Emerging Opportunities in High-Energy X-ray Science: The Diffraction-Limited Storage Ring Frontier

The worldwide march to electron storage rings with diffraction-limited photon properties in the X-ray regime is well underway. First out of the gate is MAX-IV in Sweden, scheduled for operation in 2016, followed by SIRIUS in Brazil in 2018; both are greenfield rings operating at 3 GeV with ~520 m circumference and emittances of ~250 pm-rad. They will be followed by the upgrade of ESRF, operating at 6 GeV with a target emittance of 150 pm-rad and operational date of 2020. The upgrade of the APS at Argonne National Laboratory (6 GeV, 60 pm-rad) is anticipated to follow shortly thereafter.

Taking advantage of the 2015 International Synchrotron Radiation Instrumentation Meeting in New York, a workshop at Argonne on July 13–14, 2015, entitled "Emerging Opportunities in High-Energy X-ray Science: The Diffraction-Limited Storage Ring Frontier," was organized as a satellite meeting to discuss scientific opportunities brought about by the exceptional capabilities of these light sources. Roughly 80 researchers from the U.S., Germany, Denmark, Korea, China, Japan, and France participated in a highly interactive two-day workshop.

After being welcomed by Linda Young, the plenary session was kicked off by Henning Poulsen (Technical University of Denmark), who presented hard X-ray microscopy for multiscale materials science with the aim of extending 3D movies and 3D modeling from the coarse (mm) to the very fine (nm) scales. Stimulating talks followed, by Wendy Mao (Stanford) on opportunities in high-pressure science, Matt Tirrell (U Chicago) on soft matter, Sossina Haile (Caltech/Northwestern) on electrochemical processes, Joe Hupp (Northwestern) on catalysis, and Gayle Woloschack/Tatjana Paunesku (Northwestern) on nanoprobes of biological mechanisms. The post-lunch plenary session continued with two talks in which considerations and opportunities stemming from improved transverse coherence and optics were presented by Brian Stephenson and Xianbo Shi (Argonne).

Day 1 focus sessions were held on structural materials, chemistry and industrial applications, environmental and earth science. Grand challenges in structural materials were presented by Tony Rollett (Carnegie Mellon University) and Peter Voorhees (Northwestern), both of whom stressed the need for understanding materials behavior under extreme manufacturing or operating conditions and the new opportunities afforded by characterization of stress/strain at the individual grain level with the new experimental X-ray and high-performance computational tools. Uta Ruett (DESY) described the surface diffraction beamlines, operating at energies higher than 50 keV, at PETRA III, presently the brightest X-ray synchrotron (6 GeV, 1-nmrad). It was noted that the proposed APS-U will bring a 100-fold improved brightness over that existing today at PETRA III. In the Chemistry and Industrial Applications Session, Wenbin Lin (U Chicago) described exciting applications in sustainable catalysis and artificial photosynthesis enabled by inspired design of metal-organic framework (MOF) molecules. The MOFs feature size- and enantio-selectivity, recyclability and reusability, synthetic tenability, and record high turnover number. Conal Murray (IBM) discussed the trend toward nanoelectronics and the many material and structural issues that affect device performance; e.g., strained Si channels for enhanced carrier mobility, effect of dopant density on contact resistance. In the Extreme Conditions and Environmental Science focus session, Tony Lanzirotti (U Chicago) gave examples of the diverse geoscience problems where new opportunities arise due to the ability of high-brightness X-rays to probe geosystems, which possess inherent extreme heterogeneity, from the nanoscale to mesoscale with elemental and chemical sensitivity. Jennifer Jackson (Caltech) described how synchrotron Mössbauer spectroscopy and inelastic X-ray scattering can provide insight on the dynamics of hot, dense materials at the core-mantle boundary and the impact of the timing structure for these studies. Day 1 ended with a lively reception and dinner at the Argonne Guest House.

Day 2 continued with focus sessions on Materials Synthesis/Condensed Matter and Soft Materials and Bioscience. Oleg Shpyrko (UCSD) gave a fascinating talk on "Coherent X-ray NanoVision" that showed the universality in time-length scales for exploring dynamical problems in soft materials with those in more standard materials science and the new insights available with coherent scattering. Examples presented included research in battery materials, imaging single defects in materials, and calculations for the ultimate resolution for coherent X-ray diffraction imaging. Darrell Schlom (Cornell) discussed how to realize the Materials by Design dream with the proper toolkit, which includes an *in situ* oxide MBE machine at a synchrotron in order to understand how oxide thin films grow. To put folks in the right frame of mind for further brainstorming, John Freeland (Argonne) recapped an earlier workshop on frontier experiments in condensed matter physics. In the Soft Materials and Bioscience focus session, Stephen Cheng (Akron) introduced the audience to the world of nano-atoms, compact rigid molecular particles that possess precisely defined symmetry and surface functionalities with end-to-end distances of ~1 nm. Hyunjung Kim (Sogang University) showed how coherence with hard X-rays enables probes of dynamics and structure using X-ray photon correlation spectroscopy. Bob Leheny (Johns Hopkins) recapped the earlier workshop on soft materials with specific experiments; e.g., nonlinear response to mechanical stress, interactions and assembly at fluid interfaces, and structure and dynamics of biomembranes.

The workshop turned out to be an excellent follow-up to the series of workshops on