Extreme Conditions: High Energy Diffraction
Scientific Case for the Sector 1 Upgrade

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Executive Summary

Upgraded Sector 1 beamlines will enable transformational studies in basic and applied materials science and engineering. Basic, in that many underlying principles have not yet been verified because appropriate observations have not been possible. Applied, in that they underlie the properties, lifetime, and reliability of materials that are used every day in every sector of the economy. Relevant to engineering materials, because the measurement techniques can be applied to complex materials from metallic alloys to ceramic composites to irradiated reactor components.

Phenomena occurring inside of bulk materials that have long been hypothesized and even modeled will finally become observable during processing: grain boundary motions in polycrystals; development of anisotropic, inhomogeneous stress fields due to thermo-mechanical treatments; formation of self-organized defect structures under deformation; spatially resolved stress distributions and partitioning in composite materials; phase and microstructural evolution at buried interfaces of operating batteries; and bulk dynamics associated with freezing. All these phenomena are known from ex-situ, destructive measurements, but now, for the first time, all can be directly observed under realistic conditions with currently emerging high energy x-ray techniques. This ability to follow microscopic and microstructural changes can be used to train and/or validate computational models that operate on the same variables. Model development will leverage measurements beyond anecdotal observations of individual samples.

Spatially resolved studies inside of bulk materials require high brilliance at high x-ray energies (> 40keV) with a small, stable source that allows micron scale or better focusing. This work relies on the specific characteristics of the APS that set it apart from lower energy sources. Those characteristics will be enhanced through facility and beamline upgrades. Similar high energy capabilities are currently being implemented at the European Synchrotron Radiation Facility (ESRF) and at Petra-III at Hamburg. Current strong international ties combined with comparable upgraded beamlines assure continuing mutually beneficial interactions between these efforts.

Current experimental work at Sector 1 places the APS in a world leading position in high energy x-ray applications to materials. Upgraded beamlines will maintain this position. While technique development work at Sector 1 has allowed proof-of-principle measurements, upgraded beamlines will yield greatly increased resolution (real space, reciprocal space and temporal), facilitate the combining of techniques – greatly multiplying their impact – and provide dedicated setups that result in more efficient use of beamtime and greater experimental throughput. Combined high energy diffraction microscopy (HEDM) near- and far-field measurements will result in unprecedented spatial maps of crystallographic orientation fields and lattice strain states. Addition of sub-micron resolution tomography yields correlations with inhomogeneities that play crucial roles in materials performance. Combined small beam small- and wide-angle x-ray scattering (SAXS/WAXS) will yield data sets spanning length scales from nanometers to millimeters spanning a hierarchy of structures in complex, multi-component materials. Data collection times currently on the order of 24 hours should be reducible to minutes enabling more realistic in situ investigations. Advanced data handling, image analysis, and visualization will be crucial enabling elements allowing some dedicated setups to be tailored for non-expert users and, potentially, for mail-in measurements.

Current facilities are inadequate to meet current demand. As high energy capabilities are disseminated to the materials and engineering communities, demand is accelerating. Thus, upgraded beamlines will be timely and likely oversubscribed. Users include domestic and international scientists who collaborate with beamline staff in technique development, and, increasingly, those who bring new materials and problems for study. Users come from universities, national laboratories, and industries. The breadth of this community reflects the economic, national security, and energy related impacts of a Sector 1, high energy scattering facility, upgrade.

A Scientific Case

The following subsections describe major materials science and engineering research areas that will be part of the upgraded Sector 1 portfolio. Measurement techniques, which overlap between topics, are described as needed. Specific upgrade components that will benefit each area are described and referenced to the draft Conceptual Design Report (CDR).

A.1 Thermo-mechanical response of polycrystals

The vast majority of the solid materials used in engineered systems are polycrystalline. That is, they are comprised of many single crystals (typically referred to as "grains") joined together by a three dimensional network of internal interfaces called grain boundaries. Polycrystals are complex non-equilibrium systems with history dependent properties. Scientists have been working towards a predictive understanding of this class of materials (or at least specific subsets) for over 100 years yet most structure-property relationships employed in design are largely empirical. The large over-design or "factors of safety" reflect our level of level of confidence in most failure criteria. A true predictive capability for a process like fatigue would make possible lighter, more efficient designs combined with elevated safety factors. That we rely on them in so many applications (air frames, turbine blades, nuclear energy systems, etc) makes achieving this goal critically important. Macroscopic properties of polycrystals emerge from a hierarchy of structures that begin at the nano-scale (crystal structure, lattice defects and grain boundary structures) and pass to the meso- and macro-scales (grain size and orientation and grain boundary type distributions).

Under realistic processing and application conditions, polycrystals undergo complex changes at all the above length scales. Under applied loads, lattice defects are generated and can self-assemble into complex structures within the grains. Due to anisotropic properties, the stress state experienced by each crystal varies significantly within the aggregate and evolves as the individual crystals transition from a purely elastic state into elastic-plastic deformation. Crystallographic axes within grains can rotate and grains can break up into multiple different orientations. Grain boundaries can move to allow regions with preferred orientations to grow. At elevated temperatures, crystal defects can migrate and grain boundaries can move to minimize interfacial free energy under intrinsically anisotropic forces that drive the system toward equilibrium. At elevated temperatures and under loads, complicated combinations of these ordering and disordering responses become active.

Due to the empirical nature of our current "structure-property" understanding, learning to quantitatively understand, predict and, eventually, control the above processes would enable game changing advances in process and product design. The idea of integrated computational materials engineering (ICME), [1] for example, is based on the assumption of the ability to accurately model materials behavior in realistic applied environments. The traditional paradigm of comparative studies of different samples treated differently (necessitated by the fact that essentially all probes are limited to near surface regions) needs to be augmented by the ability to track the evolution of a particular volume of microstructure as it evolves and to do so over a statistically representative volume of material. Such observations can be directly compared to modeled evolution.

With the development at third generation high energy synchrotron sources of high energy x-ray diffraction microscopy (HEDM) techniques (at APS Sector 1, ESRF and soon Petra-III), it has become possible to track internal materials responses on the length scale of single grains and at the same time to cover a large ensemble of interacting grains. This tracking of "real materials in real time" under realistic conditions lends itself to the interaction with model development just mentioned and as illustrated below.

HEDM uses a monochromatic incident beam and rotates the sample about an axis normal to the incident beam to observe many Bragg peaks from each grain in an illuminated volume. Measurements currently can be separated into two classes: strain sensitive far-field and near-field orientation mapping. [2, 3] Both use a focused (or small) incident beam and measure diffraction in transmission using one or more area detectors.

