NSLS-II Beamline Development Proposal

Type I [X] Type II

High-energy x-ray micro-mapping of materials for advanced energy and structural engineering applications beamline. (HEX)

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A. Science Case

The HEX engineering materials beamline will be a state-of-the-art facility that will not only push the boundaries of fundamental science but also enable studies on materials and systems of industrial/societal relevance. The beamline's multitude of capabilities will enable strong university/industry/national-lab collaborations. The HEX beamline will be a central component to increasing the industrial relevance of synchrotron science. A leit motif of the beamline will be to enable experiments to be done on real materials/systems designed for applications, under real in situ operating conditions, in real time. Deep-penetrating, high-energy X-rays will be used in high spatial resolution work enabling one to apply 4D (3D space + time-temperature-voltage-applied stess etc.) phase, strain and morphology mapping capabilities to the study of materials research challenges that are central to this nation's technological future. The goal of the proposed beamline is to establish a sorely needed facility contributing to the US's competitiveness in materials research and in industrial applications (see [1]).

The concept of high energy synchrotron beamlines to provide unique insight into problems of technological interest has already been embraced by a number of other technology dependent countries. Examples include: the JEEP ID12-beamline at the UK Diamond synchrotron [2,3]; Beamlines ID15A&B at the EU's ESRF [4,5]; and engineering beamlines at Germany's HASYLAB synchrotron facilities [6,7]. In the US, the Sector 1 at APS (with its planned upgrade) provides a superior high energy undulator-based set of materials science/engineering beamlines [8-10]. (See section B. below for further discussion.)

The proposed HEX wiggler beamline is intended to substantially surpass the operating parameters of the present X17-B1 wiggler beamline and to greatly enhance the end station capabilities for attacking and solving fundamental/technological problems. Consistent with world class beamline facilities, the HEX beamline will integrate multiple high energy techniques: energy dispersive x-ray diffraction (EDXRD); wide and small angle monochromatic angle dispersive diffraction; pair distribution function measurements; and tomography/radiography. The benefit integrating of such core techniques was underscored at the HEX BDP Workshop by the experience of state of the art European and APS facilities [11,12].

The European facilities include the highly flexible wiggler-based white beam EDXRD method [2,4,6]. Currently, there is no similar dedicated wiggler engineering beamline in the US. Indeed upon the scheduled 2014 shutdown of NSLS X17-B1 there will be no high-energy-wiggler materials science/engineering facility in the US. Without such a beamline the competitiveness of the US in high energy x-ray materials research is in jeopardy. An investment in HEX at NSLS-II is therefore vital to the US's worldwide competitiveness in this area of research that directly impacts both scientific breakthroughs as well as technological innovation.

The problems facing advanced technology are diverse and continually evolving. The beamline science justification presented here will be dual faceted. The first facet involves a set of fundamental science/engineering programs, which have been initiated on the X17B1 (or by the BDP participants), and which concretely illustrate the science which would be greatly expanded/enhanced at the NSLS-II HEX beamline. We will build on the experience gleaned in high energy x-ray research over the past decade to create the enhanced experimental capabilities needed for materials research in the future. The second facet emphasizes a newly evolving way of doing mechanics/materials science in which powerful high-energy x-ray measurements, from the single grain up to the macroscopic (grain averaged) length scales, are interfaced with concomitantly emerging powerful computer modeling capabilities over the same wide length scales [13].

Energy storage science: Battery research, in situ time and space characterization: The growing need for alternative energy sources and greater energy efficiency, combined with our increasingly untethered lifestyles, have made development of improved battery systems crucial to the future of the nation. These batteries span applications from large scale energy storage for electricity grid applications; to hybrid/electric vehicle applications; to portable electronic devices. Despite tremendous technical progress over decades of research and development in battery technologies, too little is known about the evolution of the internal microstructure and detailed phase changes taking place during electrochemical cycling. These limitations result from the experimental inaccessibility, during cycling, of the batteries' active components. Ex-situ (or post mortem) measurements performed on recovered battery components can lead to sample alteration and provide only a small window onto extremely complex/dynamic processes.

The pressing need to study the internal processes of batteries in their full-sized commercial embodiments and under their real operating conditions has been identified in the DOE BES report on Basic Research Needs for Electrical Energy Storage [14]. Specifically this report called for development of "in situ analytical tools" capable of characterizing the structural changes and electrochemistry inside full-sized batteries with high spatial and temporal resolution. In situ characterization of the cathode, separator, electrolyte, and anode materials as a function of time, state of charge, stress, temperature, etc. would therefore constitute a breakthrough for battery development.

Precisely such a breakthrough capability has been developed at beamline X17B1 and involves in situ, EDXRD measurements that have detailed the chemical changes, as a function of space and time (charge state) in the cathodes of two grossly different battery systems. The first system is GE's massive sodium-metal-halide battery technology intended for heavy-duty transportation and stationary power quality applications (see [15,16]). The second system involves characterizing a less than 100 µm Li_xFePO_4 thick cathode in a coin cell. Given these extreme examples, this technique appears capable of extending the benefits of such in situ studies to essentially the full panoply of prototype and production cells of all battery technologies. <u>The proposed HEX beamline should be able to increase the spatial and temporal resolution of these unique in situ battery studies by an order of magnitude. Conversely failure to proceed with the proposed beamline will constitute a setback for this emergent "in situ analytical tool", especially considering the shutdown of X17-B1 in 2014.</u>

GE sodium-metal-halide battery technology: It is important to note that this collaborative effort between GE, NSLS, and Rutgers produced fundamental research results leading to actual factory construction and commercialization of GE's "Durathon™" battery system (see [1]). In this sense the scientific results and economic fruits of this collaborative effort constitutes a paradigm for the future operation of the HEX beamline program. For details of scientific results the reader is referred to [15,16] and for the economic benefits (e.g. a new NY factory) one can refer to the "DOE Stories of Discovery & Innovation" release [1]. Only a brief illustration of the science illustration is included below.

The GE technology is based on the reaction $NaCl + M \leftrightarrow MCl_2 + M + Na$ (with M = Ni/Fe alloy). The 3.5 x 3.5 x 20 cm^3 cell consists of a central positive electrode comprising M-powder, NaCl, and $NaAlCl_4$ that is separated from a liquid Na negative electrode by a ceramic β"-alumina solid electrolyte tube [16]. It operates at 300°C, where the Na and $NaAlCl_4$ are molten. The large cell size and complex electrochemistry of this battery technology provide an excellent proving ground to establish both the penetrating power and detailed electrochemical structural insights possible with EDXRD (see [16]).

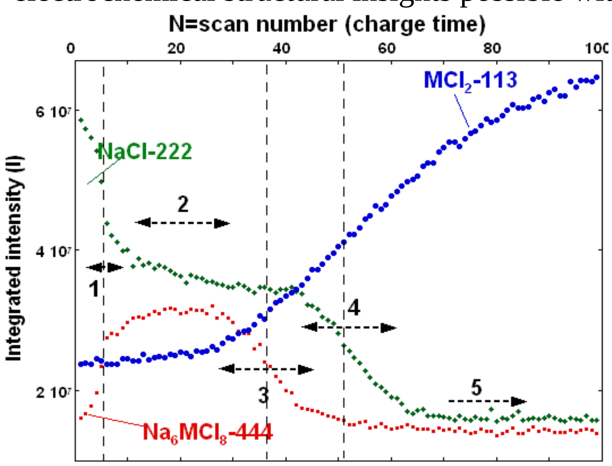


Fig. 1. The charging time (diffraction scan number) variation of the integrated spectral intensities for Bragg lines (see indices in figure) chosen to reflect the relative phase abundances of the NaCl, MCl_2, and Na_6MCl_8 phases. The vertical lines and regions 1-5 identify regions of the electrochemical kinetics discussed in reference [16].

To probe the phase evolution during cell charging, the EDXRD gauge volume was positioned in the cathode just inside the β''-alumina separator and a sequence of 99 diffraction spectra, each collected for 70 sec., were then taken as the cell was charged at constant current. In Figure 1 the integrated intensities of selected Bragg peaks, from phases involved in the cell charge cycle, are displayed versus the charging time (pattern number). One should note the transient, intermediate, Na_6MCl_8 phase formation from the NaCl phase, and its disappearance, before the conversion to the MCl_2 phase proceeds. This Bragg intensity data allowed differentiation, with respect to time, thereby yielding reaction rate curves between these different phases [16]. <u>The relevant point for this proposal is that deep within a massive production prototype battery the EDXRD technique is able to chronicle the detailed local electrochemistry involved in the temporal passage of the chemical reaction front. The appearance and disappearance of the intermediate Na_6MCl_8 phase highlights both the complexity of the electrochemistry involved and the extreme power of the characterization method.</u>

See [16] for the combined spatial and temporal profiling of these cells. Before moving on it is worth emphasizing that the x-ray path length for these in situ experiments was ~50 mm of mostly Fe/Ni alloy, confined in a steel jacket, and inside of a furnace. The white beam of the highly penetrating, high-energy x-rays, such as available at X17B1 and with much higher flux at the proposed HEX beamline, is absolutely essential for such work. <u>This work demonstrate that in-situ high energy x-ray diffraction characterization, in</u>

space and time, of advanced battery cells under realistic cycling conditions is a reality. The 10 fold increase in spatial/temporal resolution provided by the proposed HEX facility could contribute greatly to the advancement of battery technology by enabling the study of the fundamental mechanisms at work inside commercially relevant cells of almost any battery type.

$LiFePO_4$ Coin cell: $LiFePO_4$ is one of the more important and commercially viable cathode materials for Li-ion batteries for transportation and grid-storage applications (see the letter of support from C. Grey and R. Robert for more details on this section.). The microstructure of the electrode is key to its performance in batteries. The coin cell geometry studied here is directly comparable to the commercial battery geometry, hence such in situ EDXRD measurements on such cells can characterize how the relevant electrode reaction proceeds.

Recent, landmark work at X17-B1 [17] on $LiFePO_4$ based coin cells has clearly demonstrated the ability to perform high spatial resolution profiling (20 µm on a ~100 µm thick cathode) across the cathode during cycling in which the charging state is also evolving with time. Again, these results underscore the potential power that such a high-energy x-ray scattering characterization tool can bring to battery research. In order to concretely emphasize the power and feasibility of this technique selected preliminary results from this recent work are briefly discussed below.

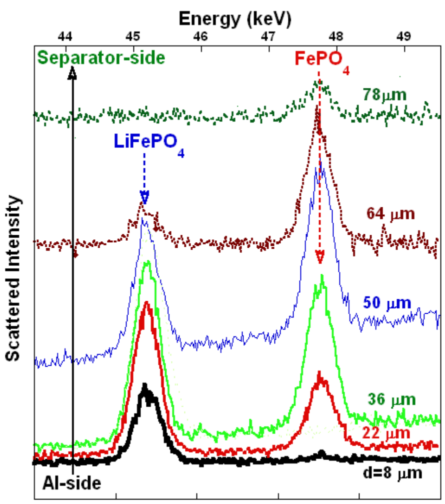


Figure 3 (below). The spatial variation across the cathode of the $LiFePO_4$ fractional phase content in various states during charge. Here phase fractions were obtained by fitting the (002) Bragg line intensities in patterns such as shown in Figure 2. The curves are labeled by their charge time in hours (h).

