coherent imaging applications

Gebhard Schertler (MRC) - Current Limitations of Low-Dose X-ray ad Electron Crystallography of Membrane Proteins

Ian Robinson (U.I. Urbana-Champaign) - Solution Scattering Studies of Protein Crystallization

Stefano Marchesini (LLNL) - Coherent X-ray Diffractive Imaging: Applications and Limitations

Breakout Session A:

(Microfocusing, imaging, powder diffraction, etc.)

Discussions and Summaries
Discussion Coordinators: Andrzej Joachimiak (ANL) and Keith Hodgson (SSRL)
Breakout Session B:
(Molecular machines, dynamics, radiation damage, etc.)
Discussions and Summaries
Discussion Coordinators: Wayne Hendrickson (Columbia U.) and Steve Durbin (Purdue U.)

Workshop on Frontier Science Using Soft X-rays at the APS

August 5-6, 2004, APS, Argonne, Illinois
Chairs: Richard Rosenberg (ANL), Juan Carlos Campuzano (ANL)

Workshop Presentations

Sessions highlight overviews of the field and potential applications in emerging areas.

Thursday, August 5, 2004
Session I: Richard Rosenberg, Chair
Efim Gluskin (ANL) - Welcome
Juan Carlos Campuzano (ANL) - Workshop Overview
David Paterson (ANL) - Scientific Highlights from 2-ID-B
John Freeland (ANL) - Scientific Highlights from 4-ID-C
Session II: Juan Carlos Campuzano, Chair
Marco Grioni (Ecole Polytechnique Fédérale De Lausanne) - Bulk Electronic Properties from High - and Higher - Energy Spectroscopies
Jim Allen (U. of Michigan) - Photoemission Experiments at SPring-8 Beamline BL25SU
John Carlisle (ANL) - Photoemission Studies o Nanocrystalline Diamond Films
Session III: John Freeland, Chair
George Sawatzky (U. of British Columbia) - Opportunities with Resonant Soft X-ray Scattering
Steve Kevan (U. of Oregon) - Coherent Soft X-ray Magnetic Scattering
Uwe Weierstall (Arizona State U.) - Coherent X-ray Diffractive Imaging a the Advanced Light Source
Peter Abbamonte (Cornell U.) - Hole Crystallization in the Spin Ladder Of Sr14Cu24O41
Session IV: George Srajer, Chair
John F Marko (U. of Illinois) - X-ray Study of Mitotic Chromosome Structure
Pupa De Stasio (U. of Wisconsin) - Spectromicroscopy of Cells, Tissues, and Minerals a the 10-100-Nanometer Scale
Stephan Rosenkranz (ANL) - Orbital Correlations in Complex Oxides
Jessica Thomas (BNL) - Probing Orbital and Magnetic Correlations in a Near Half-Doped Manganite with Soft X-ray Resonant Diffraction

Friday, August 6, 2004
Session V: David Keavney, Chair
JEff Kortright (LBNL) - Resonant Scattering Studies of Nanometer-Scale Structure-Property Relationships (Mostly Magnetism)
Atsushi Fujimori (U. of Tokyo) - Soft X-ray Photoemission and Magnetic Circular Dichroism o Correlated Systems and Nanomaterials
Jim Tobin (LLNL) - Using Higher Energy X-rays and Spin Detection to Go After Nonmagnetic Electron Correlation, Half-Metallic-Ferromagnetic Behavior and Magnetic Ordering
Michael Sing (Universitaet Augsburg) - Valence Bond Studies on Transition Metal Oxides by Soft X-Ray Photoemission

Workshop on Science with High-Energy X-rays

August 9-10 , 2004, APS, Argonne, Illinois
Chair: Dean Haeffner (ANL)

Workshop Presentations

The workshop presentations consist of plenary talks that highlight overviews of the field and identify future emerging areas. Many topical presentations include applications of high-energy x-rays to material science and materials engineering problems.

