Workshop on Emerging Scientific Opportunities Using X-ray Imaging: Summary and Recommendations August 29-September 1, 2004

The workshop on "Emerging Scientific Opportunities Using X-ray Imaging" was held from August 29 through September 1, 2004 as part of a series of workshops on the "Future Scientific Directions for the Advanced Photon Source." The scope was limited to imaging with photon energies above ~ 6 keV in order to minimize overlap with another workshop. The goals of the workshop were first to identify grand scientific challenges that can be addressed by x-ray imaging and second to define the next-generation imaging characteristics required to solve these outstanding puzzles. A diverse group of internationally renowned leaders in disciplines including geology, paleontology, biology, medicine, engineering materials (structural, electronic, magnetic), complex systems (foams, fluid flow, fuel cells, real-time processes) and x-ray imaging assembled for the workshop. The participants presented not only the frontiers in their fields but also speculated on the wilderness beyond. The participants were balanced between current and potential users of synchrotron radiation, and representatives of imaging efforts at ESRF, SPring-8, the Canadian Light Source and the Australian synchrotron contributed perspectives. The broad diversity of biological and physical sciences/engineering requiring advanced x-ray imaging dictated two parallel tracks of discussion, and this summary integrates the many imaging requirements common to both as well as discipline-specific needs.

High impact experiments addressing "grand challenges" are those producing results that: change how others do their science, have major economic impact and/or re-write textbooks. A constant refrain in the life sciences and materials science/complex systems discussions was that the dependence of function or macroscopic properties on a hierarchy of structural length scales (nm to cm) and that multiple observations on the interior of specimens are often essential.

In the materials and complex systems arena, grand challenges include understanding:

M1. *Materials deformation, fatigue and fracture:* This includes service-related deformation, texture development during processing, crack initiation, crack opening and closing phenomenon during crack propagation. In all of these areas, current models are woefully inadequate in predicting behavior across the hierarchy of structural scales. Modeling efforts are hamstrung by lack of correlated experimental data across the multiple size scales.

M2. *Failure mechanisms within engineered structures:* The two paradigms here are 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 disinterred without destroying the information of interest and subtle effects separate marginal, failure-prone ULSI 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. Following environmental attack *in situ* and noninvasively with 1 μm resolution in centimeter-sized samples is required as is 100 nm resolution in smaller samples.

M3. *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. In the life sciences domain, grand challenges enumerated include:

L1. *Developing a digital micromorphometry library*: Library for small organisms and for anatomical microstructures (e.g., plant root hairs, insect tracheal systems, microcirculation networks, bone microstructure) analogous to the National Library of Medicine “Visible Human Project” and NSF “Digital Morphology Project.”

L2. *Real time microscopic imaging of physiological processes:* In small organisms opaque to visible light, these processes (breathing, circulation, feeding, reproduction, etc.) remain almost totally uninvestigated due to the lack of a probe providing micrometer resolution for temporally changing internal structures. The necessary x-ray techniques have been demonstrated only recently, and the discovery of active respiratory pumping in certain insects invalidates current textbook treatments.

L3. *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, and x-ray image tags, analogous to luciferase, need to be developed.

L4. *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?

L5. *Discovery and description of early terrestrial (extraterrestrial?) life (micro-fossils):* In its earliest stages, life was microscopic, and these micro-fossils are difficult to find and, once found, 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 x-ray imaging will revolutionize this field.

Much world-class imaging is done at various places at APS, but a focused effort and facilities are needed to convert the scattered effort into a core activity second to none. The participants concluded the following. First, high definition x-ray imaging must be supported (large field of view + high spatial resolution + high contrast sensitivity), and this requires clean, stable optics and improved detectors (with zooming capability). Second, very high throughput is essential (i.e., it is not necessary to show one type of ants show tracheal compression but rather where it is/is not present across different insect groups). Third, many new users will not be proficient at imaging, and friendly analysis tools (shared software for remote data analysis) and local analysis team will be required for these users to exploit large amounts of unfamiliar types of data. Fourth, imaging under different environments is important. Both phase and absorption contrast techniques must be supported (other modalities are of interest), and the ability to perform multi-mode x-ray studies (i.e., x-ray microbeam diffraction/small angle scattering with absorption microCT) is crucial, either through a common sample position indexing environment or multi-purpose apparatus. The APS effort should be guided by the ESRF imaging experience: many areas of current research were not originally envisioned and their community is very heterogeneous and requires more staff support than other techniques where the users have a common physical sciences background.