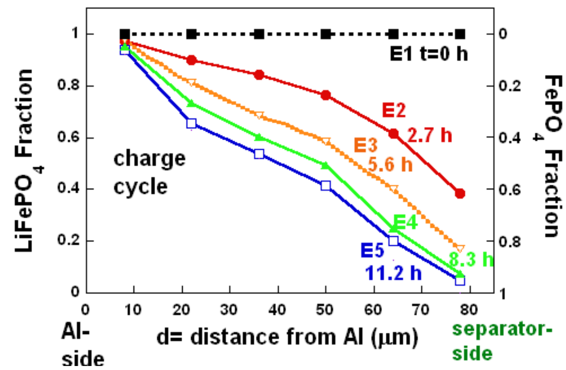


Figure 2. (above left) EDXDR in situ (002) Bragg line patterns taken at various depths in a thin $LiFePO_4/FePO_4$ cathode in a coin cell in the state of charged of ~ 17 mAh/g. The separator is the interface with the Li-reservoir and the Al-side is the electron current collector. The labeled distances are the GV position, d, traversing the cathode.

The EDXRD patterns, collected during the first charge/discharge, for a $LiFePO_4$/Li coin cell are shown in Figure 2 and reflect the transformation, as a function of position in the cathode film, between the two phases of Li_xFePO_4 in a ~17 mAh/g charge state. In Figure 3 the spatial variation, in the fractional phase content, (obtained by fitting the EDXRD patterns) is shown for a sequence of cell charge states. These results clearly show that in situ profiling of the electrochemistry in the cathode, both as a function of space (with high resolution) and time (charged state), is eminently feasible in real functioning coin cells. This last statement is provided that high energy x-ray scattering facilities, of the type proposed here, are available.

Nuclear energy materials applications: The science enabled by the beamline will have a direct impact on advanced nuclear energy systems. New, high temperature, radiation resistant materials are essential to advanced reactor designs. With better characterization techniques, one can envision a materials design cycle based on an understanding of microstructural evolution and phase stability in extreme environments. The fundamental mechanism of plastic flow and fracture properties under extreme conditions are needed to ensure safe operation for long periods at high temperatures. A more complete knowledge of dislocation processes and their impact on the materials properties can be used to engineer nano materials and grain boundaries that may create more radiation resistant materials. New, high temperature, radiation resistant materials for use in reactors are essential to advanced reactor designs. The very high temperature reactor will maintain fuel operating temperatures above 1100^{o} C to achieve efficiency and process heat production goals. New fast reactors for consuming transuranic fuels require alloys capable of withstanding 200 dpa with an irradiation temperature of 400-550^{o}C. Materials to be developed with understanding provided by the proposed beamline, such as the alloys and nano materials described in the letter of support from L. Ecker, will facilitate building these innovative reactor designs. The societal benefit is safe, more efficient nuclear power that will reduce carbon emissions while minimizing radioactive waste.

It should be noted that a novel in situ high temperature synthesis route for UN nuclear fuel material is already being studied on X17B1. Both monochromatic XRD and detailed pair-distribution function (PDF) analysis are being used to identify the long and short range order in this study. The wide range of scattering vectors available using the high energy source will be important in these studies. Moreover, the deeply penetrating character of the x-rays makes possible the robust containment of the uranium and the high temperature of the experiment.

Mechanics and Materials Science: In this section we will review the new and emerging class of science that can be addressed by the proposed HEX beamline. In recent years, high energy synchrotron radiation-based x-ray diffraction methods have been evolving, which allow such strain field profiling/ mapping of local strain field gradients, on the germane short length scales, deep in the interior of materials [18-30]. Such nondestructive cross-sectioning of the strain response, traversing a steep strain gradient, is now highly feasible for certain classes of problems in the elastoplastic deformation of solids. This capability provides a direct microscopic probe of the mechanical properties of materials on length scales down to the microns level.

Selected illustrations of such work are available from work carried on at X17B1. As a result of the "Materials Science Engineering Strategic Planning for NSLS and NSLS-II workshop" [31] a white paper on "High-energy x-ray micro-mapping of materials: engineering applications" [32 (see link)] was written. This white paper, gives specific case study applications of EDXRD strain mapping, to a range of materials deformation phenomena. Examples included were: compression processing techniques such as shot peening [22], laser peening, and split sleeve cold working (for rivet holes); residual strain profiling across a high-strength steel weld interfaces; and strain/phase profiling on plasma sprayed ceramic coatings on metals (for abrasion/corrosion resistance). The ability to profile beneficial or detrimental residual strains over the 10 μm to several cm length scale was demonstrated. Also noted were a number of examples of practical engineering applications (including for the first time in situ battery studies) where such high energy x-ray strain/phase mapping could make important contributions.

The letter of support from Proto-Manufacturing Inc. shows impressive results on the ~200 μm shot peening near-surface compression, along with the deep interior strains in Inconel 100 materials of interest to the Air Force. Moreover, the fatigue relaxation of the shot peened compressive layer under fatigue can be seen to ride upon a large, and deep residual strain field also resulting from the bending fatigue process. Without such interior strain field information from the deeply penetrating x-rays, the near surface peening fatigue relaxation could be easily misinterpreted. It is worth noting that most of the surfaces inside turbojet engines are shot peened and are subject to vibrational fatigue. <u>Importantly such DoD related work requires that a US synchrotron facility be used and without the proposed HEX beamline such resources will be severely curtailed if not, for some applications, lost.</u>

A recent paper by the Rutgers group reported EDXRD measurements in the important Ti-6Al-4V aerospace alloy under in situ four point bending [23]. This work allowed the exploration of elasto-plastic properties under both compression and tension. We have also performed similar in situ work emphasizing the anisotropic lattice elasto-plastic response on both Ti-6Al-4V and the nickel superalloy Inconel-100. This type of research provides a unique opportunity for studying plasticity phenomena in metals and alloys.

Fatigue crack studies: It is in probing both the residual and load induced strain fields in the vicinity of a fatigue crack tip that the EDXRD techniques developed at X17-B1 have been most groundbreaking [20-23]. Indications of this can be found in recent tour de force synchrotron strain mapping articles from Withers's group [28] and Korsunsky's group [33] on the fatigue cycle overload effect. Namely, Steuwer et al. [28] referred to the X17-B1 group's synchrotron strain mapping repeatedly: "Recently, elegant synchrotron X-ray diffraction experiments", "The broad profile of these compressive strains compared well with those observed by Croft et al." and "A great deal has already been learnt from the study of Croft et al.". Here it should be noted that P. J. Withers is a field leader in this area of mechanics [34-35]. Belnoue et al. [33] also devoted a generous portion of their text crediting the Rutgers group's confirming "experimentally the existence of crack closure" and "Even more importantly… showing the existence of a critical force Fc" (for the external load onset of crack tip response) "… due to the existence of crack closure". Indeed Belnoue et al. [33] extend their generous citations when discussing their own results, witness the phrases: "The compressive zone behind the crack tip that is observed by Croft et al. and our measurements is of principal importance for understanding the process of crack propagation" and "As nicely shown in Croft et al. …". Here it should be noted that A.M. Korsunsky is the head of the Diamond JEEP Beamline and that Belnoue et al. [33] (as well as Steuwer et al. [28]) could reasonably have presented their results with more passing citations.

Thermokinetics of Particulate Nanomaterials: Time evolution of densification and microstructure in multi-component and multi-phase systems is a theoretically/computationally formidable area of materials research where there is little understanding of fundamental processes governing the sintering phenomenon. Of particular interest are the thermoelastic phenomena which take place during processing of particulate nanomaterials with particle size in the 100 nm range. Although there is a wealth of empirical evidence for increased mechanical strength in sinter densified materials, the origin of these phenomena remains unknown. One such system is the Y_2O_3-MgO ceramic composite system in which such an increase in strength is observed. By using the HEX facilities, substantial advances in the understanding sintering in the <100 nm grain size range will be possible using in situ high pressure and high temperature X-ray diffraction. The time evolution of thermokinetic and thermoelastic processes will be monitored by 3D phase and strain mapping and the microscopic sintering conditions determined and thereby optimized. The mapping of phases and strain in such materials will enable one to assess the elasto-optical coupling in multi-component and multi phase systems processed at high temperatures and pressures making such studies technologically important as most particulate nanomaterials are processed by hot isostatic pressing.

Mechanical Behavior of Nanostructured Ceramic Coatings: High energy X-ray diffraction has proven to be most effective in the study of the mechanical behavior of nanostructured ceramic coatings on Ti-alloy substrates when coupled with in-situ 4-point bending. It was found that the compressive strain due to the grit-blasting pre-deposition processing was present in all of the substrate strain profiles. The elastic response of both coatings under increasing bending moment is linear to a first approximation. However, the elastic strains are smaller in the nano- than the micro-coatings, which was indicative that the modulus of elasticity is larger in the nano-coatings. Also, a strain is observed from the interface to the surface of the coating, which is generated during plasma spraying. The high energy EDXRD method's major advantage is that it allows one to assess the strain profile across the thickness of a given coating-substrate system in-situ, under load which is otherwise not possible. This, in turn, enables one to analyze the micromechanics of the deformation process in a coating-substrate system in a phase specific manner from which data based models of the macroscopic deformation can be constructed.

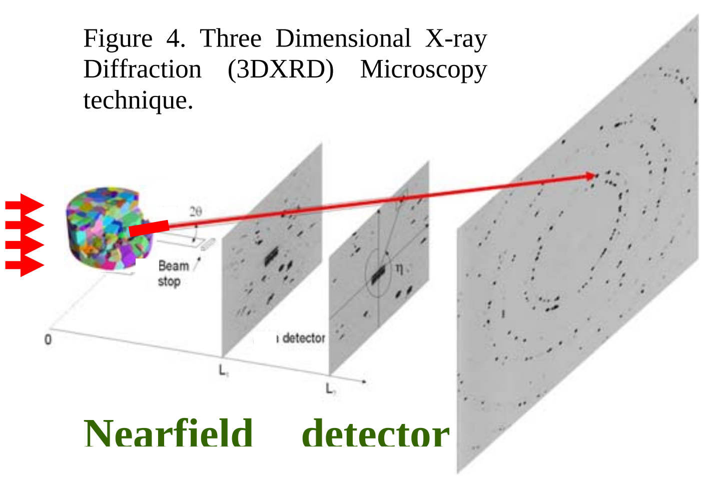
Stress-corrosion cracking of materials: Stress-corrosion cracking is encountered in virtually all aspects of structural engineering where a given load-bearing metallic member's mechanical strength decreases under the attack of the environment (water, salt water, water vapor). The HEX facility will enable US researchers to map the strains around the crack-tip in situ under stress and in the hostel environment. The crucial crack tip strain field variation from the specimen center to the hostil-environment sub-surface surface will be accessible. This, in turn, enables one to obtain the elastic and plastic strains as well as the size of plastic zone in front of the crack as a function of the environmental conditions and imposed stress. The deep penetration of HEX radiation will make it possible to obtain a microscopic picture of stress-corrosion cracking based on direct measurements which can be used in theoretical analysis.

Local Damage and Failure Studies: Unanticipated, premature failure has a wide range of deleterious consequences, including the loss of life and properties, excess replacement costs, and loss of capabilities, while replacements are put in place. Fortunately, advances in synchrotron techniques performed in-situ during mechanical testing provide significant advances in experimental information and offer the potential to revolutionize our understanding of cracking and damage evolution in complex structures under deformation and cyclic-loading conditions. Peter Liaw of Univ of Tenn. (BDP member) has used synchrotron diffraction-peak broadening/line profiles to characterize microstructures in terms of the grain-size distribution, dislocation structure, active slip systems, stacking faults, or twin-boundary densities [36]. The HEX facility will greatly expand the ability to do such studies.

Multilength scale materials-science/mechanics, from single grains to macroscopic properties: In recent years the use of high-energy x-ray diffraction to characterize the mechanical response of engineering/industrial materials, across an enormous range of length scales, has been evolving from "x-ray technique" science to "materials properties" science [13]. These evolving techniques allow 3-D orientation and lattice strain reconstructions on the grain scale [37-40], and determination of the elastic strain tensor components along with the active plastic deformation defect types/densities. <u>These powerful diffraction methods are developing with very close coupling to the modeling community in which grain scale micro-mechanics is integrated up to microscopic mechanical response.</u> The potential to co-refine multiscale experiments and modeling of 3D material response to real time thermomechanical stimuli is the future in this field. The large payoff of such powerful experiment/modeling evolution is greatly improved material selection and mechanical design.