Monday, August 9, 2004
Dean Haeffner (ANL) - Workshop Charge and Overview of High-Energy X-ray Science at the Advanced Photon Source
Plenary Session I
Sarvjit Shastri (ANL) - Optimizing the Generation of High-Energy X-rays at the Advanced Photon Source
John Parise (SUNY Stony Brook) - Studies of Short- and Long-Range Structure at High Pressures and HighTemperatures Using High-Energy X-ray Scattering
Plenary Session II
Ersan Üstündag(Ames Lab/Iowa State U.) - Micromechanics of Materials using High Energy XRD
Gregory S. Rohrer (Carnegie Mellon U.) - Characterizing the Internal Grain Boundary Network Structure of Polycrystals: the Current State of the Art and Opportunities for High-Energy X-ray Diffraction Microscopy

Dorte Juul Jensen (Risø National Laboratory) - Current and Future Applications of 3-D XRD Microscopy in Materials Science

Plenary Session III

Andrew Allen (NIST) - Characterization of Gradient Microstructures in Complex Materials by High-Energy Small-Angle and Wide-Angle X-ray Scattering

Ronald Frahm (Bergische Universität Wuppertal) - High-Energy X-ray Absorption Spectroscopy: Current Status and Future Applications

Elliot Kanter (ANL) - Investigating Atomic Inner-Shell Phenomena with High-Energy X-rays

Plenary Session IV

Yan Gao (GE Global Research) - Present and Future Use of High-Energy X-rays for Industrial Materials Research

Valeri Petkov (Central Michigan U.) - Atomic-Scale Structure of Materials with Intrinsic Disorder by the Atomic Pair Distribution Function Technique and High-Energy X-ray Diffraction

Tuesday, August 10, 2004

Session V-A: Materials Engineering

Mark Daymond (Queen's U.) - Insights into the Deformation Mechanics of Materials Using High-Energy X-rays

Anke Pyzalla (Technical U. of Wien) - *In situ* Determination of Material Behavior Under Thermal and Mechanical Loading Using High-Energy Synchrotron Radiation

Rosa Barabash (ORNL) - Understanding of Local Dislocation Structures in Deformed Materials Based on Microdiffraction

Session VI-A: Materials Engineering

Wolfgang Pantleon (Riso National Laboratory) - Emerging Order in Dislocation Structures During Metal Loading

Todd Hufnagel (Johns Hopkins U.) - Using High-Energy X-ray Scattering to Study Micromechanics of Deformation in Metallic-Glass-Matrix Composites

Session VII-A: Materials Engineering

Mark Bourke (LANL) - Mechanical Properties: Prediction and Measurement

Hans-Rudolf Wenk (U.C. Berkeley) - High-Energy X-ray Measurements of Texture in Materials

Paul Dawson (Cornell U.) - Finite Element Modeling of Lattice Strains in Polycrystalline Metals with Comparisons to Diffraction Experiments.

Workshop Summary - Discussion Leader: Ersan Üstündag

Tuesday, August 10, 2004

Session V-B: Materials Physics

Angus P. Wilkinson (Georgia Institute of Technology) - Building a Foundation for the Future, Staying Cool, and Rocket Science, All with the Aid of High-Energy X-rays

Brian Toby (NIST) - Scientific Possibilities of High-Energy X-ray Powder Diffraction

Jonathan Hanson (BNL) - *In Situ* Time-Resolved Diffraction with High-Energy X-rays from Catalyst and Metal Oxides: Results from Rietveld Refinements and Comparisons with Neutron Diffraction Studies

Session VI-B: Materials Physics

Peter Chupas (ANL) - *In situ* Pair Distribution Function Analysis Studies

Matthew Kramer (Ames Lab/Iowa State U.) - Structural Dynamics in Metallic Glasses

Lynn Soderholm (ANL) - Actinide-ion Speciation in Solution

Session VII-B: Materials Physics

Alan Goldman (Ames Lab/ Iowa State U.) - Science Using an Electrostatic Levitation Furnace in the MU-CAT Sector at the APS

Jorg Strempfer (Max Planck Institute, Stuttgart, Germany) - Magnetic Scattering Using High-Energy X-rays

Ray Osborn (ANL) - High-Energy X-ray Diffuse Scattering

Workshop Summary - Discussion Leader: Angus Wilkinson

Workshop on Membrane Science at the APS

August 17-18, 2004, APS, Argonne, Illinois

Chairs: Millicent Firestone (ANL), Tom Irving (IIT), Jin Wang (ANL), Randall Winans (ANL)

Workshop Presentations

The workshop presentations include plenary talks highlighting overviews of the field and potential future in emerging areas of (a) biomembranes and (b) organic and iorganic membranes. All the talks address the objectives of the workshop relevant to the specific topic, identifying newer needs for future capabilities at the APS.