Near field HEDM mapping measurements use a high spatial resolution ($\sim 1.5\mu$m), small area detector (say, 3×3mm^2 field of view) placed several millimeters downstream of the sample. [2, 4, 5] A line focused beam ($\sim 3\mu\text{m}\times1.3$mm) illuminates a planar section of a millimeter sized sample that is rotated about the normal to the illuminated plane. Bragg scattering generates projected outlines of grain contours on the detector. Rotation yields many images of each grain. The crystal orientation field is reconstructed via high performance computations which match scattering from simulated microstructures to that observed in the experiment. [2, 3, 4, 5] An example of a three dimensional reconstructed microstructure is given in Fig. 1a while a thermal coarsening measurement in nickel is illustrated in Fig. 1b. [6]

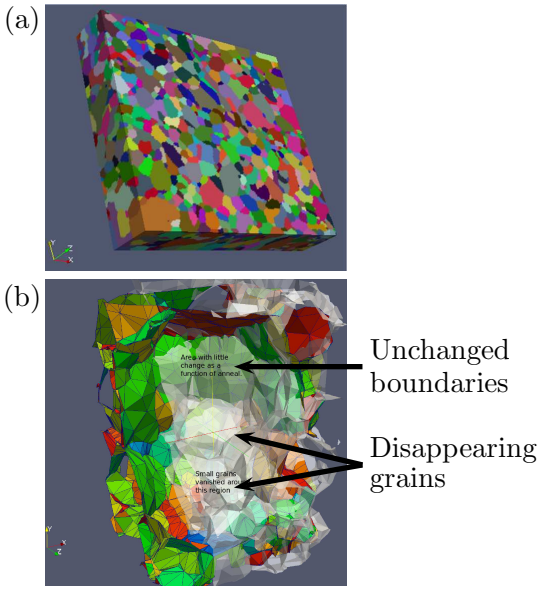

Figure 1: (a) Three dimensional grain structure of a dilute Ni-Bi alloy sample. Colors are mapped from the local orientations of crystallographic axes. The long sides are $\approx 600\mu$m while the thickness is 288μm. This same volume has been re-measured after annealing in order to observe grain boundary motions. (b) A section of three dimensional grain boundary meshes from inside a nickel sample illustrating the disappearance of small grains as the sample is annealed. Translucent white is the initial state while colors are the annealed structure with colors representing misorientation angles across the boundaries. [6] Such data sets present a unique opportunity to "train" computational models of grain growth, for example, by characterizing grain boundaries by their five mesoscopic parameters [7, 8] and allowing the energy-mobility product of each type to vary in order to optimize tracking of the experimental data.

In addition to maps of well ordered grains as in Fig. 1, it is also possible to map defected materials to determine orientation fields that include low angle boundaries that can be modeled as geometrically necessary dislocation densities. This ability means that a host of real materials and processes can be studied. One DOE/BES project is tracking damage accumulation under ductile deformation in copper [9] and zirconium. Orientation fields inside of shock deformed copper have been measured in combination with tomography measurements yielding void locations and geometries. [10] Industrially important fracture processes are being correlated with prior microstructures and damage accumulation near the fracture surface. [11] It is expected that all of these measurements will be used in model development and checking.

Far field measurements place a large detector ~ 1 meter downstream of the sample so as to detect several orders of diffraction. The use of a small beam allows separation of scattering from individual grains. Sophisticated indexing software groups together Bragg scattering from each grain yielding crystal orientations. Subtle radial motions of diffraction spots yield lattice strains in different crystallographic directions and, thus, full strain tensors that are coupled with crystal

orientations relative to sample (and, for example, externally applied tensile) axes. The following discussion illustrates such a measurement and another novel opportunity in model development involving a tight interplay between measurements and simulations.

To conduct polycrystal simulations, the single crystal elastic moduli are needed. But, for many important alloys and for new materials, they are unknown. High Energy Diffraction Microscopy (HEDM) experiments at APS Sector 1 measure lattice strains of individual crystals within a deforming polycrystalline aggregate – we measure the response of individual crystals "in the wild." Since the stress state of each crystal varies, this experiment is equivalent to testing a set of individual single crystals under different loading conditions. Figure 2 depicts the process employed. [12] Four grains were tracked during loading. Twenty or so lattice strains from each crystal (i.e., different Bragg peaks) were measured when the macroscopic stress value changed from 500 MPa to 700 MPa. The stress-strain curve is shown in Fig. 2a. The experimental setup at 1-ID-C is shown in Fig. 2c. From the measured lattice strain values we determined the lattice strain tensor associated with the load change for each of the crystals. One of the most important findings from previous HEDM work is the fact that stress states vary considerably from one crystal to the next within a sample loaded in a simple state of stress like uniaxial tension. Each crystal experiences a unique stress state due to the single crystal anisotropy and the local loading conditions. So a polycrystal actually represents a test bed of specimens.

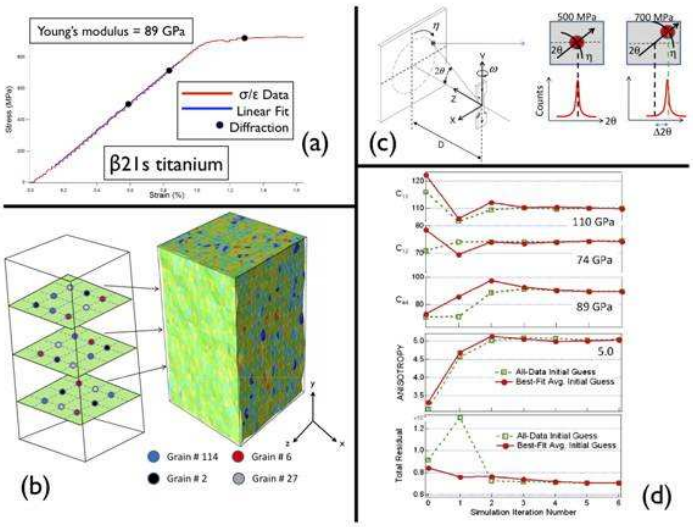

Figure 2: (a) Macroscopic stress-strain curve for the $\beta 21s$ alloy along with the linear fit in the elastic regime. Points where diffraction experiments were conducted are shown. (b) A schematic illustrating the locations of each grain within the deformed finite element simulation mesh. Each of the subject grains appears six times. The virtual sample contained 16,200 grains and 648,000 finite elements. (c) (Left) Schematic of the experimental configuration at 1-ID-C. A point on the detector is defined by η and 2θ and the diffraction experiment is conducted at a particular specimen orientation, ω. (Right) Depiction of the radial 2θ shift associated with one reflection from one crystal. This shift is converted into a normal lattice strain associated with a particular scattering vector. (d) Values of elastic moduli (GPa), the anisotropy ratio, A, and the total residual as a function of iteration number of the optimization process.

Determination of elastic moduli requires both a model (some form of Hooke's law) and experimental data. This is shown in Fig.2a where the slope of the macroscopic stress-strain curve is converted to Young's modulus. To determine the single crystal moduli, the model in this case is a polycrystal finite element simulation of the diffraction experiment conducted at Sector 1. The finite element mesh is shown in Fig.2b. The idea is to systematically vary the single crystal elastic moduli in the simulation until the simulated elastic strain tensor matches the lattice strain tensor measured using diffraction. In the experiments, we knew the location of each of the four grains (crystallites) but we did not know the orientation of the surrounding crystals. Therefore, we put the four crystals in the aggregate six times and took the average response. We formulated a residual

consisting of the difference between the measured and computed lattice strains, then implemented the fitting process within an optimization formulation - rerunning the finite element simulation each time the values were changed. The values of the elastic moduli were constrained to produce the macroscopic modulus of 89 GPa. The progress of the iteration process is shown in Fig.2d. Two different methods for approximating the initial values were employed. As can be seen, the values of the moduli converged quite rapidly. This is a good example of an application where BOTH grain resolved measurements and simulation are essential - we cannot determine moduli without both.