A good example of this experimental/modeling paradigm is the Cornell Miller/Dawson, collaboration [51] which has utilized high energy x-ray diffraction data, together with crystal-based finite element simulations, to understand deformation partitioning in deforming polycrystals [41-51]. They have used lattice strain pole figure data, under loading, to quantify the local stress distribution [41-47] and thereby demonstrated dramatic stress variations between crystallites within a polycrystal under uniaxial tension. These data are ideal for use with large scale simulations where each crystal is composed of hundreds or even thousands of finite elements. Some of their latest work has explored the evolution of crystal stresses during cyclic fatigue deformation [48] and the integration of lattice stain pole figure results with preexisting residual stresses [49]. Miller and Lienert (BDP team members) are co-organizers of a NSF funded workshop [50] to explore/promote the use of high energy x-rays with computational mechanics for understanding challenging multiscale structural mechanics problems. The workshop is already over-subscribed, which is indicative of the interest in the area. See the support letter of Matthew Miller for more details.

Figure 4. Three Dimensional X-ray Diffraction (3DXRD) Microscopy technique.



The Three Dimensional X-ray Diffraction (3DXRD) Microscopy technique can provide complete microstructural information within a gauge volume containing up to 1000's of individual grains [52-54]. The sample is illuminated by a full field beam and 2D transmission diffraction images are taken using the rotation method. Using a large area far field detector and reconstruction software, the full orientation, elastic strain tensor, volume, center of mass (5-10 microns), and unit cell refinement can be determined for every grain within the illuminated volume. In addition, by placing a high resolution semi-transparent 2D or 3D near field area detector close to the sample (~10mm) the 3D grain boundary morphology can be reconstructed using a back projection method. In this way the spatial and angular information are decoupled and more difficult samples (high mosaicity, for example) can be reconstructed in extreme cases. For low mosaicity polycrystalline materials, however, the use of just a near field detector with the appropriate analysis software allows for time resolved studies of 100's – 1000's of grains simultaneously following changes in orientation, strain, stoichiometry, and size as a function of applied forces (P/T). Although detailed local grain boundary information cannot be achieved without the use of a high resolution detector, centers of mass can be determined along with volumes allowing for a tessellation process to determine the most likely grain neighbors. In this way, correlations between kinetics and local microstructural heterogeneities can be probed. The ability to collect grain by grain kinetics on a statistically significant number of grains rather than just measuring a powder averaged value, will allow more realistic models to be developed that incorporate the true kinetic distributions of behavior due to the inhomogeneous nature of all polycrystalline materials.

The monochromatic beam mode with area detectors will enable HEX beamline to play an important role in this rapidly expanding and powerful area of research. Indeed, the grain level approach to mechanical properties is anticipated also to bear fruit in the detailed understanding of local electrochemistry (and it's in-homogeneities) in batteries. The second HEX-B2 hutch, and the forward planning external building HEX-B3 hutch, should allow the large, long setup time in situ stress apparatuses necessary for work in this field.

B. Beamline Concept & Feasibility

Novelty and Critical Mission: Diffraction and small angle scattering for engineering and material science require synchrotron x-ray beamlines which offer the required penetration lengths (e.g. 2 inches Ni super alloy as in Proto Manufacturing's letter of support). The High energy Engineering X-ray scattering (HEX) beamline will produce the hardest feasible x-rays at the NSLS-II, up to 250-300keV. A rough schematic of the beamline is shown below.

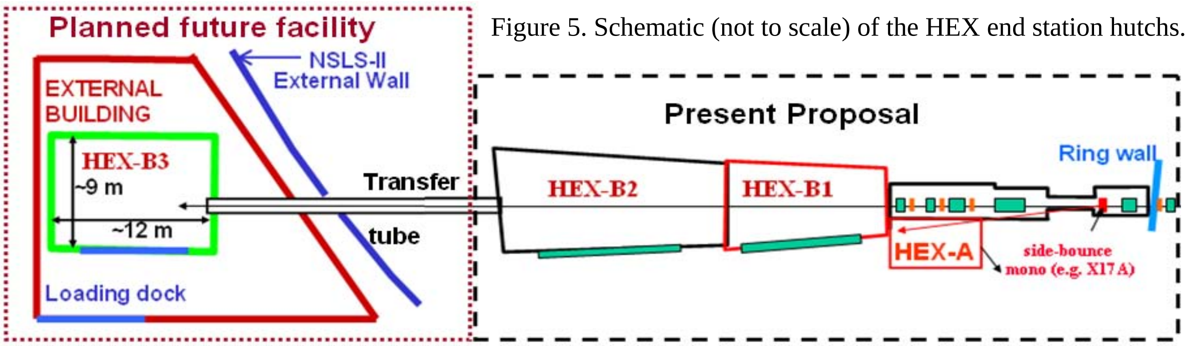


Figure 5. Schematic (not to scale) of the HEX end station hutchs.

Station HEX-A: Beam into a side station, HEX-A (in analogy to NSLS X17-A) is produced by a side bounce Laue monochromator providing a high-flux beam of ~80 keV with moderate energy resolution of 10^{-3} $\Delta E/E$ with a flux of about 10^{13} ph/s/mm^2 in a spot of less than 100(H)x50(V) μm^2. Coupled with compound refractive lenses (CRL) it will allow high-resolution experiments at high energies. This hutch will be used for pair distribution (PDF) measurements. Recall here the nuclear energy science PDF studies of Lynne Ecker noted above and in the letters of support. HEX-A can also be used for wide angle scattering on modest samples/systems where 80 keV provides sufficient penetration. This station has the advantage of continuous beam without interfering with experiments in the other stations.

Experimental Station-HEX-B1 and HEX-B2 {and eventually HEX-B3} will have white beam (30-250 keV) and monochromatic (30-150 keV) beam radiation options. **HEX-B1** will be the workhorse station of the beamline. It will support white beam EDXRD in two modes. A general-purpose multielement high resolution Ge detector (vis-à-vis the 23 element detector at JEEP Diamond see [3]) with two sets of fixed diffraction beam semicircular collimation slits. This mode allows rapid and standard sample interchange along with high data collection rates and simultaneous multiple strain component measurement. A second mode using multiple individual detectors with two sets of continuously variable slits which will be utilized where small or specialized gauge volume tailoring is needed for specific experiments. This is the mode which has been used with great success at NSLS X17-B1. The monochromatic scattering mode will utilize an area detector, or an array of area detectors (see the APS presentation [9]). For small angle scattering an area detector will be placed at the end of the **HEX-B2** station while the sample is in the **HEX-B1** station. (again see [9]). Simultaneous small and wide angle scattering, as at APS, will be possible within this arrangement. Finally when the exterior building and the **HEX-B3** station is added ultrasmall angle scattering will become possible as at the Diamond JEEP beamline [3].

The sample support for **HEX-B1** will allow limited multiple circle rotation as well as x-y-z translation with support from below leaving free access to a large volume sample/experiment-system (for example see the JEEP Diamond design [3]). A rotation stage will also allow tomography/radiography. Multiple fields of view modules with a high speed camera will allow tomography/radiography with varying magnification scales (see [3]). The eventual goal will be to be able to quantitatively specify the microscopic location of inhomogeneous regions (a crack for example) by imaging and then move to that region and profile local strain/stress fields or chemical changes.

Experimental Station HEX-B2 will be used for angle or energy dispersive diffraction on large specimens or in situ experimental systems. It will be equipped with heavy duty stage. In addition long-running experiments involving in situ mechanical fatigue or electrochemical cycling could be operated in **HEX-B2** with periodic beamtimes to monitor the system evolution. Difficult, long setup time experiments could also be prepared in **HEX-B2** while other experiments are performed in **HEX-B1**. The extended letter of support (see appendix) from Prof. Miller from Cornell provides elegant illustrations of in situ lattice strain poll studies which could be carried out in the monochromatic mode on a large stage in **HEX B2**.

Experimental Station-HEX B3 in the eventual external building would accommodate still larger industrial samples/systems. In this respect the recent work at JEEP Diamond by Rolls Royce on characterizing innovative coatings on engine fan blades for the Boeing 787 Dreamliner is noteworthy as prototype for such research (see [55]).

Dedicated multipole superconducting wiggler: The combined requirements of hard x-rays, high flux, and a wide/smooth energy spectrum mandates a multi-pole superconducting wiggler (SCW) source for the HEX beamline. As discussed in Appendix I, balancing ring energy and stability considerations with the maximal flux up to ~250 keV has led to a preliminary choice of a wiggler with: B=4.2T, ~0.8m length, 27 full field poles + 4 end poles, and a period length of 55 mm (HEX SCW55 4.2T). The specification, compare favorably to the best hard x-ray wigglers in the world. The final SCW parameters will be further optimized taking into account performance of up-to-date SC technology and detailed optimization within constraints imposed by accelerator physics.

Monochromator: We will employ a Double-Laue crystal related to the design pioneered by Z. Zhong at NSLS [56]. Such monochromators are already functioning up to the 150-200 keV range on the JEEP [60], W2 [61], and ID15 [62] wiggler sources. The energy range resolution should be $\sim 10^{-3}$. Automated switching between diffraction and imaging optimized monochromators will be included.

Permanent and removable low energy attenuators: To reduce heat load on following x-ray optics/sample and to act as primary vacuum windows the permanent water cooled CVD diamond (primary) followed by CVD SiC windows will be installed. Optional (removable as required) water cooled filters of Al and Cu (1-8 mm thick) will be used.

Compound refractive lenses (CRL): Tentatively, the focusing optics at HEX beamline will rely on Compound Refractive Lenses (CRL). Recently a tunable x-ray focusing apparatus based on compound refractive lenses, referred to as a "transfocator", has been installed in the first optics hutch of beamline ID11 at ESRF [57]. By varying the number of lenses in the beam, the energy focused and the focal length can be varied continuously throughout a large range of energies and distances. The instrument can be used in both white (albeit with chromatic aberration) and monochromatic beams to focus, pre-focus or collimate the beam. We are conducting a ray-tracing simulations based on conservative acceptance aperture of 1 mm.

Shared equipment pool

- Heavy duty multiple circle diffractometer/X,Y,Z-stages (with rotation) for large samples.
- Array Ge detectors
- Pixium 4600 (3001x3001 pixels 143x143 μm^2) or similar GE Healthcare image plate s
- Radiographic camera for microtomography. Multiple modules with different magnifications and scintillates are anticipated.
- Spiral and conical slit systems for monochromatic depth strain profiling/mapping

Sample environment: Considerable efforts will be made to ensure that a wide range of sample environments are made available to the user community. Typical equipment includes: mechanical loaders (i.e. four-point bender, tensile loader, etc), ILL furnace (T=RT-1800C), Cyberstar hot air blower (T = RT-1300K), and Oxford Cryosystem 700+ (T= 80–500K). Industrial users will enjoy a flexibility of using large scale processing chambers, chemical reactors, and loading apparatus mounted on heavy duty stage with capacity of up to 1000kg. Battery cycling equipment will also be available.