Tuesday, August 17, 2004

Jin Wang (ANL) - Introduction to the Workshop and Workshop Charge

Plenary Session I

Sol Gruner (Cornell U.) - Some Unanswered Questions in Membrane Science

Peter Pintauro (Case Western Reserve U.) - Polymeric Membranes for Fuel Cells: Overview and Future Outlook

Jeff Brinker (U. of New Mexico and SNL) - Self-Assembly of Biologically Inspired Complex Functional Materials

Plenary Session II

Jin Wang (ANL) - Grazing-Angle X-ray Techniques for Studying Membrane and Ultrathin Films

Miriam Rafailovich (SUNY Stony Brook) - Producing Low Density, Porous Polymer Films Using Supercritical Fluids

Michael Kent (SNL) - Protein Adsorption to Lipid Membranes through Metal-Ion Chelation Studied by X-ray and Neutron Reflectivity, and Grazing Incidence X-ray Diffraction

John Nagle (Carnegie Mellon U.) - Diffuse X-ray Scattering Provides More and Better Information about Membranes than Traditional Diffraction Methods

Plenary Session III

Huey W. Huang (Rice U.) - Biomembrane Problems Studied by X-ray and Neutron Diffraction

William J. Koros (Georgia Institute of Technology) - The Next Generation of Membrane Materials and Structures for Separation of Gas Mixtures with the Potential to Minimize Energy

Deborah Leckband (U. of I. Urbana-Champaign) - Molecular Design Rules for Biological Adhesion

Michael Tsapatsis (U. of Minnesota) - Molecular Sieve Membranes: Zeolite Films and Polymer-Selective-Flake Nanocomposites

Mark Schlossman (U. I. Chicago) - New Methods to Study Biomolecules at Liquid Surfaces

Wednesday, August 18, 2004

Plenary Session IV

Lukas Tamm (U. of Virginia) - Elastic Coupling of Membrane Protein Structure to Lipid Bilayer Forces

Martin Caffrey (Ohio State U.) - Membrane Structural Biology, Membrane Protein Structure

Sue Pierce (NIH) - The Role of Membrane Microdomains in Immune Cell Signaling

Adam Hammond (Cornell U.) - Are You In or Out: Biological Rafts and Biophysical Phases

Plenary Session V

Robert MacDonald (Northwestern U.) - X-ray Diffraction in the Study of Cationic Phospholipid Derivatives: Lipoplexes, Lipid Mixtures and Bilayer Fusion

Tobias Baumgart (Cornell U.) - Coexisting Fluid Phases in Model Membranes and Biological Membranes

KaYee Lee (The U. of Chicago) - Lipid Coralling and Poloxamer Squeeze-Out in Membranes

Plenary Session: VI

Larry Scott (IIT) - Lateral Organization in Lipid Bilayers: Atomistic and Coarse-Grained Simulations

Gerard C. L. Wong (U. of I. Urbana-Champaign) - Self-Assembled Complexes of Biopolymers and Charged Membranes

Giselle Sandi-Tapia (ANL) - In Situ SAXS and GISAXS Studies of Polymeric Membranes for Energy Applications

Larry Lurio (Northern Illinois U.) - Use of X-ray Coherence to Study Dynamics in Thin Films, Layered Systems, and Membranes

Plenary Session VII

Workshop Discussion and Summary - Leaders: Millicent Firestone, Tom Irving, Randy Winans, Jin Wang

Workshop on Emerging Scientific Opportunities Using X-ray Imaging

August 29-September 1, 2004, Fontana, Wisconsin

Chairs: Francesco De Carlo (ANL), Wha-Keat Lee (ANL), Stuart Stock (Northwestern U.)

Workshop Presentations

The workshop presentations include plenary talks that highlight overviews of the field and potential future in emerging scientific areas that will benefit from x-ray imaging techniques. The topical presentations cover materials science, complex systems, and life sciences.