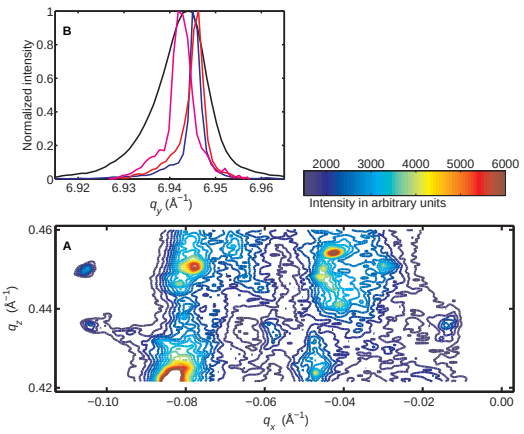

Figure 3: Three dimensional high resolution reciprocal space map of a deformed copper grain. [13] A: azimuthal projection. Sharp peaks (from almost dislocation free subgrains) can be distinguished from a diffuse background (from dislocation rich walls separating subgrains). B: radial projection. Plotted are the grain integrated profile (black) and profiles of three distinct subgrains. The narrow widths of the individual subgrain peaks indicates that they are essentially dislocation free. The relative shifts of the subgrain peaks indicate significant inter-granular strains between subgrains.

By increasing the sample-to-detector distance even further than in the conventional far-field setting, the reciprocal space resolution is increased such that peak broadening due to deformation of the undistorted crystal lattice can be quantified within individual grains. [13] The development of the high resolution reciprocal space mapping technique at the APS 1-ID beamline has been enabled by the ongoing high energy optics development program. [14] The formation of a hierarchical dislocation structure in copper has been investigated during plastic deformation. The understanding of the ordering of dislocations into structures is of fundamental and applied interest since it affects the flow stress, work-hardening rate, and fatigue behavior.

The diffraction signal from individual almost dislocation free subgrains can be separated from the diffuse contribution from dislocation rich walls that separate subgrains (Fig. 3). Information on the crystallographic orientation, volume, lattice strain, and dislocation density of the subgrains has been extracted. Measurements have been performed in situ during tensile deformation. Novel insight into strain partitioning, [15] subgrain formation and evolution, [16] and evolution under load path change [17] has been gained. Together with the near- and far-field HEDM modes, length scale coverage extends from individual dislocations to macroscopic averages.

Single grain HEDM measurements can be applied to a wide range of samples and materials problems. In addition to the case studies presented here, recent work includes Martensitic phase transformation, [18] the stress state of emerging twins, [19] phase transformation and electric loading in a ferroelectric. [20] Ongoing work includes yield surface mapping, high pressure variant selection during phase transformations, strain mapping around a crack tip, and granular materials.

Upgrade opportunities. A major shortcoming of the work described above is that the near-field measurements do not resolve strain fields and the far-field measurements do not yield precise spatial information. Whereas currently the measurements are performed in separate hutches, the beamline upgrade will bring them both into the E-hutch (CDR Fig. 4.5.4-2) and optimize apparatus

for combined measurements. A dual screen near-field detector will be semi-transparent and allow diffracted beams to propagate to the far-field detector(s). Optimizing the measurement so that intra-granular strain gradients can be spatially resolved is challenging. This may require a more highly monochromatic incident beam (CDR Fig. 4.5.4-5) which will reduce the on-sample flux. Since near-field measurements are already count rate limited, tailored undulator sources will be required (CDR 4.5.4.2 and 4.5.4.5). Focusing optics (CDR Sec. 4.5.4.4) require improvement to reach isotropic one micron resolution. Beam and apparatus stability are critical to achieving micron or better resolution. Large far-field detector arrays (CDR Figure 4.5.4-6) will directly yield improved strain resolution.

While tomographic resolution of a few microns can be obtained and registered with near-field measurements, an important class of work requires even better resolution. Short fatigue cracks that form along grain boundaries, for example, may have sub-micron dimensions. The upgrade will allow for very long path length tomography achieved by putting a sample stage in the B hutch followed by an expanding refractive lens. An area detector in the D or E hutch should then obtain ~ 100 nm resolution. A similar system is being built at Petra-III. Tomography combined with HEDM local measurements offers the possibility for a "zoom-in" capability in which a large sample region is quickly surveyed to locate interesting features (cracks, inclusions, precipitates) and then local structural measurements (orientation and/or strain mapping) are concentrated on these regions.

Very high demand can be expected for the broadly applicable (to basic and applied materials) techniques described here; information they provide is unique, is required for modeling, and is broadly sought. User demand is already on the rise and will accelerate as early results become broadly disseminated. Increased capacity represented by expansion to two beamlines is needed for the flexibility, for instance, to use a side station hutch to house a "service" facility for measurements in relatively standard sample environments.

A.2 In-situ studies of coatings and buried interfaces

Coatings in applied materials systems contain complex microstructures, multiple phases, and structural gradients through multiple layers. Buried interfaces play critical roles in these systems (coherence, cohesion, cracking) as well as in a host of other synthetic layered structures including electronically interesting ceramic interfaces. [21] These complex systems need to operate in extreme environments of temperature, chemistry, and strain and need to do so with high reliability. Relevant applications include batteries, fuel cells, and environmental barrier coatings used in turbine parts for both electricity production and propulsion. Both porosity and grain size can span a broad range of size scales, from nanometers to hundreds of microns. The morphology of inter-phase interfaces plays an important role in performance, for example, determining the strain response of buckled vs. flat interfaces. Combined small and wide angle x-ray scattering (SAX/WAXS), as developed at Sector 1, using a small, high energy incident beam in combination with large area detectors allows one to probe the entire range of length scales within a single, spatially resolved measurement. Additional information on interface morphology can be gleaned with high energy x-ray reflectivity (XRR), while crystallographic structure transitions can be probed by crystal truncation rod scattering. These powerful tools will be brought together with the upgrade, using high energy x-rays which are essential to probe deep inside of thick ($\sim$ mm scale) samples as needed to be statistically representative. High brilliance allows small focal spots to be achieved and allows for rapid measurements yielding time resolved information. Measurements of this technologically important class of system thus rely on the unique characteristics of the APS. As in the case of Sec. A.1, similar capabilities for high energy SAXS/WAXS/XRR are being developed at ESRF and Petra-III on beamlines that will be similar to the upgraded Sector 1.

Recent work at 1-ID includes studies of solid oxide fuel cells [22], thermal-barrier coatings [23] and hard coatings [24]. Measurements reveal strain and phase evolution over many grains simultaneously but with spatial resolution typically smaller than the coating layer thickness. The thermo-mechanical environments developed for these studies have allowed materials behavior to be studied under realistic conditions providing critical and unique information for materials engineers. For example, the ability to perform mechanical loading up to 1200°C provided Northwestern scientists and their partners at Rolls-Royce unique thermo-mechanical data needed to evaluate new and existing environmental barrier coatings. [25] APS-U provides an opportunity for ever more advanced in-situ environments where needed to best simulate service conditions. In the case of the environmental barrier coatings (EBCs), for example, one would like to perform the high-temperature studies under steam environments (Keiser cells), which is a crucial test to evaluate EBCs but, because of added complexity, requires dedicated setup space APS-U would provide.

One of the key systems to be studied with these capabilities will be batteries, as illustrated in Fig. 4. In order to create battery systems to meet developing and future needs, new materials need to be observed in operando to understand why they fail and how to improve them to achieve the desired technological demands. Such studies of full battery cells, several mm thick including casing, are only possible with the penetrating high energy x-rays. Similar to the solid oxide fuel cell studies mentioned above, microstructural heterogeneity can be mapped in 4d (space + time) to resolve internal strain, grain size and phase evolution. Particular issues in Li-based batteries which can be addressed include the identification and growth kinetics of solid-electrolyte interfaces, and strain and microstructural development during lithiation/delithiation of the electrodes. Using a focused x-ray beam, the component layers and interfaces within the battery can be examined during charge/discharge cycling. Both external and especially, internal ANL collaborations will be fostered to ensure the most relevant batteries are studied, including lithium-ion and lithium-air systems.