Worldwide beamlines with overlap with HEX: The newest and most relevant facility to HEX is the Joint Engineering, Environmental and Processing (JEEP) ID12-beamline at the UK Diamond synchrotron [2,3]. This beamline/program incorporates many of the objectives of the HEX beamline: its energy range, its selection of techniques, its external building, and its emphasis on industrial/economic relevance. The absolutely key point here is that JEEP serves the UK/EU industry and economic well-being. Without the HEX beamline no comparable facility is on the horizon in the US. JEEP has a wiggler source with an energy range of 50 keV – 150 keV for energy dispersive and monochromatic (2-D detector) scattering. It also provides small angle scattering SAXS and ultrasmall angle scattering (by placing the detector in the exterior building). JEEP has radiographic and tomographic imaging over the similarly high-energy range. The external building accommodates extremely large industrial components. See for example their recent report of a turbojet fan blade study [55] wherein the following prescient comment was made: "Diamond provides world-leading experimental facilities for UK science and industry. By enabling large-scale components to be studied in such incredible detail, JEEP marks a real advance in our technological capabilities." **Absent HEX no such comment will be possible in the US.**

The EU's European Synchrotron Radiation Facility (ESRF) [4,5] has several beamlines for high-energy x-ray science/engineering studies. Beamline ID15A&B has a wiggler source for white beam or monochromatic x-rays in the 30-750 keV range. Energy dispersive diffraction, angle dispersive diffraction (with spiral slit for depth of the resolution) along with an ultrafast micro-tomography are also supported on this beamline. The undulator beamline, ID 11 provides monochromatic x-rays over the 18-140 keV range. Being a particularly long beamline it can supply nano focusing for 3-D single grain diffraction and diffraction contrast tomography. The monochromatic beamline ID31 is useful for high resolution engineering/industrial samples where below 60 keV x-rays can be used.

The HASYLAB synchrotron facilities in Germany have two high-energy beam lines involved in engineering/industrial materials [6,7]. The HARWI-II, W2 wiggler, High-Energy X-Ray Material Science beamline on the DORIS ring, accommodates x-ray scattering (energy and angle dispersive), along with imaging/tomography. With varying details the energy ranges for these techniques are 20-200 keV [6]. The High Energy Materials Science Beamline, on the PETRA-III ring, has an undulator source providing monochromatic x-rays in the 60-200 keV range [7]. The beamline supports both wide and small angle x-ray scattering as well as imaging/tomography.

In the US the Sector 1 at APS (with its planned upgrade) provides a superlative set of high energy, undulator-source materials science/engineering beamlines [8,9]. Beamline 1 ‐ ID provides monochromatic x-rays in the 50 ‐ 130 keV range for science/engineering/industrial research. It supports high-energy diffraction microscopy, and wide/small angle scattering in a wide variety of in ‐ situ environments. Indeed the wide and small angle scattering can be run simultaneously with 2-D area detectors in two separate hutches [9]. Pair distribution function (PDF) and tomography measurements are also supported. It should be noted that this beamline is fivefold oversubscribed [9]. In the upgrade additional1-ID D, E,F,G hutches will be served by new canted undulators. It should be noted that in a tapered mode the APS undulator can be used to generate a high-energy white beam. This however does not appear to be the standard mode of operation.

NSLS-II beamlines with overlap with HEX The 40keV-80keV scattering energies supported by the X-ray Powder Diffraction (XPD) beamline overlaps the HEX capabilities at the low end. These energies are less than those typically needed for engineering studies. The XPD will moreover be heavily oversubscribed with basic science users.

The 4-Dimensional Studies in Extreme Environments (4DE) with its x-ray scattering in the 20–100 keV range and with both monochromatic and energy dispersive diffraction provides some overlap with the HEX beamline capabilities. The HEX beamline, however, emphasizes work above 100 keV energies as needed for engineering studies. Moreover, the heavy geology user load on 4DE would preclude extensive (indeed all but token) engineering studies. A meaningful (non-parasitic) material science/engineering requires a dedicated HEX beamline.

The Superconducting Wiggler Long Beamline for Full-field Imaging (FXI) with its energy range of 5-60 keV will impinge on the lower energy range of the imaging/tomography of the HEX line. Again, for a real engineering program, higher energy and non-parasitic mode running are required. The FXI line will also be heavily oversubscribed by basic science users for imaging.

C. Required Technical Advances (if any)

The impact of the high field SCW on the beam dynamics of the NSLS-II will be investigated and mitigated if required. The wide horizontal beam may require special vacuum chamber design. Further advancements in CRL optics are required for maximizing the acceptance aperture and RMS. High energy detectors and energy-discriminating area detector development (in the range 50-200 keV) would be very desirable but is not required to accomplish the basic scientific goals.

D. User Community and Demands

The demand for HEX can be found in the prior/ongoing work by the Rutgers Group, by the battery groups, industrial representatives, and by representatives of the nuclear energy materials science. A series of letters of support and/or endorsement testifying to the need and applications for the proposed HEX facility are presented in the appendix. These include letters from a number of industrial, university, and synchrotron representatives, and the ONR. The proposed HEX will be multi-purpose and will serve a diverse group of scientists working in high-priority areas of research that will directly benefit of the nation.

A compelling case for the importance of the HEX facility for battery/energy storage studies is made in the support letters from Clare Grey (Stony Brook & Cambridge), Esther Takeuchi (SUNNY Buffalo), and Mark Little (Senior VP of GE Global Research). The work and statements of these battery field leaders make it clear that high-energy x-ray diffraction (and EDXRD in particular) provides a heretofore missing and important analytical tool for battery research. Namely, it opens a window on the local in situ electrochemistry transpiring in real prototype batteries. It should be noted that this window has been opened at X17B1 and that, to the proposers knowledge, this is the first and only such initiative in the world. In this sense NSLS and NSLS-II appear to have a substantial edge in this area.

The importance of the HEX facility for characterizing advanced engineering alloys and ceramics was emphasized in the letters from M. Little (GE), M. Brauss (Pres. Proto. Mfg.), F. Preli (Pratt & Whitney/UTC), R. Ayer (ExxonMobil), and E. Johnson (John Deere). The ceramic and nano material facets of the unique HEX capabilities were emphasized in the letters from G. Kim (Perpetual Tech.), R.S. Burnhouse (Pres. A&A Co. Inc.), G. Skandan (CEO, NEI Corp.), C. S. Nordahl (Raytheon) and L. Kabacoff (Prog. Officer ONR). In a number of these materials applications the Department of Defense interests/funding explicitly requires characterization at US-based facilities which would be greatly reduced absent the proposed HEX beamline.

The call for a new generation of nuclear reactors in this country is loud from the scientific community, to the halls of government, and from the future energy needs of the general population. The appendix letters of support from Lynn Ecker and N. Simos clearly outlines the urgent need for a wide spectrum of advanced materials research to accomplish these urgent societal needs. They emphasize that fundamental research on these materials, and importantly their properties after radiation damage, is clearly in the outline goals of the DOE and Brookhaven laboratory. Additional users in this area can also be anticipated.

The support letter from V. Honkimaki and T. Buslaps (grounded in long direct experience) emphasizes the growing and potentially very large engineering/industrial science community for HEX type high-energy beamlines. Moreover, they imply that, absent HEX type infrastructure investment, the upward inflecting importance of synchrotron science that has begun in Europe, could leave US scientific/economic interests behind. The support letter from U. Lienert (APS Sector 1 Beamline) also emphasizes that the HEX beamline is “absolutely required” for competiveness with the European community. Moreover, he underscores HEX as complementary to and facilitating a synergy with the APS undulator program. Finally he notes that the combined the HEX and APS programs help to achieve the “critical mass” needed to exploit the great potential of simotaneous advances in high energy x-ray hardware/software and materials modeling.

Finally we would like to emphasize the support letters from M. Miller (Cornell) and R. Suter (Carnegie Mellon) which touch on the new and rapidly expanding field of bottom-up grain scale to macroscopic mechanical properties co-refinement of high energy x-ray measurements with theoretical modeling/simulations. Revolutions in both the massive experimental data reduction and the modeling computational power are underway. The massive over subscription of the APS facilities means that the HEX facility could play an important role in carrying this revolution forward.

E. Proposal Team Expertise and Experience

As indicated in the bios the Team Members cumulatively possess the necessary expertise and experience to implement the state-of-the-art HEX at the NSLS-II. Z. Zhong is the beamline scientist at X17-B1, has vast experience in hard x-ray applications and instrumentation, and is fundamentally responsible for all of the work that has come out of this beamline. M. Croft, an experimental solid state physicist, brings 30 years of experience in X-ray based research in materials science and also possesses experience in instrumentation design and development. T. Tsakalakos, an experimental as well as computational materials scientist, also brings 30 years of experience in X-ray based materials research, and has a record of accomplishments in the field of mechanical behavior of materials, nano- and biomaterials, micromechanics, phase transformations, among others. E. K. Akdogan, a experimental materials scientists with a strong background in thermodynamics and kinetics, brings 16 years of experience in the fields of nanomaterials, functional materials, materials processing an characterization. A. Ignatov has nearly 20 years of experience in synchrotron radiation experiments, advanced data analysis and instrumentation.

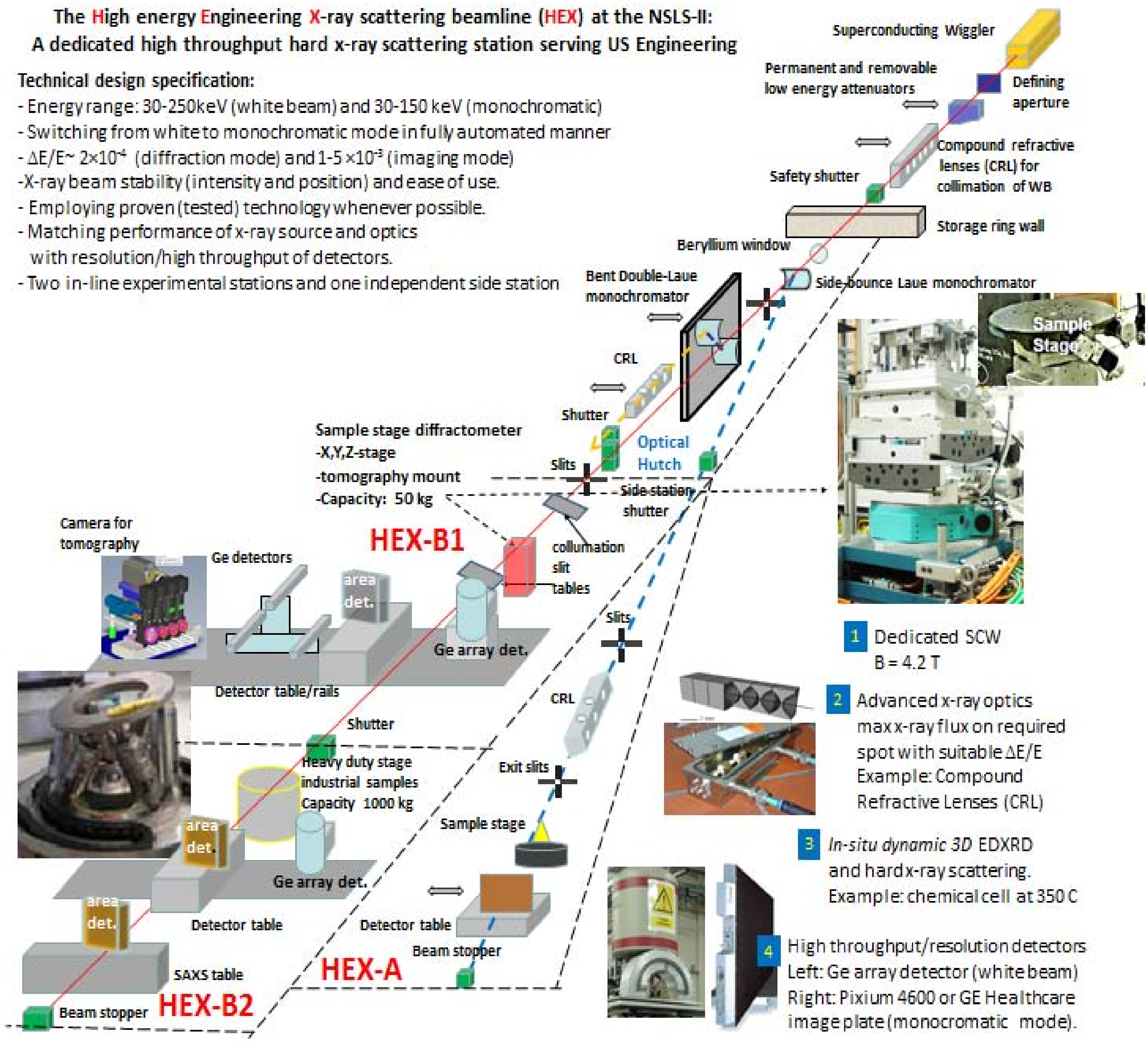
The battery group includes C. Gray and E. Takeuchi who are important leaders in the battery research field with large groups and positions in research consortia. R. Robert is a synchrotron specialist working with this battery group. J. Rijssenbeek is a task leader on GE's NaMx battery program, and is in charge of a global team of scientists and engineers that is developing fundamental understanding of the degradation mechanisms and the operational conditions that affect NaMx battery performance over life under application specific duty cycles. Y. Gao is a synchrotron experimentalist whose 30 years' experience is almost unparalleled in depth and breadth. Lynne Ecker is an expert in materials science as applied to nuclear power.