Sunday, August 29, 2004

Stuart Stock (Northwestern U. Medical School) - Introduction to the Workshop and Grand Challenges of Emerging Science Using X-ray Imaging

Gabrielle Long (ANL) - Introduction to the Advanced Photon Source

Monday, August 30 , 2004

Plenary Session I - Overviews

Wah-Keat Lee (ANL) - Welcoming Remarks and Charge to Participants

Jose Baruchel (ESRF) - Emerging Scientific Opportunities with X-ray Imaging at ESRF

Yoshiro Suzuki (SPring-8) - Emerging Scientific Opportunities with X-ray Imaging at SPring-8

Wah-Keat Lee (ANL) - Emerging Scientific Opportunities with X-ray Imaging at APS

Plenary Session II - Overviews

Erik Ritman (Mayo Clinic, Rochester) - Research Needs and Opportunities for Micro-CT of Microcirculatory Structure and Function

Ersan Üstündag (Iowa State U., Ames Lab) - Imaging Composite Materials Using X-rays

John Spence (Arizona State U.) - Lensless Imaging in Materials Science and Biology

Mark Rivers (The U. of Chicago) - Complexities in Astrogeological Systems

Session A-1: Materials Science and Complex Systems

Harry Martz (LLNL/Center for Nondestructive Characterization) - X-ray Nondestructive Characterization of Mesoscale (mm Extent with Micrometer Features) Objects

Jan Ilavsky (ANL) - Challenges in Microstructure Characterization of Engineered Materials by X-ray Microtomography

Session A-2: Life Sciences

Mark Westneat (Field Museum) - X-ray Imaging of Small Animal Functions

Kathleen Donohue (Harvard U.) - The Evolution of Novel Fruit Morphology in a Tribe of Mustards: Can Structural Changes in the Pericarp Influence Geographic Distribution?

J. W. Hagadorn (Amherst College) - Tentative: Understanding Paleocommunities from Sedimentary Structures and Fossils

Plenary Session III: Overviews

Stuart Stock (Northwestern U. Medical School) - Complementarity of X-ray Techniques

Steve Wilkins (CSIRO) - Emerging Scientific Opportunities for Hard X-ray Phase-Contrast Imaging Using Synchrotron Radiation

Tuesday, August 31, 2004

Plenary Session IV - Overviews

Christoph Rau (U. of I. Urbana-Champaign) - Imaging and Tomography on the Nanometer Lengthscale

Chris Jacobsen (SUNY Stony Brook) - Lensless X-ray Imaging Using Computational Phasing: Progress at Stony Brook

Jin Wang (ANL) - Hydrodynamics of Fluid Jets

Session B-1: Materials Science and Complex Systems

I. C. Noyan (IBM) - X-ray Microtopography: Mapping Deformation Fields in Integrated Circuit Metallization

Kimberley Kurtis (Georgia Institute of Technology) - X-ray Characterization of Cement-based Materials: Previous Applications and New Opportunities

Bernie Koziozemski (LLNL/NIF) - Inertial Confinement Fusions Target Characterization

Session B-2: Life Sciences

Beth Brainerd (U. of Massachusetts) - *In Vivo* X-ray Imaging in Biomechanics and Developmental Biology

Jon Harrison (Arizona State U.) - X-ray Imaging as a Tool to Investigate Insect Gas Exchange: Questions, Initial Results, and a Wish List

Charles Boyce (The U. of Chicago) - The Evolution of Cell Wall Biochemistry in Fossil and Living Plants

Session C-1: Materials Science and Complex Systems

Michael Pivovaroff (LLNL) - Hard X-ray Optics for Astronomy and the Laboratory

James Glazier (Indiana U., Bloomington) - The Properties and Problems of Liquid Foams

Lyle Levine (NIST) - Imaging of Deformed Metals

Yong Chu (ANL) - Time-Resolved X-ray Diffraction Imaging of Ferroelectric Domains in Barium Titanate Single Crystals

Session C-2: Life Sciences

Dean Chapman (U. of Saskatchewan) - Tentative: The Contrast Mechanisms in Biological X-ray Imaging

Steve Cook (U. of Utah) - Liquid Feeding in Ants (Formicidae): Using X-ray Imaging to Study Mechanisms of Ingestion

Wednesday, September 1, 2004

Session D-1: Materials Science and Complex Systems: Report from Breakout Session Leader : Stuart Stock

Session D-2: Life Sciences

Workshop on Time Domain Science Using X-ray Techniques

August 29-September 1, 2004, Fontana, Wisconsin

Lin Chen (ANL), David Reis (U. of Michigan), Steve Milton (ANL)

Workshop Presentations

The workshop presentations include plenary talks that highlight overviews of the field and potential future in emerging scientific areas in time domain science. Additional topical presentations cover the area of (1) gas phase dynamics, (2) chemical and biological science, and (3) condensed matter. A special session is dedicated to two presentations that address the limitations of the storage ring in compressing electron bunches in the APS below about 40 ps, and on a new scheme to reduce the bunch width by an order of magnitude.