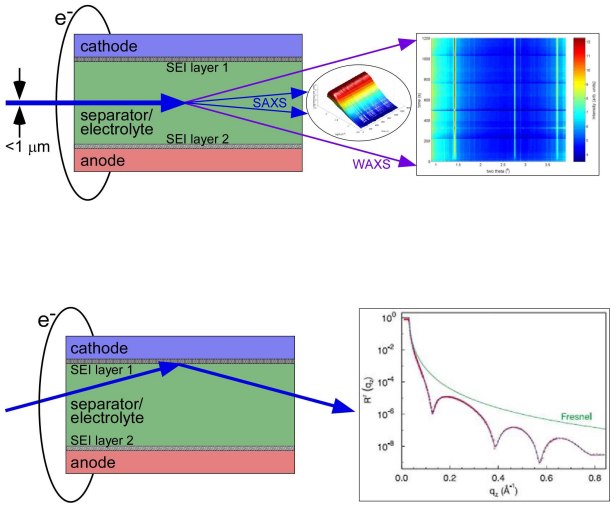

Figure 4: Buried interfaces in batteries and other layered systems can be investigated in-situ with proposed APS-U techniques. Bulk structural information can be simultaneously recorded using (a) high-energy SAXS, providing nano-particle/porosity size and shape and WAXS, providing crystallographic phase, texture and strain. By translating the sample with respect to the focused x-ray beam, structural gradient information can be directly measured. Images from reference [26]. (b) Enhanced surface/interface sensitivity can be obtained with the same probe beam using x-ray reflectivity (shown providing an electron density profile normal to an interface) as well as glancing-incidence SAXS and WAXS and crystal truncation rod measurements.

In addition to battery systems, these high energy x-ray techniques will benefit the scientific community by providing a tool to probe deeply into systems that require millimeter length-scale of thickness to operate effectively, as well as materials that contain medium to heavy elements.

Recently, the high-energy x-ray reflectivity technique has been successful in probing fundamental questions regarding the behavior of water in nature, such as the existence and quantification of a vapor gap between hydrophobic surfaces and liquid water and in the melting of solid water in contact with mineral surfaces [27]. In addition, the SAXS/WAXS probe has been used to investigate the kinetics of nano-particle formation in a variety of systems ranging from bulk metallic glasses [28] to nanostructures at liquid/semiconductor interfaces [29]. Amongst the large volume of potential studies using these techniques are liquid-solid interfaces involved in electrochemical processes, such as electroplating, and liquid-liquid interfaces involved in environmental remediation, such as the oil-liquid interface present in the separation process used for actinides. The ability to couple these measurement modes offers exciting possibilities for studying the dynamics of complex systems.

Upgrade opportunities. The microfocused, high-energy x-rays available through APS-U will provide unique characteristics to probe buried interfaces in a number of technologically-relevant material systems. A short-period undulator, ideally a superconducting type for the highest brilliance, (CDR 4.5.4.2) and 2-d optics (CDR 4.5.4.4) will provide a sub-micron and fixed-energy (70keV) probe. This will be coupled to a goniometer, select sample environments, and a flexible detector system to allow complementary measurement modes of transmission SAXS/WAXS, x-ray reflectivity, crystal truncation rods, and grazing incidence scattering. The system will accept a monochromator able to tilt the beam and permit measurements without the need to move the specimen, of particular relevance for liquid/liquid and liquid/gas interfaces. This will enable a new suite of in-situ and in-operando studies which are complementary to, but distinct from, the APS-U planned lower-energy surface and interface beamlines.

A.3 Advanced Composite Materials: Synthetic and Biological

The proposed high energy SAXS/WAXS (see above) probe offers unique opportunities to study the individual phases of advanced composites, which can give a wealth of unique information relevant to their structural integrity. The properties of composites depend on the distribution, orientation, shape and connectivity of the strengthening phase as well as the bonding between the reinforcement and the matrix which may decrease due to damage accumulation (e.g. cavitation, delamination) or increase (due to matrix plasticity, or reaction during heat treatments). This is reflected in the load partitioning between matrix and reinforcement which can be determined by WAXS and SAXS. One area of interest is the material response during creep and fatigue of advanced composites in gas turbine engines, for which higher-temperature operation is desired to increase engine efficiency. A number of existing and proposed composites may be used in such applications including (i) superalloys (Ni based, and containing gamma prime and carbide second phases), (ii) metal-matrix composites [30] (iii) ceramic matrix composites and (iv) advanced ceramics such as $MoSi_2$ with second phases. In all systems, the load bearing capacity is dictated by load transfer from the relatively compliant, soft matrix to the stiff, hard reinforcements. For even higher temperature operation, these materials can act as substrates for ceramic coatings (e.g. TBCs), mentioned in the previous section, for which load transfer across the substrate/coating interface is of prime interest. The proposed beamlines will permit studies of the phase-specific strain responses under relevant thermo-mechanical conditions. Sub-second temporal resolution will allow scientists to track the responses close to the origin of deformation, with sufficient spatial resolution (micron-level) to track damage gradients, particularly in coated systems.

With longevity increasing for populations both in the US and worldwide, biomaterials are becoming key elements in maintaining mobility and quality of life. One bottleneck in this area is inadequate understanding of how implant materials interact in biological systems, particularly at

the tissue/material interface. For example, a critical concern for implant materials (e.g. for hip replacements) is stress-shielding by the implant material, which weakens bonding with the growing tissue. In-situ, 3D-resolved scattering methods, combined with imaging, will provide gradient information of strain and microstructure needed to better understand and optimize such implant materials. Another area of interest is biomedical stents. Stents, which are typically made of superelastic NiTi, are increasingly being utilized in surgical applications, yet fatigue failure remains an important issue. In such case one would like to fatigue cycle the stent within a simulated artery, and study the cyclical phase transformation and associated strain responses. In addition, improved understanding of bone nano-mechanics is needed to understand the underlying mechanisms of such failures at ultra-structural and molecular levels.

1-ID has demonstrated capability to study the phase response within biomaterials including bone [31] and teeth [32] using sequential SAXS/WAXS. One important issue for such studies is to minimize radiation dose, and associated radiation damage, [33] in order to decouple possible effects from load-induced damage. Recent systematic investigations have identified that sequential SAXS/WAXS data can be collected at doses of 500 Gray which is below critical levels which affect load transfer between collagen and mineral phases [34]. The advanced detector arrays provided by APS-U will allow for more efficient collection of simultaneous SAXS/WAXS data, on the order of 10 times below current doses, which may even make possible in-vivo studies (for reference, typical doses in human cancer therapy are on the order of 0.1 Gray while sterilization levels are at 100 kGray). These arrays will also eliminate the need for detector motion, opening possibilities for new studies of relevant physiological processes such as fracture and high-cycle fatigue.

A.4 Nuclear materials

Nuclear power has enjoyed a renewed interest of late. Generation 4 reactors which more efficiently burn fuel to higher levels and reduce radioactive waste will run at higher temperatures and expose materials to higher levels of irradiation than previous reactor technology. No material currently exists that can withstand the challenges associated with these conditions. Research directed at understanding the evolution of microstructures and the associated materials response (i.e. the structure property relations) under these operating conditions, and eventually informed design of materials is required to realize the benefits of generation 4 nuclear reactors. High energy synchrotron radiation is uniquely capable of probing the microstructure of the relevant materials, i.e. advanced steels, zircalloy alloys, high Z-number metallic and oxide fuel materials under high temperature, stress, and possibly, simulated irradiation conditions.