M. Miller is a world expert in hard x-ray diffraction applied to the microscopic mechanics of materials. L. Margulies is a world expert in the area of 3-D x-ray diffraction microscopy and more than a decade of experience at multiple synchrotron facilities. U. Lienert has more than 16 years experience in cutting edge high energy x-ray synchrotron research and is a world leader in the diffraction microscopy field. Moreover, he establishes a direct/synergistic connection with APS program. .P. Liaw: holds a named chair in Materials Science and Engineering the Univ. of Tenn.; is co-author on more than 500 papers and coeditor of more than 30 books in this area; and is an ASM fellow. O.Tchoubar (Chubar) is a scientist with more than 19 years' experience in synchrotron radiation simulations and insertion device design.

HEX Appendices

Appendix I Beamline details: optics, equipment, flux and background

Figure AI.1 A schematic poster illustrating the HEX beamline optics, hutches, and end station equipment.



HEX wiggler: Flux, power and ring perturbation considerations

In making a preliminary choice for the HEX wiggler three factors were weighed: the highest flux possible in the 100-250 keV range; the heat loading levels; and the beam spreading effects on other insertion devices. A preliminary optimization of these factors has yielded a B=4.2T unit, ~0.8m long, with 27 full field poles + 4 end poles, with a period length of 55 mm (“HEX SCW55 4.2T). As seen in Figure AI.2 this choice yields a flux curve essentially identical to the most recently established engineering beamline JEEP at the 3 GeV Diamond synchrotron light source. Achieving higher fluxes in a 3GeV machine would require detailed consideration by the NSLS-II machine scientists. The flux at 150 keV will be 19 fold higher than the current NSLS X17.

In terms of the power load the HEX SCW55 4.2T is (as noted in the Figure AI.2 caption) far less than the powder diffraction beamline (XPD) and only slightly larger than the SCWC60 wiggler. Thus, we can use experiences gained by the XPD facility beamline and the ISS beamline (both of which use DW100) to guide our front end and optical design, especially regarding heat-load management.

Figure AI.2 Comparisons of wiggler fluxes: European Diamond JEEP, ESRF ID15, and DORIS W2; NSLS X17; the NSLS-II SCWC60 design; and the preliminarily optimized NSLS-II HEX SCW55 B=4.2 T choice. The total wiggler power, for the various B choices are indicated. Note that the power load of the HEX SCW55 is only 8% larger than the SCWC60 and is 34% less than the powder diffraction beamline (XPD) damping wiggler (DW100) [59]. Curves calculated with WS/XOP2.3 [58]

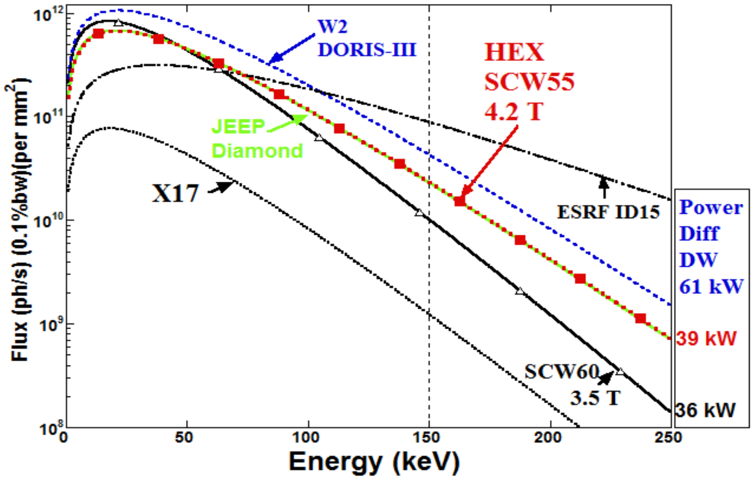


Table I.1 The parameters used in these calculations are in the following table.

Wiggler	**SCW55 HEX**	ID12 Diamond	W2, DorisIII	ID15, ESRF	~SCW60
Total Length (m)	**~0.8**	~1.2	~4.0	~1.9	~1.1
Period Length (mm)	**55**	48	110	230	45
Peak field (T)	**4.2**	4.2	1.98	1.84	3.5
Number of poles + 4 side poles	**27**	45	70	7	45
Critical energy (keV)	**25.2**	25.1	26.1	44.1	21.0
Power*(kW)@I(mA)	**39@500**	33@300	27@140	15@200	36@500

Calculated using WS/XOP2.3 [58] by A. Ignatov.

We have calculated the effect of the proposed HEX wiggler, given and assumed set of wiggler insertion devices, on the RMS horizontal electron beam emittance, ε_x, the crucial RMS relative energy spread parameter, σ_δ, and the electron energy loss per turn, U_{tot} The energy spread including the SCW55 (4.2T) falls below the critical "tolerable" 0.1% level. Additional iterations on the wiggler design to potentially tweak the flux up and the energy spread down will be considered with the NSLS-II machine design group.

Table I.2 The illustrative ring parameters with the HEX SCW55 B=4.2 T includes.

Wiggler Configuration	ε_x [nm•rad]	σ_δ [%]	U_{tot} [keV]
3DW+SCW40(3T)+SCW60(3.5T)+SCW55(4.2T)	0.69	0.099	877

Calculated by J.Bengtsson (NSLS-II Accelerator Physics Group) and O.Tchoubar (Photon Division, Photon Sciences Directorate).

HEX BDP modifications actions in response to 2010 Review Panel comments.

In the last BDP proposal round the HEX proposal had a 1.1 out of 1.0 (best) rating on the scientific case. Nevertheless in this round is scientific case has been strengthened greatly by the addition of significant discussion of the monochromatic scattering grain by grain and multiscale material property capabilities. To strengthen the proposal in the monochromatic scattering and multiscale material area L. Margulies and U. Lienert (both world experts in this area) were added to the BDP team. Moreover U. Lienert also reinforces a more direct/synergistic connection with APS. The GE battery work has also come to fruition both in publication [16] and in commercialization [1] since the last proposal round.

The HEX group also had a workshop in May of 2011 [11] in which high-energy engineering beamline representatives (among others) from APS [9, 10], ESRF [5], and Diamond-JEEP [3] presented summaries of their various programs/beamlines. As a result of this workshop the monochromatic wide and small angle scattering techniques and the imaging/tomography techniques have been made more prominent in the current proposal. These techniques meet the needs of a rapidly expanding high-energy engineering community, and are standard in the engineering beamline's worldwide.

In the present proposal a more modest, but still world-class, wiggler has been proposed. As noted above the power dissipation (raised as an issue in last review proposal round is now well below the high end range already planned for NSLS-II. The effect of the HEX wiggler on the overall ring and insertion device has been quantitatively taken into consideration in our current proposed SCW55 4.2T HEX wiggler source. The machine scientist O. Tchoubar has been added to the BDP and has helped refine our preliminary wiggler choice. It will also help to refine the wiggler parameters to match the NSLS-II ring requirements.

Appendix II References and Links

{for some some links : User Name: croftcomm Password: fall2010

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[3] HEX May 2011Workshop JEERP-Diamond Presentation, M. Drakopoulos "The New High Energy Beamline for Engineering, Material Science and Processing at the Diamond Light Source" http://www.physics.rutgers.edu/~croft/BDP11/HEX-WS-presentations/JEEPpresented-HEX-WS.pdf
[4] See http://www.esrf.eu/UsersAndScience/Experiments/StructMaterials/ID15/
[5] HEX May 2011Workshop ESRF Presentation link http://www.physics.rutgers.edu/~croft/BDP11/HEX-WS-presentations/NSLS2_workshop_Buslaps.pdf
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See enlarged poster at http://hasylab.desy.de/e70/e231/e33691/e33901/e33907/infoboxContent106814/SRI09_Melbourne_eng.pdf
[8] see Advanced Photon Source Sector 1 http://www.aps.anl.gov/Sectors/Sector1/
[9] see J. Almer "High Energy X-ray Studies of Engineering Materials at the APS 1-ID-C-E Beamline" presented at HEX Workshop http://www.physics.rutgers.edu/~croft/BDP11/HEX-WS-presentations/Almer_NSLS_Workshop_May11.pdf
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[12] HEX May 2011Workshop Presentations link http://www.physics.rutgers.edu/~croft/BDP11/HEX-WS-presentations/
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[51] HEX May 2011Workshop M. Miller Presentation link http://www.physics.rutgers.edu/~croft/BDP11/HEX-WS-presentations/NSLS_miller_2011.pdf
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[60] Diamond JEEP monochromator http://www.diamond.ac.uk/Home/Beamlines/I12/specs/optics.html#mono
[61] Desy Lab W2 monochromator http://www.mf.mpg.de/en/abteilungen/dosch/hemd/optics.shtml
[62] ESRF ID15 monochromator http://www.mf.mpg.de/en/abteilungen/dosch/hemd/optics.shtml

Appendix III Proposal Team Member Bios (alphabetical)

Enver Koray Akdoğan

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Rutgers-The State University of New Jersey
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Education

Ph.D.; Materials Science and Engineering, Rutgers University, New Brunswick, New Jersey (1999) Thesis Advisor: Professor A. Safari (Ph.D. Penn State University)
M.Sc.; Metallurgical and Materials Engineering, METU, Ankara, Turkey (1994) Thesis Advisor: Professor M. Timucin (Ph.D. University of Missouri-Rolla)
B.Sc.; Metallurgical and Materials Engineering, METU, Ankara, Turkey (1991)

Areas of Research: Mechanical behavior of engineering materials (bulk, coatings and thin films). Environmental effects on mechanical behavior of engineering materials with emphasis on Titanium alloys, ferrous alloys, amorphous Iron, TiO_2 and Al_2O3-TiO_2. Phase and strain mapping and interfacial phenomena (phase evolution, diffusion etc.) in batteries. Phase and strain mapping in nanostructured films, coatings and bulk materials. Deformation mechanics, dislocation phenomena and plasticity. Micromechanics and nanomechanics of thin films and coatings (experimental and computational). Use of eigenstrain formalism in the study of films and coatings (experimental and computational) Dislocations, strain relaxation, nonlinear elasticity phenomena in thin films, heterostructures, nanoisland and nanotubes, and their effect on phase stability and/or evolution. Evolution of electronic, optical, magnetic and cross-coupled properties (second and third harmonic generation, electrooptic, photoelastic, piezooptic properties, electrocaloric, magnetostrictive properties etc) with finite size, defects and strain.Electroactive monolithic bi-layer structures for asymmetric and low-hysteresis actuation, conformal actuators and sensors, strain coupling and interfacial phenomena in elecrostrictive-ferroelectric heterostructure thin films, thick films and co-sintered macro-composites.Protonic conductors based on H^+ doped ferroelectric and paraelectric media, effect of H^+ and defects on nonlinear dielectric characteristics of host, and the effect of host media on ionic transport. Nano-self Assembly of multiphase functional oxides and strongly correlated systems, nonequilibrium processing, spinodal decomposition under biaxial stress (isotropic and anisotropic) and their effects of electronic, optical, magnetic and cross-coupled properties.Nonlinear dielectric materials with emphasis on electric field-induced nonlinearity and loss phenomena (especially extrinsic loss), anisotropic epitaxy, strain-modulated phase equilibria, microwave soliton propagation in nonlinear dielectric media in the context of nonlinear transmission lines for rf/microwave device applications.