Sunday, August 29, 2004

David Reis (U. of Michigan) - Introduction to the Workshop: Synchrotron Radiation Investigations and Grand Challenges of Time Domain Science

Lin Chen (ANL) - Introduction to the Advanced Photon Source

Monday, August 30, 2004

Plenary Session I

Linda Young (ANL) - Welcoming and Charge to Participants

Phil Bucksbaum (U. of Michigan) - Opportunities for Ultrafast X-ray Physics

Phillip Anfinrud (NIH) - Watching Proteins Function with Picosecond Time-Resolved X-ray Crystallography

Roberto Merlin (U. of Michigan) - Tentative: Collective Excitations in Condensed Matter

Session A-1: Gas Phase Dynamics

Steve Southworth (ANL) - Pump-Probe Studies of Atomic Inner-Shell Photoionization and Vacancy Decay

Chii-Dong Lin (Kansas State U.) - Probing Auger Decays in the Time Domain

Nora Berrah (Western Michigan U.) - Probing Dynamic in Correlated Systems

Session A-2: Chemical and Biological Science

Gerald Meyer (The Johns Hopkins U.) - Photoinduced Charge Transfer with Transition Metal Coordination Compounds

Jeffery Zink (U.C., Los Angeles) - Molecular Machines: Rotational Motion, Molecular Impellers, and an Operational Nanovalve

David Tiede (ANL) Measuring Molecular Structure and Dynamics in Liquids Using Wide-Angle Scattering/Diffraction

Session A-3: Condensed Matter

T. K. Sham (Western Ontario U.) - Time-Dependence X-ray Excited Optical Luminescence in Nanoscaled Systems and Related Phenomena

Justin Wark (Oxford U.) - Modelling of Time-Resolved X-ray Diffraction from Laser-Shocked Crystals

Andrea Cavalleri (LBNL) - Tentative: Insulator-Metal Transitions

Plenary Session II

Keith Moffat (The U. of Chicago) - Ultrafast Time-Resolved Macromolecular Crystallography

Shin-ichi Adachi (Photon Factory) - Time-Resolved X-ray Diffraction at the Photon Factory Advanced Ring (PF-AR) to Probe Photo-Induced Phase Transition in Organic CT Crystals

Marcos Dantus (Michigan State U.) - Coherent Laser Control of Physicochemical Processes

Larry Lurio (Northern Illinois U.) - Coherence and Time-Resolved Studies

Plenary Session III

John Byrd (LBNL) - Tentative: Potential for Ultrashort Electron Bunches from Storage Rings

Alexander Zholents (LBNL) - Possibilities for Obtaining Subpicosecond X-ray Pulses at the Advanced Photon Source

Tuesday, August 31, 2004

Plenary Session IV

Philip Coppens (SUNY Buffalo) - The Potential of Time-Resolved Diffraction at Atomic Resolution: What is Needed for its Further Development?

Eric Collet (U. of Rennes) - Photo-Induced Phase Transition Probed by Time-Resolved X-ray Diffraction

Tamar Seideman (Northwestern U.) - Controlling External Molecular Modes with Intense Light

Session B-1: Gas Phase Dynamics

Steve Pratt (ANL) - Geometry-Dependent Molecular Photoionization Dynamics

Stefan Vajda (ANL) - Gas Phase Dynamics in Small Molecules: From Analysis to Control

Session B-2: Chemical and Biological Science

Christoph Rose-Petruck (Brown U.) - Ultrafast Laser-Pump XAFS-Probe Measurements of Solvated Transition Metal Coordination Complexes Using a Table-Top X-ray Source

Mike Wasielewski (Northwestern U.) - Photochemistry, Molecular Devices, and Utrafast Molecular Dynamics

Session B-3: Condensed Matter

Susan Dexheimer (Washington State U.) - Ultrafast Electronic and Vibrational Dynamics in Quasi-One-Dimensional Molecular Solids

Nitash Balsara (U.C., Berkeley) - Formation of the Critical Nucleus in Phase-Separating Polymer Blends