Recent in-situ neutron diffraction measurements on irradiated zirconium alloys during deformation (unpublished) have demonstrated two clear effects: 1) the microstructure of the material was dramatically affected by ten years of service in reactor (evidenced by diffraction line shape), and 2) the balance of the active deformation mechanisms was shifted by the change in microstructure. It is reasonable to assume that these types of effects are pervasive in irradiated materials and understanding the development of the microstructure is critical to designing materials which either resist or are more tolerant of these changes. Unfortunately, due to the small quantities of activated materials which can be used in these experiments as dictated by personnel radiation safety, the neutron measurements are prohibitively slow (4 hours per line profile measurement) to allow the real-time measurements necessary to understand the evolution of the microstructure.

The high flux of the 3rd generation synchrotron x-ray sources coupled with optimized detector designs (CDR Figure 4.5.4-6) will allow real-time in-situ measurements on very small quantities of materials (milligrams). Keeping with the above example of irradiated zirconium, the obvious next step is diffraction line profile measurements during heating, which will allow us to understand the

mobility of the defects introduced by irradiation. These measurements are not possible with neutron diffraction because of the slow measurement rate. However, the proposed detector design (CDR 4.5.4.6 and Fig. 5) will allow the experiments to be completed on a sample with sub-millimeter dimensions on sub-minute time scales. This capability, which is not currently available, would allow us to monitor the defect population in real time as the material is annealed under heating conditions similar to those it might experience in service.

While this is one specific example, one can imagine many possible experiments on different materials under relevant environmental conditions. The proposed 1-ID beamline upgrade would allow for diffraction measurements which, when optimized in different ways, allow one to follow the evolution of internal stress, texture, dislocation density and character, under multiple environmental conditions. Further, small angle x-ray scattering (SAXS) will be used to provide information about larger scale (1nm-100nm) heterogeneities such as voids or He bubbles. The penetration of high energy x-rays allows them to probe structural materials (e.g. steel, zirconium), fuel materials (metallic uranium, UO_2), and waste materials (e.g. mixed trans-uranic oxides). Relevant environmental conditions certainly include high temperature and applied stress, but could easily also include magnetic and electric field, or, if one stretches ones imagination, under simulated (with ion beams) irradiation conditions.

Currently, post irradiation examination, is the only routinely used mechanism to glean information about irradiated materials. Synchrotron x-rays could provide the first routine access to real time in-situ experiments. The difference is analogous to the difference between archaeology, i.e. understanding a civilization by what it left behind, and observing an existing civilization. Thus, the impact of this capability could be huge, providing never before available glimpses into the behavior of nuclear power relevant materials under relevant conditions.

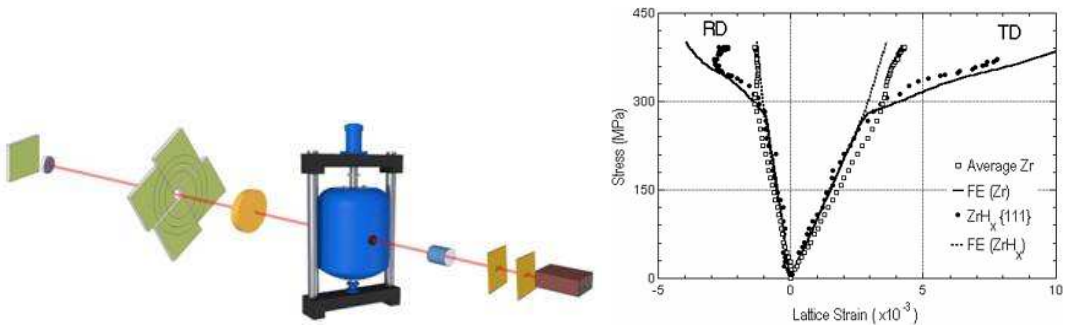

Figure 5: New detector arrays for simultaneous SAXS/WAXS will enable thermo-mechanical studies of irradiated materials as illustrated in (a). This will build on and enhance existing studies of non-irradiated nuclear materials such as Zr-alloys, as illustrated in (b), in which in-situ deformation response of both bulk (Zr) and minority ($ZrH_x, < 1\%$ vol. fraction) phases were determined with sufficient fidelity for FE model comparison and to provide estimates of fundamental properties such as critical hydride failure length. [35]

A.5 Dynamics of undercooled systems

Liquids and glasses are probably the least understood phases of matter. Our understanding of how they crystallize and, in some cases, become glasses with cooling is incomplete. Furthermore, novel liquid/liquid phase transitions at temperatures below their melting temperatures (supercooled) are largely unexplored. Since most elements are liquids only at elevated temperatures and react strongly with container materials, experimental studies of their structures and properties, which

could guide fundamental theoretical efforts, are difficult or impossible to make. To address these and related questions, Washington University in St. Louis and Iowa State University have designed and constructed an electrostatic-levitation (ESL) x-ray scattering facility (Beamline ESL or BESL) to allow structural and kinetic studies of high temperature liquids, both above and below the equilibrium melting temperature. The liquids are levitated in high vacuum using electrostatic levitation, thus avoiding container contamination and minimizing the potential for heterogenous nucleation. This chamber, and its predecessor at NASA, has been used successfully in a series of pioneering experiments that correlate physical measurements such as density and calorimetry, with the microscopic liquid structure. [36, 37, 38, 39, 40, 41]

Upgrade opportunities. The proposed upgrade of 1-ID will strongly enhance this program in very specific ways. Currently, at 6-ID,[1] the ability to measure a full diffraction pattern using a 2D detector is flux limited. In liquid Si, for example, useable data can be obtained on a timescale of 100 msec. With an expected increase of a factor of at least 100 in incident flux at high energy (CDR Sec. 4.5.4.5), the data collection time will be correspondingly reduced. This finer temporal resolution will reveal kinetic processes in liquids in greater detail, which are critical to investigate proposed liquid-liquid phase transitions in the undercooled state and transient metastable solid phases that occur upon the initial stages of crystallization. Second, the simultaneous SAXS/WAXS probe (CDR 4.5.4.6 and Secs. A.2 and A.3) will provide details of phase separation in undercooled liquids and metastable solid products of crystallization over a large range of length scales which, to date, is relatively unexplored territory. Finally, the continuous energy coverage provided by the in-line D and E hutches can be used for anomalous scattering to extract partial pair distributions for heavier elements in undercooled liquids. These partial pair distributions are critical for a successful modeling of multi-component liquids using, for example, reverse Monte Carlo techniques.

A.6 Imaging the reciprocal space of single crystals

A key distinguishing feature of the Advanced Photon Source (APS) is the capability for high-energy scattering, which has been exploited for numerous applications including pair distribution studies, high pressure studies, and investigations of the mechanical behavior of materials. Coupled with the new generation of two-dimensional area detectors, high-energy diffraction studies of powder samples provide an important and complementary path to conventional powder diffraction measurements. The capabilities for high-energy single-crystal diffraction measurements at the APS, however, remain somewhat underdeveloped and there is an emerging need for this technique. Recently, a crystal oscillation technique, using high-energy x-rays to image planes of reciprocal space has been developed. This method has been applied, to a variety of systems including the new iron arsenide superconductors [42, 43], quasicrystals [44], and for the study of crystallographic phase transitions [45]. Most recently, a Partner User Agreement with the APS to extend this technique to full precession camera capability has been established. This enhanced instrumentation will provide unique capabilities at a third generation light source for examining bulk single-crystal samples under extreme environments.