Professional Work Experience

Jan 2010-present: Co-Director, Nano-Structured Materials Laboratory,
Nov 2001-Jan2010, Research Assoc., Rutgers Univ., Dept. of Materials Science and Eng'g
Jan 1999-Nov 2001, Postdoctoral Fellow on J-1 Status, Rutgers Univ., Dept. of Materials Science and Eng'g
Aug 1994-Jan 1999 NATO Fellow and doctoral student, Rutgers Univ., Dept. of Materials Science and Eng'g

Publication Articles (Total: 60 published, 7 in preparation)

1) M. Croft, V. Shukla N. Jisrawi, Z. Zhong, R. Sadangi, A. Ignatov, L. Balarinni, ***E. K. Akdoğan***, K. Horvath, and T. Tsakalakos, "*In situ strain profiling of elasto-plastic bending in Ti-6Al-4V alloy by synchrotron energy dispersive x-ray diffraction,*" Journal of Applied Physics,. **105**, 093505 (2009).
2) J. Sun, P. Ngernchuklin, M. Vittadello, ***E.K. Akdoğan***, and A. Safari "*Development of 2-2 piezoelectric ceramic/polymer composites by direct-write technique,*" Journal of Electroceramics,
DOI 10.1007/s10832-009-9561-3 (2009).
3) A. Safari, M. Abazari, K. Kerman, N. Marandian-Hagh, ***E.K. Akdoğan***, "$(K_{0.44}, Na_{0.52}, Li_{0.04})(Nb_{0.84}, Ta_{0.10}, Sb_{0.06})O_3$ Ferroelectrics, IEEE Transactions on Ultrasonics, Ferroelectrics Frequency Control, 56, 8,1586-94 (2009).
4) P. Ngerchuklin, ***E.K. Akdoğan***, B. Jadidian, A. Safari, IEEE Transactions on Ultrasonics, Ferroelectrics Frequency Control, 56 , 6, 1131-1138 (2009).
5) P. Ngerchuklin, ***E.K. Akdoğan***, B. Jadidian, A. Safari, "Electromechanical displacement of piezoelectric-electrostrictive monolithic bilayer composites," Journal of Applied Physics 105, 034102 (2009).
6) M. Abazari, ***E.K. Akdoğan***, A. Safari, "Effects of background oxygen pressure on dielectric and ferroelectric properties of epitaxial $(K_{0.44}, Na_{0.52}, Li_{0.04})(Nb_{0.84},Ta_{0.10}, Sb_{0.06})O_3$ thin films on $SrTiO_3$, Applied Physics Letters, Appl. Phys. Lett. 93, 192910 (2008).
7) M. Abazari, ***E.K. Akdoğan***, A. Safari, "Dielectric and ferroelectric properties of strain-relieved epitaxial lead-free KNN-LT-LS ferroelectric thin films on $SrTiO_3$ substrates," Journal of Applied Physics, 103, 104106 (2008).

Biographical Sketch: Mark C. Croft, Professor, Dept. of Physics and Astronomy Rutgers University

Education: B.A. (69), Johns Hopkins University : M.A. (71), Ph.D. (76) University of Rochester
Positions: Teaching/Research Assistant, University of Rochester 1969-71, 1973-77
Physical Sciences Assistant, US Army Electronics Com., Electronic Materials 1973
Rutgers Univ. :Instructor 1977-79; Assist. Prof. 1979-83; Assoc. Prof. 1983-96, Prof. 1996-present
Rutgers Synchrotron Radiation Facility Coordinator for Materials Science 1990-2006
Member of Participating Research Team X19-A/X18B: National Synchrotron Light Source (NSLS) 1990-2006
Contributing User Materials Science Beamline X17B1: NSLS 2006-2008,2008-2011

Awards
Fellow of the American Physical Society (2007): for seminal contributions to correlated electron physics and electronic structure of rare earth and transitional metal compounds; novel applications of synchrotron radiation.
Rutgers McMahon Award (2000) for community service in the form of ongoing lectures bringing the excitement and wonder of science to children and the public at large (with D. Maiullo).
Patents: "Analysis methods for energy dispersive x-ray diffraction patterns." pat. no. 6118850 issued on 9/12/00

Selected Relevant Publications (180 as of 7/11)

83. "Mercuric Iodide Detector Systems for Identifying Substances by X-Ray Energy Dispersive Diffraction", J. Iwanczyk, B. Patt, Y. Wang, M. Croft, Z. Kalman, W. Mayo, IEEE Trans. on Nucl. Sci. **42**. 606 (1995)

123. "Stress Distribution and Tomographic Profiling with Energy Dispersive X-Ray Scattering", M. Croft, I. Zakharchenko, Z. Zhong,T. Tsakalakos, Y. Gulak, Z. Kalman, J. Hastings, J. Hu, R. Holtz, and K. Sadananda, in MRS Proc. Vol. 678, [Edr.'s P. Allen, S. Mini, D. Perry, S. Stock]. Application of Synchrotron Radiation Techniques to Materials Science VI. Symposium (Materials Research Society Symposium Proceedings Vol.678). Mater. Res. Soc., pp.EE2.1.1-6. (2001)

128. "Strain Field and Scattered Intensity Profiling with Energy Dispersive X-Ray Scattering", M. Croft, I. Zakharchenko, Z. Zhong, Y. Gulak, J. Hastings, J. Hu, R. Holtz, M. DaSilva, and T. Tsakalakos, J. App. Phys. **92** ,578-586 (2002)

130. "Methodology of Synchrotron EDXRD Strain Profiling" I. Zakharchenko, Y. Gulak, Z. Zhong, M. Croft, and T. Tsakalakos, Advances in X-ray Analysis, Vol. 46, 98-105 (2003)

131. "Application of Synchrotron EDXRD Strain Profiling in Shot Peened Materials", I. Zakharchenko, Y. Gulak, Z. Zhong, M. Croft, and T. Tsakalakos, Advances in X-ray Analysis, Vol. 46, 338-345 (2003)

146. "Strain Profiling of Fatigue Crack Overload Effects Using Energy Dispersive X-Ray Diffraction" M. Croft, Z. Zhong, N. Jisrawi,I. Zakharchenko, R.L. Holtz,Y. Gulak, J. Skaritka, T. Fast, K. Sadananda, M. Lakshmipathy, and T. Tsakalakos. Int. J. Fatigue 27, 1409 (2005) http://www.physics.rutgers.edu/~croft/papers/146-OL-effect-IJF-27-1409-2005.pdf

157. "Fatigue history and in-situ loading studies of the overload effect using high resolution x-ray strain profiling", M. Croft, N. M. Jisrawi,Z. Zhong, R. Holtz, K. Sadananda, J. Skaritka, and T. Tsakalakos, International Journal of Fatigue 29 (issues 9-11) 1726-1736 (2007) http://www.physics.rutgers.edu/~croft/papers/157-IJFatigue29-1726-2007.pdf

160. "Stress Gradient Induced Strain Localization in Metals: High Resolution Strain Cross Sectioning via Synchrotron X-Ray Diffraction" M. Croft, N. Jisrawi, Z. Zhong, R. Holtz, M. Shepard, M. Lakshmipathy, K. Sadananda, J. Skaritka, V. Sukla, R. Sadangi and T. Tsakalakos, Engineering Materials and Technology, **130**, 021005 (2008) http://www.physics.rutgers.edu/~croft/papers/160-strainloc-JYT-130-021005-2008.pdf

168 "Mapping and load response of overload strain fields: synchrotron x-ray measurements", M. Croft, V. Shukla, N. M. Jisrawi,Z. Zhong, R. K. Sadangi, R. L. Holtz, P. Pao, K. Horvath, K. Sadananda, A. Ignatov, J. Skaritka, and T. Tsakalakos , Int J. of Fatigue 31, 1669-1677 (2009) http://www.physics.rutgers.edu/~croft/papers/168-Mapping-loadresp-IJF2009.pdf

169 "In situ strain profiling of elasto-plastic bending in Ti-6Al-4V alloy by synchrotron energy dispersive x-ray diffraction" M. Croft, V. Shukla, K. Akdoğan, N. Jisrawi, Z. Zhong, R. Sadangi, A. Ignatov, L. Balarinni, E., K. Horvath, T. Tsakalakos, J. Appl. Phys. 105, 093505 (2009) http://www.physics.rutgers.edu/~croft/papers/169-bend-Ti64-JAP-2009.pdf

171a. (extended abstract) "In-situ Spatial and Temporal Studies of Electrochemistry in Advanced High Temperature Batteries Under Operating Conditions" *Microscopy and Microanalysis,* 15 (Suppl. 2) , pp 1394-1395 doi:10.1017/S1431927609099486 http://www.physics.rutgers.edu/~croft/papers/171a-Micro%20and%20Microanal-15-1394-2009.pdf

177. "In situ x-ray diffraction of prototype sodium metal halide cells: time and space electrochemical profiling" J. Rijssenbeek, Y. Gao, Z. Zhong, M. Croft, N. Jisrawi, I. Ignatov, T. Tsakalakos, Journal of Power Sources, 196, 2332-2339 (2011) http://www.physics.rutgers.edu/~croft/papers/177-pre-Insitu-sodium-metal-halide-cells.pdf
Also available at http://dx.doi.org/10.1016/j.jpowsour.2010.10.023

Lynne E. Ecker
Scientist, Advanced Nuclear Concepts

EXPERIENCE

BROOKHAVEN NATIONAL LABORATORY, Upton, NY
Associate Scientist/Scientist; November 2004 - Present, *Advanced Nuclear Concepts*

- Demonstrated the laboratory-scale production of Infiltrated Kernel Nuclear Fuel and preformed experiments at the National Synchrotron Light Source using XANES to identify the chemical composition and uranium distribution. (team accomplishment)
- Developed a quantitative model to predict the fuel loading in Infiltrated Kernel Nuclear Fuel from fundamental material properties.
- Proficient in GAmma Detector Response and Analysis Software (GADRAS) and PeakEasy for analyzing gamma-ray spectrum – Alternate on the Reachback Team
- Derivative Classifier for the Energy Sciences Department

KNOLLS ATOMIC POWER LABORTORY, LOCKHEED MARTIN, Schenectady, NY, Naval Reactors Program
Scientist/Senior Scientist; October 1995 – October 2004, *Computational Materials Science*

- Performed advanced finite element modeling of materials related phenomenon (elastic-plastic materials, thermal and irradiation creep, anisotropic swelling, fracture mechanics parameters, failure mechanisms, crack growth and contacting surfaces) in complex mechanical systems and corrosion films.
- Imported and developed new finite element technologies, including ABAQUS, a general purpose finite element code that has become the company standard, OOF, an object oriented finite element mesh generator for micrographs to model microstructural features, and Python, a scripting language used to automate and customize the finite element modeling process with ABAQUS. Combined capabilities to generate multiple finite element models with computational design of experiments and response surface methods for characterizing parameter uncertainty and design optimization in advanced nuclear fuel systems. Performed statistical analysis for robust design.
- Calculated the material properties of ZrC using atomistic modeling.
- Chair - KAPL/Bettis System Mechanical Performance Consortium.
- Project Management: Lead for 3 Engineers for project on modeling the effect of crystal plasticity during large deformation manufacturing processes; Mentoring: Lead for Naval Nuclear Propulsion Fellowship on Probabilistic Design Methodology and risk/safety assessment.

