1-ID Phase II Upgrade

The 1- ID beamline currently supports three programs, (1) high-energy diffraction microscopy (HEDM), (2) high-energy SAXS/WAXS studies and (3) high-energy structural studies. These programs share the 1-ID-C hutch, with some HEDM work also performed in the 1-ID-B hutch, and are enabled by the high brilliance, high-energy x-rays available at 1-ID. Similar to other programs originated at 1-ID which have subsequently moved to other have dedicated instruments at other beamlines (for example, phase contrast imaging and Rapid-PDF), these three programs have experienced significant growth in recent years. This growth has led to high oversubscription rates (~5 as of run 2009-2). With such high levels of demand for beamtime, outreach to potential user communities is not possible. Furthermore, the need to share limited hutch real-estate has restricted the quality of scientific output by diverting staff efforts towards set-up/tear-down modes at the expense of measurement quality and optimization and staff productivity for data analysis.

In order to alleviate this situation, we propose to build a new white-beam hutch (1-ID-D) downstream of 1-ID-C which will house the HEDM program. The high-energy SAXS/WAXS program will remain in the 1-ID-C hutch, while the structural science work will primarily move to the 1-ID-B hutch. These plans are consistent with the larger goal of increasing high-energy capability to the APS, as presented in a number of scientific cases in the APS renewal. This upgrade will not fully solve the problem of oversubscription, but can allow for more productive use of beamtime, since instruments will remain in their optimized modes and beamtime will not be needed to track down setup artifacts.

Further justification for this proposal can be broken down to four key areas:

- A. Strengthen scientific output
 - a. HEDM. A significant part of the development work on HEDM over the past 2 years and certainly since being awarded a PUP has been to lower the barriers to new users. For example, Prof. Armand Beaudoin at the University of Illinois – who is deeply entrenched in the modeling community with very little experimental background – has recognized the potential represented by the data from the HEDM experiments and is now writing GUP proposals to validate plasticity, fracture and dislocation mechanics theories. The development of dedicated experimental facilities for HEDM would further lower these barriers by allowing better instrument optimization and would allow more resources to be applied to improved data analysis – the other significant bottleneck in the field. There is considerable potential for application of the HEDM technique to other user communities such as ceramics, geology, high pressure, and small (and possibly large) molecular crystallography, so the ability for greater accessibility to more users, combined with greater participation from the materials modeling community will strengthen the scientific case to provide more beamtime access for this technique.

- b. HE-SAXS/WAXS. This program is already heavily oversubscribed and productive, with a diverse scientific base including bio-materials deformation, chemistry/synthesis, layered systems for energy applications (fuel cells / thermal-barrier coatings, etc) and nuclear materials. All of the studies benefit from the unique high-brilliance, high-energy x-rays available at 1-ID, and would likely grow if additional beamtime were available. For example, the nuclear materials community has a key need for non-destructive, in-situ thermo-mechanical characterization of microstructural and strain evolution in extant and novel materials for fuel cladding and related structural applications, which can be uniquely met with this probe. A dedicated hutch will enhance the efficiency of available beamtime and somewhat enhance availability
- c. HE structural studies. This program will remain unique at the APS with energy tunability at high-energies, which enables resonant scattering studies of high-Z elements. This program will continue it's focus on studies of fundamental structures and structural changes under various environmental conditions that relate to properties, activities and functionalities of materials.

B. Automation

HEDM necessitates accurate sample alignment, positioning control during deformation, and detector synchronization during data acquisition. Essentially all procedures are repetitive and the potential for automation has been demonstrated. However, further progress is inhibited by the lack of dedicated hardware. Automation would significantly facilitate to accommodate non-expert users, reduce setup and data acquisition time, and improve data quality. Although automation is somewhat less of an issue for the other high-energy programs, similar arguments hold and automation will be pursued.

C. Efficiency and data quality

The rebuilding of instrumental setups during beamtime is highly inefficient and compromises data quality. Beamtime is consumed to find and remove sources of spurious scattering that change each with each reconstruction of the experimental environment and would reduce data quality. When these artifacts cannot be eliminated due to the pressure to start experimental, their recognition and removal from the large data sets is often the most time consuming part of the analysis and often impairs the scientific value of experiments. Development of dedicated instrumental setups would allow many of these problems to be addressed and solved permanently.

D. Ability to advance experimental techniques

a. HEDM: At present the separation of the near- and far-field techniques in the 1-ID B and C-hutches does not allow the simultaneous observation of strain and grain boundary topology/orientation during deformation. Such data would establish a new level of interaction with the modeling community. One of the most important frontiers in the area of micromechanical testing is the determination of the spatially resolved stress tensor during in-situ loading. An important modeling question is the deconvolution of orientation vs. neighborhood effects during the deformation of polycrystals. The near+far experiment would enable that understanding. A significant software development will be required on both sides to exploit the enormous data sets. Real data is required, noting that highest resolution is not needed initially, to initiate these developments.

- b. HE- SAXS/WAXS. Hutch dedication will have a number of positive effects. First, since this technique is often used with advanced sample environments (e.g. MTS thermo-mechanical device), it will aid in the optimization and development of such ancillary equipment. Second, it will enable detectors to be optimized for simultaneous SAXS/WAXS studies, which are currently limited to sequential mode for most cases. This will open up a number of time-resolved studies in the msec regime not currently available. Third, it will allow more efficient setup and use of diffracted beam apertures (conical and spiral slits) for three-dimensional mapping, which have often been requested by users. Finally, it will provide an improved framework to add further operational modalities, including radiographic imaging and laser spectrometry, which have been recently requested by users.
- c. HE structural studies. Dedicated instruments will provide opportunities to conduct a range of experiments including resonant scattering, high-resolution single crystal or powder diffraction, diffuse scattering and charge density studies. As for the other programs, the use of high-energies will enable use of a variety of environmental chambers to study these materials in extreme conditions of pressure, pressure and high electric and magnetic fields.

E. Future work

Additional upgrade work will be needed to continue this upgrade to 1-ID. Several options are being considered for white-beam delivery to 1-ID-D and await availability of engineering resources to explore further. However, the main impact from lack of ability to delivery white beam to this hutch is to limit the range of focusing options available for the HEDM program.