The combination of high-energy x-rays, a suitably designed precession camera, and fast area detectors will enable a "big picture" of reciprocal space for a single crystal, yet maintain high enough resolution to study twinning in the newly discovered iron arsenide superconductors. The data shown in Figure 6, for example, were key to elucidating the nature of structural twin domains in the parent

[1] Note that APS-U plans may include removing the 6-ID high-energy program as required by the short pulse x-ray (SPX) program. Hence, the measurements described here may be moved to 1-ID; an upgraded Sector 1 may dictate such a move in any case.

$AEFe_2As_2$ (AE = Ca, Sr, Ba) compounds associated with the tetragonal-to-orthorhombic distortion observed in these materials and their doped, superconducting daughters [42]. Furthermore, diffuse scattering measurements of chemical short-range order, phonons and structural instabilities will also benefit from the proposed upgrade. Fig. 7, for example, shows diffuse scattering (performed at 6-ID-D) from Fe-Ga alloys with large magnetostriction, showing features arising from both chemical order and thermal vibrations.[46] More quantitative analysis of the diffuse scattering would be possible if measurements were performed in high symmetry planes of the crystal, rather than over the surface of the Ewald sphere. The proposed precession technique provides a unique approach that could be applied to diffuse scattering problems to allow measurements in such high symmetry planes. Upgraded and expanded facilities at 1-ID (CDR 4.5.4.3, 4.5.4.6) will provide the flexibility to implement this technique.

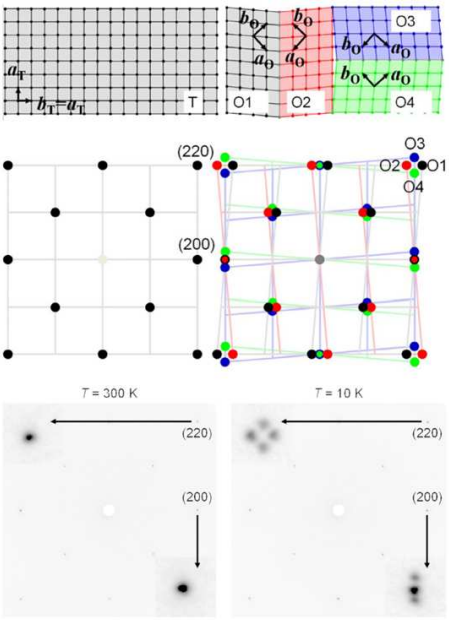

Figure 6: In $BaFe_2As_2$ a pattern of domain walls is formed below the tetragonal-to-orthorhombic transition due to formation of twin boundaries. The top panels show schematics of the displacements of atoms in the tetragonal lattice (above T_{SM}, left) during structural transition, leading to orthorhombic distortion and the formation of domain walls. In the orthorhombic phase (right) the unit cell of the lattice doubles in size in the $a-b$ plane, with new lattice vectors a_O and b_O of different length ($a_O > b_O$), rotated by approximately 45 degrees. The third row shows the expected transformation of the x-ray diffraction pattern during domain formation in the (HH0) plane. The bottom row shows actual x-ray data acquired on station 6-ID-D, zooming in on the (200) and (220) reflections. [42].

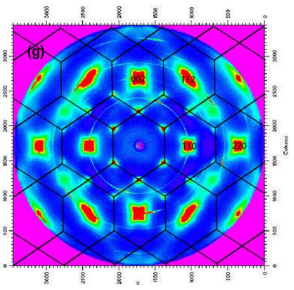

Figure 7: Diffuse x-ray scattering measurements performed on magnetostrictive $Fe_{82}Ga_{18}$ alloys using the Sector 6 high-energy side station with an energy of 100 keV. With fixed crystal orientation, scattering occurs on the Ewald sphere tangential to the $(1\bar{1}0)$ crystallographic direction. Strong thermal diffuse scattering is observed near allowed Bragg reflections of the BCC structure ($h+k+l$ = even). Chemical short-range-order peaks are observed near (001) and $(1/2, 1/2, 1/2)$-type reflections due to incipient D03 alloy ordering. [46].

B APS Relevance

Each of the science cases described above map seamlessly onto the APS Upgrade theme of "real materials under real conditions in real time." They exploit the unique APS characteristic of having

the highest brilliance in the nation in the high energy (> 40 keV) spectral range. Internationally it is rivaled only by ESRF, Petra III, and SPring-8, all of whom continue to develop similar programs to those described in the science themes. In Europe in particular a number of high-energy beamlines are being upgraded and/or built including at the ESRF (even with the reduced ESRF upgrade scope, an ID-11 upgrade and a new high-energy beamline are planned), and PetraIII (the HEMS beamline). Substantial synergy can be achieved through continued collaboration between these institutions, particularly with APS having comparable capabilities as APS-U would provide. While neutron sources offer comparable penetration power to high-energy x-rays, the newly-built SNS has substantially lower brilliance (~ 2 orders of magnitude), as will high-energy beamlines at the only newly planned national synchrotron source, NSLS-II.

The above sections have pointed to specific upgrade components that are relevant to particular measurements. To summarize, upgraded APS 1-ID sources and optics will deliver a unique combination of high (i) penetration power, (ii) spatial resolution, (iii) temporal resolution, and (iv) reciprocal space range and resolution to probe the most complex "real" materials. The higher brilliance associated with the upgraded beamlines will substantially increase the spatio-temporal resolution of delivered beams, to $\leq$500nm and msec levels, allowing "real" time investigations and opening new frontiers in materials research. Increased beam stability will enhance spatially resolved measurements. In addition, APS-U at 1-ID will provide a new high-energy surface and interface scattering capability for studies of buried interfaces rivaled only by the ESRF and distinct and complementary to the surface scattering efforts at other APS beamlines. Equally important, the increased specialization and number of experimental stations will allow unique in-situ environments and increase user throughput to address oversubscription rates (see Sec. C).

The microstructural probes will be synergistic with strategic laboratory initiatives including Materials for energy and energy storage. Indeed the need for non-destructive microstructural probes, capable of observing gradients on the 1-10 micron level, was articulated by Jeff Chamberlain in the ANL "future states" energy storage lecture (Nov, 2010). Both HEDM and the buried interface methods (Secs. A.1, A.2, and A.3) are expected to fill this targeted need through combining bulk penetration capabilities with micron-level resolution of structure. In addition, the SAXS/WAXS probe in particular can interface the Materials for Energy initiatives by providing rapid (sub-second) structural information on nano-scale processes, [29] which is the relevant size-scale where the majority of synthesis and design of novel materials will occur. Finally, the ability to study irradiated materials, particularly in response to external stimuli including thermo-mechanical deformation, will provide unique information relevant both for ANL initiatives as well as national energy and security needs.

C User Community: existing, potential, specific requirements

The 1-ID user community is international and is comprised of academic, national laboratory, and industrial researchers in the fields of materials science and engineering, other engineering disciplines (primarily mechanical and biological), physics and chemistry. The GUP oversubscription rate has ranged from three to five over the past five years, discouraging outreach efforts which could lead to appreciably higher numbers of proposals. Interest in the types of science and the unique capabilities described herein can be expected to increase demand significantly as these capabilities become better developed and known in the community. This potential demand has and will continue to guide a significant part of the effort at Sector 1. Upgraded beamlines and the resultant improvements in measurement techniques and capabilities will allow expansion beyond the community of x-ray experts (see Sec. D).