Plenary Session V

James Norris (The U. of Chicago) - Tentative: Investigating Photosythesis

Paul Evans (U. of Wisconsin, Madison) - Nanosecond Switching Dynamics in Ferroelectric Devices

Lin Chen (ANL) - Capturing Transient Molecular Structures in Photochemical Reactions by Laser Initiated Time-resolved X-ray Spectroscopy

Peter Abbamonte, (BNL) - Imaging Electronic Motion with Attosecond Time Resolution

Wednesday, September 1, 2004

Session C-1: Gas Phase Dynamics

Ali Belkacem (LBNL) - Pump-Probe Studies of K-Shell Photoionization and Vacancy Decay of Alkali Atoms at the ALS

Robin Santra (JILA) - Xenon Clusters in Intense VUV Laser Fields

Session C-2: Chemical and Biological Science

James McCusker (Michigan State U.) - Ultrafast Spin and Structural Isomerization Dynamics in Transition Metal Complexes

Bob Schoenlein (LBNL) - Development of an Undulator Beamline for Ultrafast X-ray Science at the ALS

Session C-3: Condensed Matter

Larry Lurio (Northern Illinois U.) - Tentative: Dynamics of Polymer Films

Robert Leheny (The Johns Hopkins U.) - XPCS and the Nanoscale Dynamics in Soft Glassy Colloidal Systems

Plenary Session VI

Workshop Report Presentations - Leaders: Lin Chen, Davis Reis, Linda Young

Workshop on Mesoscopic and Nanoscopic Science

August 29-September 1, 2004, Fontana, Wisconsin

Chairs: Sunil Sinha (U.C., San Diego), Eric Isaacs (ANL/The U. of Chicago)

Workshop Presentations

Plenary sessions highlight overviews of the field and potential future in emerging scientific areas of mescopic and nanoscopic science. The sessions address the objectives of the workshop, which is to conduct a truly interactive dialogue between experts in the field of mesoscopic/nanoscopic science from various perspectives and work towards focused recommendations for future synchrotron-based studies and capabilities, specifically identifying newer needs for future capabilities at the APS.

Sunday, August 29, 2004

Dennis Mills (ANL) - Welcoming Remarks

Sunil Sinha (U.C., San Diego/LANL) - Introduction to Workshop: Synchrotron Radiation Investigations and Grand Challenges of Mesoscopic and Nanoscopic Science

Eric Isaacs (ANL/The U. of Chicago) - Introduction to the Advanced Photon Source

Monday, August 30, 2004

Plenary Session I: Frontier Examples of Nanoscale Characterization

Chair: Heinrich Jaeger (The U. of Chicago)

Sunil Sinha (U.C., San Diego/LANL) - Welcoming Remarks and Charge to Participants

Paul Voyles (U. of Wisconsin, Madison) - Future Nanocharacterization with Electrons: Sub-Angstrom, Sub-eV, and Single Atom

Miquel Salmeron (LBNL) - Tentative: Physical Methods to Understand the Behavior of Nano-Droplets
Zhonghou Cai (ANL) - X-ray Diffraction Studies of Internal Structures of Individual Nanoscale Materials
Mark Sutton (McGill U.) - Mesoscopic Characterization Using X-ray Speckle Spectroscopy
Ross Harder (U.I. Urbana-Champaign) - Nanoscale Imaging Through Coherent X-ray Diffraction
Mark Ratnar (Northwestern U.) - Tentative: Properties of Molecular Assemblies

Plenary Session II: Synthesis, Transport, Granular Systems - St. Moritz

Chair: Mike Bedzyk (Northwestern U.)
Massimiliano Di Ventra (U.C., San Diego) - Transport in Molecular Structures: An Overview of Present Understanding
Avi Ulman (Brooklyn Polytechnic Institute) - Tentative: Novel Methods of Synthesis of Nanomaterials
Heinrich Jaeger (The U. of Chicago) - TBD
Stephen Gray (ANL) - Theoretical Modeling of Nanoscale Confined Light: From Metal Nanoparticles to Nanoholes
Eric Isaacs (ANL/The U. of Chicago) - Overview of Center for Nanoscale Materials at Argonne