RECENT PUBLICATIONS

- Podobedov, B., L. Ecker, D. Harder and G. Rakowsky. “Eddy Current Shielding by Electrically Thick Vacuum Chambers.” Particle Accelerator Conference, Vancouver, CN. May 2009.
- Ecker, L. et al. “An Infiltration Manufacturing Process for Nuclear Fuels.” ASME High Temperature Reactor Conference, Washington, D.C. October, 2008.
- Ecker, L. “Materials in Extreme Conditions.” Presented to the EENS Visiting Committee and Commissioner of the NRC, July 2008.
- Ludewig, H., L. Cheng, L. Ecker and M. Todosow. “An Integrated Analysis of a NERVA Based Nuclear Thermal Propulsions System.” Space Technology and Applications International Forum, Albuquerque, NM, February, 2006.

EDUCATION

SYRACUSE UNIVERSITY, Syracuse, NY,
Ph.D. in Solid State Science and Technology, May 1996

- Dissertation Topic: Fatigue Crack Propagation During Rolling Contact - Developed a new failure mechanism for rolling contact fatigue using rolling contact fatigue tests, finite element methods and microstructural analysis.

M.S. in Mechanical Engineering, December 1992
B.A. in Physics, May 1988

Clare P. Grey - Biographical Sketch

Professor, Department of Chemistry; Stony Brook University
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(a) Education and Training:

University of Oxford	Chemistry	BA (*First Class Honors)* 1987
University of Oxford	Chemistry	D. Phil. 1991
University of Nijmegen	Physical Chemistry	Royal Society Post-doctoral

(b) Research and Professional Experience:

Director, Northeastern Center for Chemical Energy Storage, a Department of Energy Frontier Center, Stony Brook University (Aug. 2009-present)
Head, Inorganic Sector, Cambridge University, (Aug. 2009-present)
Geoffrey Moorhouse Gibson Professor in Inorganic Chemistry, University of Cambridge, UK, (July 2009-present)
Visiting Professor, Université de Picardie Jules Vernes, Amiens, 2006-07; 2007-08
Associate Director, NSF Center for Environmental Molecular Science, Stony Brook University, (Oct 2002 - present)
Professor, Department of Chemistry, Stony Brook University (Sept. 2001 - present)
Visiting Professor, Université Louis Pasteur, Strasbourg, (2000)
Associate Professor, Department of Chemistry, Stony Brook University (Sept. 1997 - Aug. 2001)
Assistant Professor, Department of Chemistry, Stony Brook University (Jan. 1994 - Aug. 1997)
Visiting Scientist at DuPont CR&D (Feb. 1992 - Jan. 1994)

(c) Honors and Awards:

Ampere Award (2010); RSC John Jeyes Award (2010); Vaughan Lecturer (2008); Research Award of the Battery Division of the Electrochemical Society (2007); NYSTAR Award (2007); United University Professions Individual Development Award (2006); NSF POWRE Award (2000); Camille and Henry Dreyfus Teacher-Scholar Award (1998); Alfred P. Sloan Foundation Research Fellow (1998); Cottrell Scholar (1997); DuPont Young Professor Award (1997). NSF National Young Investigator (1994); Royal Society European Post-doctoral Fellowship (1991); Junior Research Fellowship, Balliol College, University of Oxford (1990).

(d) 10 Recent Relevant Publications:

1. "High Resolution X-ray Diffraction, DIFFaX, NMR and First Principles Study of Disorder in the Li_2MnO_3 – $Li(NiMn)_{1/2}O_2$ Solid Solution", J. Breger, M. Jiang, N. Dupré, Y. S. Meng, Y. Shao-Horn, G. Ceder, C. P. Grey, *J. Solid State Chem.*, 178, 2575-2585, (2005).
2. "Electrodes with High Power and High Capacity for Rechargeable Li Batteries," K. Kang, Y. S. Meng, J. Breger, C. P. Grey and G. Ceder, *Science,* 311, 977-980 (2006).
3. "Cation ordering in $Li[Ni_xMn_xCo_{(1-2x)}]O_2$-Layered Cathode Materials: A Nuclear Magnetic Resonance (NMR), Pair Distribution Function, X-ray Absorption Spectroscopy, and Electrochemical Study", D. Zeng, J. Cabana, J. Breger, W.-S. Yoon, and C. P. Grey, *Chem. Mater.,*19, 6277–6289 (2007).
4. "Real-time NMR Investigations of Structural Changes in Silicon Electrodes for Lithium-ion Batteries", B. Key, R. Bhattacharyya, M. Morcrette, V. Seznéc, J.-M. Tarascon and C.P. Grey, *J. Am. Chem. Soc.*, 131 (26), 9239-9249, (2009).
5. "Electrochemical and Structural Study of the Layered, "Li-excess" Lithium-Ion Battery Electrode Material $Li[Li_{1/9}Ni_{1/3}Mn_{5/9}]O_2$", M. Jiang, B. Key, Y.S. Meng, C.P. Grey, *Chem. Mater.,* 21, 2733-2745, (2009).
6. "Investigation of the Conversion Reaction Mechanisms for Binary Copper (II) Compounds by Solid-State NMR Spectroscopy and X-ray Diffraction", N. Yamakawa, M. Jiang and C.P. Grey, *Chem. Mat,* 21, (14), 3162-3176, (2009).
7. "Identifying the Local Structures Formed during Lithiation of the Conversion Material, Iron Fluoride, in a Li Ion Battery: A Solid-State NMR, X-ray Diffraction, and Pair Distribution Function Analysis Study", N. Yamakawa, M. Jiang, B. Key and C.P. Grey, *J. Am. Chem. Soc.,* 131, (30), 10525-10536, (2009).
8. "Investigation of the Structural Changes in Li[NiyMnyCo(1−2y)]O2 (y = 0.05) upon Electrochemical Lithium Deintercalation", D. Zeng, J. Cabana, W-S Yoon and C. P. Grey, *Chem. Mater.*, 22, (3), 1209-1219, (2010).
9. "MAS NMR Study of the Metastable Solid Solutions Found in the LiFePO4/FePO4 System", J. Cabana, K. Shirakawa, G.Y. Chen, T. J. Richardson, C.P. Grey. *Chem. Mater.,* 22, (3), 1249-1262, (2010).
10. 210. "*In situ* NMR Observation of the Formation of Metallic Lithium Microstructures in Lithium Batteries", R. Bhattacharyya, B. Key, H. Chen, A.S. Best, A.F. Hollenkamp, and C.P. Grey, *Nature Materials*, article AOP (2010).

Dr. Yan Gao
Senior Scientist - Materials Characterization
Chemical and Structure Analysis Laboratory
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Dr. Gao has over 25 years experience in x-ray diffraction, and is an active and experienced synchrotron and neutron user. His early work included analysis of incommensurately modulated crystal structures for high-temperature superconductors, and x-ray anomalous scattering. Since joining GE in 1994, he expanded his expertise to broader areas ranging from diffraction (XRD) to x-ray absorption spectroscopy (XAS) and to small-angle x-ray scattering (SAXS). He is a key member of the GE team that pioneered the in-situ diffraction techniques for hydrogen storage materials at the NSLS. He is an advocate and practitioner for using high-energy x-rays for non-invasive characterization of materials such as thermal barrier coatings (TBC), metals and alloys, and at present, sodium metal chloride battery. He is among a few active industrial researchers nowadays who frequently travels to NSLS and APS, and performed innovative experiments on a wide variety of industrial materials. He was invited to speak on industrial use of synchrotron and neutrons in various conferences and workshops.

Education
Ph.D., Chemistry, State University of New York at Buffalo, 1990.
B.S., Chemistry, Jilin University , 1982.

Research & Professional Experience
July 1994 – present: Senior scientist, GE Global Research, Niskayuna, New York
January 1990 – June 1994: Staff Scientist, SUNY Beamlines at NSLS, Brookhaven National Laboratory

Selected peer-reviewed publications and presentations

Y. Gao, P. Lee, P. Coppens, M. Subramanian & A. Sleight, "The Incommensurate Modulation of the 2212 Bi-Sr-Ca-Cu-O superconductor", *Science* (1988), 241, 954-956.

P. Lee, Y. Gao, H. Sheu, V. Petricek, R. Restori, P. Coppens, A. Darovskikh, J.C. Phillips, A. Sleight & M. Subramanian, " Anomalous Scattering Study of the Bi Distribution in the 2212 Superconductor: Implications for Cu Valency", *Science* (1989), 244, 62-63.

Y. Gao, "Modulated Structures of Bismuth-Based Superconductors", in *Incommensurate Sandwiched Layered Compounds*, Ed. A. Meerschaut, Trans Tech Publication Ltd, (1992), 273-308.

S. M. Loureiro, Y. Gao & V. Venkataramani, "Stability of Ce(III) Activator and Codopant Effect in $MHfO_3$ (M = Ba, Sr) Scintillators by XANES", *J. Am. Ceram. Soc.,* (2005), 88 [1] 219–221.

J. Her, P.W. Stephens, Y. Gao, Grigorii L. Soloveichik, J. Rijssenbeek, M. Andrus and J-C. Zhao, "Structure of unsolvated magnesium borohydride $Mg(BH_4)_2$", *Acta Cryst*. (2007) B63, 561–568.

J. Rijssenbeek, Y. Gao, J. Hanson, Q. Huang, C. Jones, B. Toby, "Crystal structure determination and reaction pathway of amide–hydride mixtures", *J. Alloys and Comps*. 454 (2008) 233–244.

G. Soloveichik, J. Her, P. W. Stephens, Y. Gao, J. Rijssenbeek, M. Andrus & J.-C. Zhao, "Ammine Magnesium Borohydride Complex as a New Material for Hydrogen Storage: Structure and Properties of $Mg(BH_4)_2 \cdot 2NH_3$", *Inorganic Chemistry*, 47(10), 2008, 4290-4298.

R. Gilles, M. Hofmann, Y. Gao, F. Johnson, L. Iorio, M. Larsen, F. Liang, M. Hoelzel, B. Barbier, "Probing the Relationship of Long-range Order in Nanodomain FeCo Alloys with Ternary Additions using Neutron Diffraction", *Metallurgical and Materials Transactions A*, 2009, in print.

Curriculum Vitae
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Personal U.S. Citizen

Education

10/2000 – 12/2004: Postdoctoral, Department of Physics, New Jersey Institute of Technology (NJIT), NJ
05/1991 – 05/1995: Ph.D. in Condensed Matter Physics, Moscow Engineering Physics Institute (MEPI), Moscow, Russia
09/1985 – 03/1991: M.S. in Laser Physics (MEPI)

Appointments

06/2008- present: Research Associate, Materials Science & Engineering, Rutgers, NJ
10/2006-10/2007: Assistant Professor of Research (not tenure-track), CAMD, Louisiana State Univ., LA
02/2005- 08/2006: Beamline scientist, Case Western Center for Synchrotron Biosciences at the National Synchrotron Light Source, Brookhaven National Laboratory
10/2000 - 12/2004: Postdoctoral research associate, Department of Physics, NJIT, NJ

Research Experience and Managing Skills

(1) Materials Characterization. Years of experience in solving challenging problems of Materials Science, Physics, and Engineering by use of synchrotron x-ray absorption and scattering techniques as well as advanced simulations. Specifically, 8 years of experience with perovskites and HTSCs; 3-6 years of experience with magnetic materials, CMRs, ferroelectric and catalytic support materials, 2-3 years of experience with hydrogen energy-related materials and metal proteins. 1-2 years of experience in thermal-sprayed ceramic coatings.

