Workshop on Science with High-Energy X-rays: Executive Summary

by Dean R. Haeffner, workshop chair

A workshop entitled "Science with High Energy X-rays" was held on August 9 and 10, 2004, at the Advanced Photon Source. This workshop was one of the eight workshops in the series on defining the Future Scientific Directions for the Advanced Photon Source held during the summer of 2004. The goal of this workshop was to identify the emerging scientific areas that could benefit from the use of high energy x-rays at the Advanced Photon Source. The statements of scope, objectives, and charge to participants for the workshop are given in Appendix A.

The 49 participants of 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 well represented. Topics for the 28 presentations ranged over a large variety of scientific areas, including materials science, condensed mater 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 program for the workshop is given in Appendix B and the scientific advisory committee, local organizing committee, and list of participants in Appendix C.

The first day of the workshop consisted of a series of plenary talks that highlight major areas of high-energy x-ray research (3D x-ray microscopy, micromechanics of materials, rapid pair distribution function measurements), and several other talks that showed the breath 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 session, 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* 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 materials engineering 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 materials engineering 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.

Relating 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 *inter*-granular mechanics,
- Microstructure characterization (dislocation structures, etc.),
- Kinetics studies,
- Coatings,
- Buried interfaces,
- Residual stresses (in small structures, components, welds, etc.), and
- High-rate deformation (with μsec 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 to 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 is chemistry/structure for the bulk versus the surface in concrete).

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 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.

Appendix A
Scope, Objectives, and Workshop Charge

1. Scope

The synchrotron radiation facilities based 6-8 GeV storage rings are well suited to deliver high-energy x-rays in the 50 keV to 150 keV range. The high energy x-rays not only penetrate through highly dense materials, but with the wavelength being shorter than the inter-atomic separation in materials, the processes involved in their interaction with matter change. Hence when the traditional x-ray scattering and absorption techniques are used with high energy x-rays one obtains newer insights in to material science. For example, diffuse scattering measurements will permit a quantitative analysis of several Brillouin zones since the Ewald sphere is flat at high x-ray energies. The complex terms in the x-ray magnetic scattering cross-section are simplified when the x-ray energy is high, thus simplifying the data analysis on magnetic structures. High-energy x-rays can penetrate deeply into a sample and can be used to measure true bulk properties. Also, they can probe through environmental chambers that are inaccessible to lower energy x-rays, allowing for experiments in extreme conditions and for many types of *in situ* studies. In many cases, high-energy x-rays have penetration capabilities comparable to neutrons, but with much better spatial resolution and considerably higher flux. Examples of high-energy x-ray research include measurements of stress/strain in materials, powder diffraction of compounds containing heavy elements, diffuse scattering of defects in complex oxides, pair-distribution-function measurements of amorphous materials, and high-energy small-angle scattering from thermal-barrier coatings.

The workshop focuses one following topics:

- Interaction of high energy x-rays with matter
- Grand challenges in the field of materials science and technology in the next decade
- Use of high energy x-rays to meet grand challenges in material science and engineering.
- Unique application of high energy x-rays to atomic science, chemical science, and condensed matter physics.
- Science at extreme environments

The user demand for high-energy x-ray experiments is growing rapidly, and current capabilities for some of the techniques are heavily oversubscribed. Opportunities exist to further enhance the high-energy x-ray capabilities at the APS through optimization of optics and insertions devices, and through the development of dedicated instrumentation. Such optimization will increase the available high-energy flux by more that an order of magnitude.

The purpose of this workshop is to explore the emerging scientific opportunities using high energy x-rays, and to seek input from both instrumentation experts and interested scientists on possibilities for the development of future high-energy x-ray facilities at the APS.

2. Objectives

a) Explore new and emerging scientific and technological areas defined in the scope of this workshop.
b) Broaden the community interaction by including researchers from various methodologies (E.g., EM, Neutron Scattering, Etc,)
c) Identify new scientific proposals/programs specific to the emerging areas which can benefit from the use of high energy x-rays that the participants will bring to the APS during next 5 to 10 years. Also evaluate the capital and operational requirements for these proposals/programs.
d) In addition to available beamline capabilities at the APS, identify future needs to support research in this area of science and technology.
e) Address the need and support for theoretical work to strengthen the experimental research.
f) Prepare a summary document for the archival literature to serve as a roadmap for the future applications of high-energy x-rays and suggest the role of the Advanced Photon Source towards this objective.

3. Charge to the Participants

a) Identify “Grand Challenges” (science and technological) to be addressed during the next 5-10 years which require or high-energy x-rays
b) Identify and justify the technical requirements to meet the Grand Challenges
    - New instrumentation and techniques that need be developed on existing beamlines to perform new kind of science.
    - Need for a new dedicated beamline(s) for this community
c) Identify R&D areas that will prepare the community to address the Grand Challenges