Tuesday, August 31, 2004

Plenary Session III: Soft and Hard Matter

Chair: Paul Voyles (U. of Wisconsin, Madison)
Detlef Smilgies (CHESS) - Nanostructured Functional Materials via Self-Organization in Organic Thin Films - What Can We Learn from Synchrotron X-ray Scattering?
Miriam Rafailovich (SUNY Stony Brook) - Tentative: Bio-nano Composites
Woowon Kang (The U. of Chicago) - Tentative: Reentrant Insulating Phase and Fractional Quantum Hall Effect in a Two-Dimensional Electron System
Alex Groisman (U.C., San Diego) - Tentative: Microfluidics and Applications to Biophysics
Yao Lin (U. of Massachusetts) - Studies of Nanoparticle Assemblies at Fluid Interfaces
Jin Wang (ANL) - Kinetics of Nanoassemblies
Carol Thompson (Northern Illinois U.) - X-ray Studies of Ferroelectrics

Plenary Session IV: Magnetism, Photonics

Chair: Woowan Kang (The U. of Chicago)
Ivan Schuller (U.C., San Diego) - Tentative: Confined Magnetism - An Overview
Gabriel Aeppli (U. College, London) - Tentative: Quantum Magnetism in Nanosystems
David R. Smith (U. of C. San Diego) - Tentative: Materials with Negative Refractive Index

Wednesday, September 1, 2004

Plenary Session V: Summary and Wrap-Up

Chairs: Sunil Sinha (U.C., San Diego/LANL and Eric Isaacs (ANL/The U. of Chicago)

Workshop on Nanomagnetism Using X-ray Techniques

August 29-September 1, 2004, Fontana, Wisconsin

Sam Bader (ANL), Laura Lewis (BNL), George Srajer (ANL)

Workshop Presentations

The workshop presentations include plenary talks that highlight overviews of the field and potential future in emerging scientific areas of nanomagnetism. A set of topical presentations covers the areas of (a) confined magnetism, (b) cluster magnetism, and (c) phase-separated systems/complex oxides.

Sunday, August 29, 2004

Sam Bader (ANL) - Introduction to the Workshop: Synchrotron Radiation Investigations and Grand Challenges of Nanomagnetism
George Srajer (ANL) - Introduction to the Advanced Photon Source

Monday, August 30, 2004

Plenary Session I

Laura Lewis (BNL) - Welcoming Remarks and Charge to Participants
Ivan Schuller (U.C., San Diego) - Emerging Areas of Magnetism in Confined Structures
Art Epstein (Ohio State U.) - Tentative: Emerging Areas of Cluster Magnetism
Elbio Dagotto (Florida State U.) - Complexity in Transition Metal Oxides

Sessions A-1: Confined Magnetism

Paul Crowell (U. of Minnesota) - Spin Dynamics in Ferromagnetic Microstructures
Axel Hoffmann (ANL) - Magnetic Structure at Buried Interfaces
T. C. Schulthess (ORNL) - Studying Nanomagnetism with Computational Techniques
Caroline L'Abbe (Katholieke Universiteit, Leuven) - New Perspectives for Site- Selective Magnetization Measurements Using Nuclear Resonant Scattering
David Keavney (ANL) - Studies of Confined Systems Using Soft X-ray Magnetic Microscopy

Sessions A-2: Cluster Magnetism

Mark Freeman (U. of Alberta) - Ultrafast Magnetization Dynamics from Continuous Films to Nanoparticles
R. Kawakami (UC, Santa Barbara) - Molecule-Based Spintronics and Possibilities for X-ray Spectroscopy
Klaus Attenkofer (ANL) - How Can X-ray Studies Contribute to the Field of Molecular Magnets?

Sessions A-3: Phase-Separated Systems / Complex Oxides

Myron Salamon (U. of I. Urbana-Champaign) - Phase Separation or Griffiths Phase in Doped Manganites?
Thomas Rosenbaum (The U. of Chicago) - Non-Linear Dynamics in Spin Liquids
Peter Schiffer (Penn. State) - Defect-Controlled Ferromagnetism in the Canonical Ferromagnetic Semiconductor (Ga,Mn)As
Daniel Haskel (ANL) - Beyond Element Specific Magnetism: Magnetic Spectroscopy in the Diffraction Channel

Plenary Session II

Caroline Ross (MIT) - Magnetic Behavior of Small Patterned Structures
Gabriel Aeppli (U. College, London) - Quantum Magnetism in Novel Materials and Geometries
Chris Leighton (U. of Minnesota) - Intergranular GMR in a Spontaneously Phase-Separated Perovskite Oxide
Jonathan Lang (ANL) - Overview of Synchrotron Techniques for Nanomagnetism Studies

