Workshop on Scientific Opportunities in Soft Matter and Biophysics at NSLS-II

September 5-6, 2003
Student Activity Center, Stony Brook University
Stony Brook, NY

Workshop Discussion Leaders and Organizers -- *Front Row*: Dave Litster, Simon Mochrie, Nitash Balsara, Chi-Chang Kao, Lin Yang; *Second Row*: Janos Kirz, Sol Gruner, Stephen Cheng, Ben Chu, Timothy Lodge; *Third Row*: Ben Ocko, Noel Clark, Richard Register; *Back Row*: Mathias Lösche, Ron Pindak, Christian Burger, Paul Heiney; *Missing from photo*: Robert Austin, Ben Hsaio, Ian Robinson, Helmut Strey

Workshop Organizers:

Ben Chu, *Stony Brook University*

Ben Hsiao, *Stony Brook University*

Ben Ocko, *Brookhaven National Laboratory*

Ron Pindak, *National Synchrotron Light Source*

Helmut Strey, *Stony Brook University*

Workshop Coordinators:

Corinne Messana, *National Synchrotron Light Source*

Jane Wainio, Stony Brook University

A workshop on "Scientific Opportunities in Soft Matter and Biophysics at NSLS-II" was held on September 5th and 6th at the Student Activity Center at Stony Brook University, Stony Brook, NY. Evening sessions and the workshop banquet were held at the nearby Danford's Inn in Port Jefferson, NY. 32 participants attended the workshop representing the subfields of polymers, complex-fluids, liquid-crystals, colloids, and biophysics. Although these subfields are distinct, researchers in these subfields utilize similar synchrotron x-ray techniques so a joint workshop was organized to promote a cross-fertilization of ideas between the different groups.

The first discussion topic of the workshop was the new source. This discussion session began with a presentation by Steve Dierker (*NSLS*) on the review process that lead to the recommendation to Brookhaven National Laboratory to submit a proposal for a new synchrotron source and the specifications of the proposed NSLS-II source. The next two discussion sessions focused on the critical components involved in doing synchrotron research; namely, the beamlines and optics, lead by Lonny Berman (*NSLS*), and fast, large-area, detectors, lead by Peter Siddons (*NSLS*).

The workshop participants unanimously agreed that NSLS-II has the opportunity to distinguish itself from other third generation sources by taking an integrated project approach that involves, from the earliest stages, *parallel development* of all the key project components including:

- optimized insertion devices
- fast x-ray area detectors
- optics for focusing hard and soft x-ray beams
- user friendly data reduction and analysis software
- manipulators for nano-samples
- integral in-situ probes such as a high-resolution optical microscope incorporated into a x-ray nano-probe beamline
- ancillary facilities for handling bio-hazard samples
- sample handling assemblies as flow cells fabricated using the facilities of the Brookhaven Center for Functional Nanomaterials

Moreover, it was decided that, achieving measurements out to length scales that overlapped what could be achieved with visible light and eliminating the need for optics, would require the installation of an extra-long beamline. This beamline would be used for x-ray photon correlation spectroscopy and ultra small-angle scattering (USAXS) studies. Moreover, it was suggested that pairs of canted permanent magnet undulators in longer straight sections be evaluated as potential replacements for single, continuously tuneable, superconducting undulators. It was also suggested that a higher energy ring be evaluated as a potential way to achieve single, continuously tuneable, permanent magnet undulators.

Discussions then turned to the scientific challenges that would be addressed using the high-brightness NSLS-II source. The workshop was fortunate to have, among its discussion leaders, researchers with editorial positions at three of the major journals in the field: “Polymer”, Senior Editor, Stephen Cheng (*Univ. of Akron*), “Macromolecules”, Editor-in-Chief, Timothy Lodge (*Univ. of Minnesota*), and “Liquid Crystals”, Editor, Noel Clark (*Univ. of Colorado*). Also, leading one of the discussion sessions was Sol Gruner, Director of *CHESS*, a synchrotron facility noted for strong programs in soft matter and biophysics. The remaining discussion sessions were lead by equally distinguished scientists each with considerable synchrotron x-ray experience:

Robert Austin (*Princeton Univ.)*
Nitash Balsara (*U.C. Berkeley*)
Christian Burger (*Stony Brook Univ*.)
Paul Heiney (*Univ. of Pennsylvania*)
Janos Kirz (*Stony Brook Univ*.)
David Litster (*M.I.T.*)
Mathias Lösche (*NIST and Johns Hopkins Univ*.)
Simon Mochrie (*Yale Univ.*)
Richard Register (*Princeton Univ*.)
Ian Robinson (*Univ. of Illinois, Urbana*)
Lin Yang (*National Synchrotron Light Source*)

Science challenges in soft matter and biophysics were identified and discussed, but the workshop participants agreed that the exciting problems identified were only ‘the tip of the iceburg’. Because soft matter and biophysics are rapidly growing research areas, a steady stream of new, challenging structural problems were anticipated well into the future.

On the second day of the workshop, the participants formed two working groups: one in Soft Matter (polymers, complex-fluids, liquid-crystals, colloids) and the other in Biophysics. Based on discussions of the previous day, each group identified the main research directions in which significant breakthroughs were most likely to occur. These research directions included:

In Soft Matter (Polymers, Complex Fluids, Liquid Crystals, Colloids) --

- Processing
- Nanocomposites
- Kinetics of phase transitions
- Ultra thin organic films
- Hierarchical structures in polymers
- Complex phases
- Interfaces between different phases and confined geometries
- Liquid crystals and colloids
- Complex solutions
- Dynamics of fluctuations

In Biophysics --

- Dynamics of biomolecules in solution
- Ultra-fast dynamics in biomolecules

- Hierarchical biological systems
- Counterions clouds
- Structural studies of membrane proteins using two-dimensional crystals
- Signal transduction, neuron plasticity
- Biomimetic devices
- Synthetic biomolecular systems
- Nanofluidics and coherent imaging
- Imaging of organelles

The discussions leaders agreed to summarize developments and future perspectives in each of these research directions for inclusion in the NSLS-II science case.

Finally, the working groups also identified the different types of synchrotron beamlines that would be required to address the science challenges in the field. The forefront problems invariably required the source brightness provided by undulators so these devices were emphasized. A fraction of an undulator beam, since it preserves the source brightness, was preferred to bending magnet beam. The table below contains the suite of insertion device beamlines needed for soft matter and biophysics research, the features enabled by a high-brightness source that each beamline would utilize, and the techniques for which each beamline would be optimized.

Suite of Soft Matter and Biophysics Insertion Device Beamlines		
ID Beamline	Features emphasized	Techniques
SAXS	Small (μm) mirror-focused beam	Small and Wide Angle X-ray Scattering (SAXS and WAXS)
GISAXS	Small (μm) mirror-focused beam, downward-deflection	Glancing Incidence SAXS and diffraction, Liquid scattering
Nanoprobe 1	Ultrasmall (~30nm) optic-focused beam of hard x-rays (3-20 keV) Integral in-situ probes (high-resolution microscopy)	High-res tomography, High-res anomalous and fluorescence imaging, Diffraction-imaging
Nanoprobe 2	Ultrasmall (~15nm) optic-focused beam of soft x-rays (0.5-3 keV)	Spectromicroscopy, Diffraction-imaging
ASAXS	Energy tunability	Low-energy, Anomalous SAXS, Resonant scattering
USAXS	Optics-free operation	XPCS, Ultra Small Angle Scattering (USAXS)
IXS	Energy resolution	Inelastic X-ray Scattering