One user community which is largely untapped to date is in the nuclear field. The potential is illustrated by the interest generated at the APS workshop on irradiated materials studies ($\sim$ 150 member attendance) in 2009. The workshop organizers summarized: "Synchrotron studies hold enormous potential to answer questions central to all aspects of nuclear energy production, from simulation validation, to quantifying materials problems, to environmental remediation...Major experimental challenges remain including...design and execution of in situ experiments (particularly those under extreme environments)...The construction of dedicated high energy ($>$ 60 keV) X-ray beamlines for experiments on radioactive samples would accommodate the relevant requirements associated with handling nuclear materials (radiation levels, safety, security) and provide capabilities unavailable elsewhere in the world. This recommendation is considered consistent with APS capabilities and its plans for an overall upgrade."

The upgrade will increase the quality and quantity of experiments to attend to the needs of these communities. The strong user base will grow, particularly in the areas of in-operando studies of materials processing and synthesis, deformation studies of advanced materials used for a variety of applications including nuclear and lightweight, energy-efficient materials, and spatially resolved microstructural studies of basic and engineering materials. Stronger ties with computational scientists have been emphasized above; these ties will further leverage novel in-situ data sets.

sort this out after letters come. Finally, we anticipate that the upgrade will enhance current ties to industrial partners, particularly in the areas of HEDM imaging and SAX/WAXS measurements. The non-destructive 3D resolved strain mapping capabilities can be used, for example, to verify surface treatments (e.g. peening, case hardening) often applied industrially, but typically measured using layer-removal techniques. Existing industrial partners include GE (see attached support letter), John Deere, Ormond and Caterpillar. Industrial users for SAX/WAXS have been limited primarily by beamtime availability, but could range from orthopaedic implant manufacturers (e.g. Zimmer) to firms involved in nanoparticle synthesis. Similarly, and as described above, a significantly larger community can be expected with more user-friendly HEDM measurements, with a wide array of potential industrial ties ranging from battery evaluation to thermo-mechanical process (stamping, forging, welding, etc) investigations.

D Required Technical Advances/Technical Feasibility

With the facility upgrade (higher electron beam current and better beam stability) and the beamline upgrade (new canted undulator sources in a long straight section with a side-station beamline and new hutches) will come challenges associated with increased data rates, new environmental chambers, and new detector configurations. Further, to gain the full impact of new capabilities, it will be important to develop a user friendly environment for non-experts.

Undulators. Technical advances in undulator design will allow the highest possible brilliance to be delivered to the upgraded hutches in canted geometry. For one section of the cant, a permanent magnet undulator is proposed, able to produce beam with continuous coverage in the energy range of 40-140 keV. A particularly attractive device would be the "revolver" undulator, which would allow discrete short-periods to be used (e.g. 2.1 and 2.3 cm), with a significantly longer length as compared to the alternative of two shorter undulators in series. For the second section, an undulator is proposed with a period and gap to produce a third harmonic at 60-75 keV, such as the APS prototype superconducting 1.6 cm device. This would deliver between 1-2 orders of magnitude more flux for time-resolved experiments such as those described in Secs. A.2 and A.5 as well as enabling near-field HEDM microstructure mapping measurements to become time resolved.

Optics. Optics development will be undertaken to provide the highest possible beam quality as well as flexibility for different types of resolution (spatio-temporal and reciprocal space, line or point focus) demanded by the broad array of scientific and technological demands and related measurement techniques described above. A cryogenically cooled, bent double-Laue monochromator will be used to provide a fully-tunable energy range with preserved source brilliance, while a single bent Laue crystal will be used for the fixed-energy branch. The former monochromator will be an upgraded version of the highly successful system used at 1-ID for over 10 years, with added energy range (40-140keV). A high-energy-resolution monochromator system will be placed downstream of this tunable monochromator to allow users to tradeoff flux for energy resolution (needed e.g. for resonant scattering or very high strain resolution). A number of focusing optics (primarily parabolic refractive lenses) will be dedicated for both short ($\sim$ 1 m) and long ($\sim$ 20 m) focal lengths to give users the option to choose the highest spatial resolution (ex., submicron beams) or more moderate resolution ($10 - 20\mu$m) with increased flux and reciprocal space resolution.

Detectors. All proposed techniques rely on area detectors. The availability of efficient multi-mega-pixel detectors with fast read out is another key advantage as compared to neutron diffraction techniques. Dramatic progress has been made over the last years and is likely to continue. For example, even with present technology a semi-transparent dual near-field detector could be engineered that would allow simultaneous near- and far-field HEDM. Such a detector system may make possible tomographic strain mapping within individual grains.

Sample environment. We anticipate that new science will be enabled by sample environments that will provide extreme conditions that are not yet available. While the proposed diffraction techniques pose some constrains on sample environments (in particular near-field techniques), it is clear that technological limits have not been reached and that ample potential exists for developments. A variety of efforts are underway including DOE funded SBIR partnerships.

Data handling and computational environment. A common theme in the described measurements is the use of area detectors. In several cases, multiple detectors (as many as five) will be used simultaneously and, with upgraded x-ray flux, will have to be read out rapidly and in synchronism with sample and other motions. Mechanical hardware-to-detector-to-software interfacing is a significant challenge that will require investment. Fast and reliable data streaming from experimental hutches to massive data storage devices (on- and/or off-site) will be essential as will fault tolerant data collection software. High performance computing, already used HEDM reconstructions, will be required for on-line data analysis so that experimenters can tune sample treatments based on knowledge of prior behavior. Detailed collaboration between instrument scientists and software developers will be required. As is the case in high energy physics measurements, it may be impractical to keep all full detector images; this limitation re-emphasizes the need for real-time image reduction and/or interpretation. Significant local computing power will be required.

Measurements will need to make the transition from being run solely by developers to being tools that non-experts can use. The described measurement modes hold the potential to be extremely useful tools to broad materials communities. The potential broad user base has been pointed out above. However, this broad user base will not consist entirely of x-ray experts or people who want to become experts in doing the measurements. It will be essential to develop essentially a "turn-key" capability for at least some instruments and/or measurement modes. Making this transition will be demanding both of hardware and software design.

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Professional Preparation

• *Post-doctoral:* IBM Research, Physical Sciences, 1979 - 1981.
• *Graduate:* Clark University, Physics, Ph.D., 1978.
• *Undergraduate:* North Carolina State University, Electrical Engineering, BSEE, 1970.

Appointments

1. 2006-present, Professor of Materials Science and Engineering
2. 1996-present, Professor of Physics, Carnegie Mellon University
3. 1987-1996 Associate Professor of Physics, Carnegie Mellon University
4. 1987 Visiting Scientist, Schlumberger-Doll Research (summer)
5. 1985 Visiting Scientist, IBM Research (nine month leave from CMU)
6. 1981-1987 Assistant Professor of Physics, Carnegie Mellon University
7. 1978-1979 Research Associate and Instructor, Clark University
8. 1970-1972 Electronics Engineer, U.S. Patent Office

Recent Publications: (see here for re- and pre-prints)

1. C.M. Hefferan, S.F. Li, J. Lind, U. Lienert, A.D. Rollett, P. Wynblatt, R.M. Suter, "Statistics of High Purity Nickel Microstructure From High Energy X-ray Diffraction Microscopy," Computers, Materials and Continua, **14**, 209-219 (2009).
2. C.M. Hefferan, S.F. Li, J. Lind, and R.M. Suter, "Tests of Microstructure Reconstruction by Forward Modeling of HEDM Data," Journal of Powder Diffraction, **25**, 132-137 (2010).
3. U. Lienert, M.C. Brandes, J.V. Bernier, M.J. Mills, M.P. Miller, S.F. Li, C.M. Hefferan, J. Lind, R.M. Suter, "3DXRD at the Advanced Photon Source: Orientation Mapping and Deformation Studies," Risoe 2010 Symposium proceedings (2010).
4. S.R. Wilson, C.M. Hefferan, S.F. Li, J. Lind, R.M. Suter and A.D. Rollett, "Microstructural Characterization and Evolution in 3D," Risoe 2010 Symposium proceedings (2010).
5. U. Lienert, S.F. Li, C.M. Hefferan, J. Lind, R.M. Suter, J.V. Bernier, N.R. Barton, C. Brandes, M.J. Mills, M.P. Miller, C. Wejdemann, and W. Pantleon, "High-Energy Diffraction Microscopy at the Advanced Photon Source," J. of Matls, (invited issue), submitted (to appear in July 2011).