Tuesday, August 31, 2004

Plenary Session III

Eric Fullerton (Hitachi Global Storage Technologies) - Nanostructured Magnetic Materials for High-Density Storage Applications
Myriam Sarachik (CCNY-CUNY) - Quantum Tunneling in a Single Molecule Magnet
Kenneth Gray (ANL) - Surface Magnetic and Electronic Properties of Layered Manganite Single Crystals

Sessions B-1: Confined Magnetism

Jon Slaughter (Freescale Semiconductor, Inc.-a subsidiary of Motorola) - Properties of Magnetic Tunnel Junction Bits for MRAM
Hendrik Ohldag (SSRL/ALS): Nanomagnetism and Polarized Soft X-ray Spectromicroscopy - How Sensitive Can We Be?
David Lederman (U. of West Virginia) - Tentative: Understanding of the Exchange Bias Systems

Sessions B-2: Cluster Magnetism

Kannan Krishnan (U. of Washington) - Magnetic Material Function and Size
Sara Majetich (Carnegie Mellon U.) - X-ray Investigation of Magnetic Nanoparticle Assemblies
Jeff Kortright (LBNL) - Tentative: Resolving Magnetic and Chemical Heterogeneity in Thin Films with Soft X-Ray Resonant Scattering

Sessions B-3: Phase-Separated Systems/Complex Oxides

Soonyong Park (Rutgers U.) - Magneto-Electric and Magneto-Dielectric Effects in REMn 2O5
John Freeland (ANL) - Loss of Ferromagnetism and Intrinsic Insulators at the Surface of Naturally Layered Manganites
Charles Fadley (U.C., Davis) - Synchrotron Radiation Studies of Colossal Magnetoresistive Oxides and Buried GMR and MTJ Interfaces

Plenary Session IV

Theme Discussion Leaders Present Preliminary Summary of Emerging Ideas
Chia-Ling Chien (The Johns Hopkins U.) - Tentative: Spin Torque and Nanorings
Talat Rahaman (Kansas State U.) - Tentative: Tailoring of Properties of Magnetic Clusters
Jonathan Sun (IBM) - Spin-Transfer Induced Switching in Magnetic Nanopillars

Wednesday, September 1, 2004

Pleanary Session V

Presentation of Summaries - Leaders:
Sam Bader (ANL), Laura Lewis (BNL), George Srajer (ANL)

Strategic Planning Meeting

September 2-3, 2004, Fontana, Wisconsin

Thursday, September 2, 2004

Session I: Murray Gibson (ANL) - Welcoming remarks

Gabrielle Long (ANL) - Charge to participants

Lin Chen (ANL), David Reis (U. of Michigan), Linda Young (ANL) - Report from the Workshop on Time Domain Science using X-ray Techniques

Ercan Alp (ANL) - Report on Inelastic X-ray Scattering

Session II: Wah-Keat Lee (ANL), Stuart Stock (Northwestern U. Medical School) - Report from the Workshop on Emerging Scientific Opportunities Using X-ray Imaging

Eric Isaacs (ANL/The U. of Chicago) - Report from the Workshop on Mesoscopic and Nanoscopic Science

Session III: Millicent Firestone (ANL), Randall Winans (ANL) - Report from the Workshop on Membrane Science

Gabrielle Long (ANL) - Report from XOR sectors (Slides)

Session IV: Steve Sutton (The U. of Chicago), Ken Kemner (ANL), Shelly Kelly (ANL) - Report from the Workshop on Future Directions in Synchrotron Environmental Science

Juan Carlos Campuzano (ANL) - Report from the Workshop on Frontier Science using Soft X-rays at the APS

Friday, September 3, 2004

Session V: Sam Bader (ANL), Laura Lewis (Brookhaven National Laboratory), George Srajer (ANL) - Report from the Workshop on Nanomagnetism Using X-ray Techniques

Greg Boebinger (NHMFL) - A Big Magnet at the APS?

Session VI: Dean Haeffner (ANL) - Report from the Workshop on Science with High-Energy X-rays

tba - Report from the Workshop on Emerging Areas in Biological Crystallography

Session VII: Murray Gibson and Gabrielle Long - Discussion and Wrap-up