Related Activities

• Suter's research group has developed the High Energy X-ray Diffraction Microscopy (HEDM) microstructure mapping technique at the Advanced Photon Source through collaboration with Sector 1 personnel (primarily Ulrich Lienert). Hardware and data collection macros have been and continue to be refined. Reconstruction software has been developed that uses high performance computing on the NSF Teragrid and other HPC facilities. Through a Partner User Program beam time allocation (with Lienert and Matthew Miller of Cornell University), we are working to make the technique accessible to non-expert users and to combine tomography and strain sensitivity with orientation mapping. The user base is currently expanding through collaborations with scientists at national laboratories and universities. Outreach presentations have been given in 2010 at the CMU NSF/MRSEC 3D Microstructures Summer School, PowderMet 2010, and in Japan (Japan Iron and Steel Symposium at Hokkaido University, SPring-8 synchrotron facility, and Kyoto University).
• Suter was elected to the Adv. Photon Source Users' Organization Steering Committee in 2009.
• Suter is chair of the "Engineering-Applied Materials" proposal review panel at the APS.
• Suter has served as Director of Outreach for the CMU NSF/MRSEC program and as Director of the Undergraduate Program in the Physics Department at Carnegie Mellon University.

Jonathan D. Almer

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Professional Preparation

- Post-doctoral research assistant, Engineering Materials Group, Linkoping University, Sweden, 1998-1999.
- Northwestern University, Evanston, IL. Ph.D., Department of Materials Science and Engineering, 1998. Advisor Jerome B. Cohen.
- North Park University, Chicago, IL. B.S. in Physics with minor concentration in English. *Summa cum laude,* 1991.

Appointments

- 2009-pres Leader, Materials Physics and Engineering Group, Argonne, Il.
- 2006-pres Physicist, Argonne National Laboratory, Argonne, IL.
- 2000-2006 Assistant Physicist, Argonne National Laboratory, Argonne, IL.
- 1999-2000 Instructor, Linkoping University, Sweden.
- 1994-1998 Graduate research assistant, Mat. Sci. Eng. Dept, Northwestern University
- 1991-1992 Research assistant, Mat. Tech. Div., Argonne National Laboratory.

Selected Publications (total over 130)

1. Wang, Y.M., R.T. Ott, A.V. Hamza, M.F. Besser, J. Almer, M.J. Kramer, “Achieving large uniform tensile ductility in nanocrystalline metals, Phys. Rev. Lett., **105**, 215502 (2010).
2. Almer, J. and S. Stock, "Internal strains and stresses measured in cortical bone via high-energy x-ray diffraction", Journal of Structural Biology, **152**, pp. 14-27 (2005).
3. Jakobsen, B., H.F. Poulsen, U. Lienert, J. Almer, S.D. Shastri, H.O. Sorensen, C. Gundlach, and W. Pantleon, "Formation and subdivision of deformation structures during plastic deformation", Science, **312**(5775), pp. 889-892 (2006).
4. Hufnagel, T.C., R.T. Ott, and J. Almer, "Structural aspects of elastic deformation of a metallic glass", Physical Review B, **73**(6), pp. 64204-1-8 (2006).
5. Almer, J. and R.A. Winholtz, “X-ray stress analysis”, in Springer Handbook of Experimental Solid Mechanics, Ed. W.N. Sharpe, pp. 801-820 (2008).

Thesis Advised Students (all from Northwestern University)

- Chris Weyant, Stonybrook University, NY.
- Yana Qian, Western Digital Corp, CA
- Bryan Harder, NASA Glenn
- Anjali Singhal (current student)
- Fabian Stoltzenberg (current student)
- Fang Yuan (current student)

Carnegie Mellon

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Anthony D. Rollett

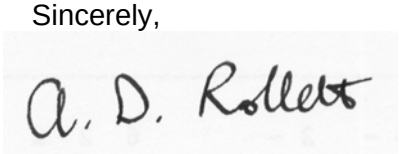
January 22, 2011

Subject: Support for 1-ID Upgrade

To Whom It May Concern:

I am writing to express my strong support for the 1-ID upgrade and any associated upgrades in the accelerator as a whole that may affect this. I am a materials scientist and a rather recent new user. The reason for my new found enthusiasm for using APS is simple: it can do things that literally cannot be done anywhere else, with the possible exception of ESRF. Namely, it is possible to map out the internal structure of polycrystalline solids using diffraction to obtain the local crystal orientation to high accuracy over volumes of order $1mm^3$, which typically yields thousands of grains. It is also proving possible to perform tomography with the same beamline, which opens up an enormous range of very challenging materials problems and especially having to do with damage initiation and growth. This then means that this capability makes it feasible to examine problems such as ductile fracture, fatigue, creep, hot shortness, weld cracking, whisker growth, to name but a few. An additional near-term prospect is the capability to measure elastic strains throughout a polycrystalline sample, which further expands the range of materials problems that the community will want to investigate using this facility. As one example, there are many questions about the performance of advanced carbon fiber composites such as those being employed in advanced airplanes (such as the Boeing Dreamliner) and their damage tolerance; the ability to probe buried interfaces and elastic strains (and therefore stresses) points again to data that cannot be obtained any other way. I am personally very excited about the difference that APS can make to materials science and the proposed upgrades will substantially increase the impact.

Sincerely,



Anthony D. Rollett
Professor, Materials Science and Engineering

UTSA The University of Texas at San Antonio
College of Engineering
Department of Mechanical Engineering

January 24, 2011

Robert M. Suter
Professor of Physics and Materials Science and Engineering
Carnegie Mellon University
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Re: Support to the APS upgrade proposal to DOE

Dear Dr. Suter:

I am writing this letter to indicate my full support for the Sector 1 beam line upgrade proposed in the APS upgrade proposal to the Department of Energy. In the past years, I have been a user of the Sector 1 beam line for my research regarding the ultrastructural characterization of hard tissues during the deformation and failure process. Such information will provide yawning insights into the structure-function relationship of these tissues, which will help bridge the gap between hard tissue biomechanics and biology and greatly advance our knowledge for prediction and prevention of osteoporotic bone fractures of woman and elderly populations.

The proposed upgrade will Increase the beam brilliance and add new hutches, which will decrease measurement times and allow a variety of improvements to techniques. More importantly, this upgrade has the potential to reduce oversubscription and the difficulty of obtaining beam time, which my research team has encountered in the past few years. I believe that the Sector 1 beam line upgrade will make a significant contribution not only to advancing basic sciences, but to new technology development that is crucial for the economy of the country.

Sincerely yours,

Xiaodu Wang, PhD
Professor
Mechanical and Biomedical Engineering

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