(2) Experimental. 12 years of *hands on* experience in XAFS, 2-12 years of hands on experience in other the synchrotron x-ray techniques (XRD, IXS, x-ray diffraction PDF analysis, XAS, XMCD, and XPS).
- Served as a beamline scientist at X9b (XAFS) and U2b (FTIR microscopy) at the NSLS;
- Experience in construction and implementation of XAFS beamline instrumentation upgrades;
- Some experience in hardware and software for use in computer control/data collection systems;
- Experience in materials synthesis (ceramic TMOs, HTSCs, CMRs, epitaxial films grown by PLD, thermal sprayed ceramic coatings) and their in-house characterization (TGE, four-probe resistivity, SQUID, specific heat, XRF, SEM, FTIR- and optical microscopy, Raman, and several mechanical tests).

(3) Modeling and Simulations. More than 8 years of experience in first-principles calculations of long-range ordered and locally disordered solids using DFT and multiple scattering (MS) for large clusters of atoms, respectively. 3 years of experience in many-body calculations for small clusters of atoms by exact diagonalization. 1 year of experience in linear response calculations of the collective lattice excitations (phonons).
- Multi-scale *ab-initio* simulations from conventional continuum (long-range ordered) down to atomic scales;
- High performance MPI computing (at clusters running under Linux).

(4) Administrative and managing skills. Rapidly adaptive, capable to work under pressure in a dynamic goal oriented environment. Proven ability to collaborate with diverse groups of scientists and users, to initiate new research programs, and to serve users community. 2 years of experience in planning and directing work of technical staff and junior scientists.

41 peer reviewed publications (three selected publications are listed below)

1. "*X-ray absorption study of Ti-activated sodium aluminum hydride*" J. Graetz, A.Yu. Ignatov, T.A. Tyson, J.J. Reilly and J. Johnson, Applied Physics Letters, **85** 500 (2004). (Cited more than 100 times)
2. *" In situ strain profiling of elastoplastic bending in Ti–6Al–4V alloy by synchrotron energy dispersive x-ray diffraction",* M. Croft, V. Shukla, E. K. Akdoðan, N. Jisrawi, Z. Zhong, R. Sadangi, A. Ignatov, L. Balarinni, K. Horvath, and T. Tsakalakos, J. Applied Physics **105**, 093505 (2009).
3. "*Superconductivity near the vibrational-mode instability in* $MgCNi_3$", A. Yu. Ignatov, S. Yu. Savrasov, and T. A. Tyson, Phys. Rev. B **68**, R220504 (2003).

Grants

$130k, "Hydrogen Storage Materials for 21st Century", Research Competitiveness, Louisiana Board of Regents

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The University of Tennessee, Knoxville, TN 37996-2200, USA.
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PROFESSIONAL PREPARATION

National Tsing Hua University, Taiwan, ROC	Physics	B.S.	1972
Northwestern University	Materials Science and Engineering	Ph.D.	1980

APPOINTMENTS

1993-Present	Professor and Ivan Racheff Chair of Excellence, Department of Materials Science and Engineering, The University of Tennessee.
1980-1993	Senior and Fellow Engineers, Westinghouse Research and Development Center.
1974-1979	Research Assistant, Department of Materials Science and Engineering, Northwestern University.

PUBLICATIONS CLOSELY RELATED TO THE PROPOSED PROJECT

Editor or co-editor of more than 30 books and author or co-author of more than 500 papers.

[1] Y. D. Wang, H. Tian, A. D. Stoica, X. L. Wang, P. K. Liaw, and J. W. Richardson (2003), "Evidence on the Development of Large Grain-Orientation-Dependent Residual Stresses in a Cyclically-Deformed Alloy," *Nature Materials*, 2(2), pp. 101-106.

[2] H. Q. Li, H. Choo, Y. Ren, T. A. Saleh, U. Lienert, P. K. Liaw, and F. Ebrahimi (2008), "Strain-Dependent Deformation Behavior in Nanocrystalline Metals," *Physical Review Letters*, Vol. 101, No. 1, p. 015502 (2008).

[3] L. Li, T. Ungár, Y. D. Wang, J. R. Morris, G. Tichy, J. Lendvai, Y. L. Yang, Y. Ren, H. Choo, and P. K. Liaw (2009), "Microstructure Evolution during Cold Rolling in a Nanocrystalline Ni–Fe Alloy Determined by Synchrotron X-ray Diffraction," *Acta Materialia*, Vol. 57, Issue 17, pp. 4988-5000.

[4] L. Li, T. Ungar, Y. D. Wang, G. J. Fan, Y. L. Yang, N. Jia, Y. Ren, G. Tichy, J. Lendvai, H. Choo, and P. K. Liaw (2009), "Simultaneous Reductions of Dislocation and Twin Densities with Grain Growth during Cold Rolling in a Nanocrystalline Ni-Fe Alloy," *Scripta Materialia*, Vol. 60, Issue 5, pp. 317-320.

[5] Y. Yang, J. C. Ye, J. Lu, F. X. Liu, and P. K. Liaw (2009), "Effects of Specimen Geometry and Base Material on the Mechanical Behavior of Focused-Ion-Beam-Fabricated Metallic-Glass Micropillars," *Acta Materialia*, 57(5), pp. 1613-1623.

[6] S. Cheng, A. D. Stoica, X. L. Wang, Y. Ren, J. Almer, J. A. Horton, C. T. Liu, B. Clausen, D. W. Brown, P. K. Liaw, and L. Zuo (2009), "Deformation Crossover: From Nano to Mesoscale," *Physical Review Letters*, Vol. 103, No. 3, p. 035502.

[7] S. Cheng, Y. D. Wang, H. Choo, X. L. Wang, J. D. Almer, P. K. Liaw, and Y. K. Lee (2010), "An Assessment of the Contributing Factors to the Superior Properties of a Nanostructured Steel using In Situ High-Energy X-ray Diffraction," *Acta Materialia*, Vol. 58, Issue 7, pp. 2419-2429.

GRADUATE ADVISEES

Z. An, B. R. Barnard, M. L. Benson, M. Borst, N. Chawla, B. Chen, C. L. Chiang, C. P. Chuang, J. A. Cook, Q. Feng, M. W. Freels, L. Garimella, E. Garlea, B. A. Green, M. Hemphill, E. Huang, Lan Huang, Lu Huang, S. Huang, J. W. Jeon, H. Jia, F. Jiang, L. Jiang, J. Kim, S. Lee, L. Li, F. Liu, Y. C. Lo, Y. Lu, W. M. Matlin, R. L. McDaniels, J. Miller, N. Miriyala, M. L. Morrison, J. A. Oberhaus, W. H. Peter, G. Porter, D. C. Qiao, J. W. Qiao, W. Ren, T. A. Saleh, L. J. Santodonato, S. Shanmugham, E. Shen, R. V. Steward, M. Stoica, J. Sun, Z. Sun, Z. Tang, K. Tao, Z. Teng, C. B. Thomas, H. Tian, J. Tian, J. Wall, G. Wang, T. Wilson, W. Woo, L. Wu, X. Xie, B. Yang, Z. Yu, W. Yuan, Y. Zhang, W. Zhao, and J. Zhu. **TOTAL** = 66 Graduate Advisees.

AWARDS AND HONORS

1997	Fellow, ASM International.
2010	L. R. Hesler Award, The University of Tennessee.
2011	Moses E. and Mayme Brooks Distinguished Professor Award, The University of Tennessee.

Ulrich Lienert
Physicist

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Education

Ph.D. Physics, Feb. 1995, University of Manchester, England, and European Synchrotron Radiation Facility (Grenoble, France).
M.S. Physics, Feb. 1990, Technische Universität Berlin, Germany
B.S. Physics, Oct. 1986, Technische Universität Berlin, Germany

Professional experience

04-present Physicist, Argonne National Laboratory, Argonne, IL
01–04 Assistant Physicist, Argonne National Laboratory, Argonne, IL
98–01 Beamline Scientist, European Synchrotron Radiation Facility, Grenoble, France
96–98 Post Doc, Risø National Laboratory, Roskilde, Denmark.
94–96 Post Doc, European Synchrotron Radiation Facility, Grenoble, France

Selected publications

1) Efstathiou, C., Boyce, D.E., Park, J.S., Lienert, U., Dawson, P.R., Miller, M.P. (2010) “A method for measuring single-crystal elastic moduli using high-energy X-ray diffraction and a crystal-based finite element model,” Acta Mater. 58 (17), pp. 5806-5819.

2) Wejdemann, C., Liener,t U., Pantleon, W. (2010) “Reversal of asymmetry of X-ray peak profiles from individual grains during a strain path change,” Scripta Mater. 62 (10), pp. 794-797.

3) Hedström, P., Han, T.S., Lienert, U., Almer, J., Odén, M. (2010) “Load partitioning between single bulk grains in a two-phase duplex stainless steel during tensile loading,” Acta Mater. 58 (2), pp. 734-744.

4) Aydiner, C.C., Bernier, J.V., Clausen, B., Lienert, U., Tomé, C.N., Brown, D.W. (2009) “Evolution of stress in individual grains and twins in a magnesium alloy aggregate,” Phys. Rev. B **80**(2), 024113.

5) Lienert, U., Brandes, M.C., Bernier, J.V., Weiss, J., Shastri, S. D., Mills, M.J., Miller, M.P. (2009) “In situ single-grain peak profile measurements on Ti-7Al during tensile deformation,” Mater. Sci. Eng. A **524** , pp. 46-54.

6) Paradowska, A.M., Price, J.W.H., Finlayson, T.R., Lienert, U., Walls, P., Ibrahim, R. (2009) “Residual stress distribution in steel butt welds measured using neutron and synchrotron diffraction,” J. Phys.: Condens. Matter **21**, 124213.

7) Lienert, U., Almer, J., Jakobsen, B., Pantleon, W., Poulsen, H. F., Hennessy, D., Xiao, C., Suter, R.M. (2007) “3-Dimensional Characterization of Polycrystalline Bulk Materials Using High-Energy Synchrotron Radiation,” Mater. Sci. Forum **539-543**, pp. 2353-2358.

8) Jakobsen, B., Poulsen, H. F., Lienert, U., Almer, J., Shastri, S. D., Sorensen, H. O., Gundlach, C., Pantleon, W. (2006) “Formation and subdivision of deformation structures during plastic deformation,” Science **312**, pp. 889-892.

9) Suter, R. M., Hennessy, D., Xiao, C., Lienert, U. (2006) “Forward modeling method for microstructure reconstruction using x-ray diffraction microscopy: Single-crystal verification,” Rev. Sci. Instrum. **77**, 123905.

10) Lienert, U., Han, T.-S., Almer, J., Dawson, P.R., Leffers, T., Margulies, L., Nielsen, S.F., Poulsen, H.F., Schmidt, S. (2004) “Investigating the effect of grain interaction during plastic deformation of copper,” Acta Mater. **52**, pp. 4461-4467.

Scientific interests

Synchrotron optics and instrumentation, micromechanics, phase transformations, peak profile analysis.

Lawrence Margulies

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Professional Experience:

2009-	Associate Physicist, Brookhaven National Lab, NSLS-2
2001-2009	Senior Scientist, Risø National Laboratory
1999-2001	Post-Doc, Risø National Laboratory
1999-2007	Visiting Beamline Scientist, European Synchrotron Radiation Facility

Awards

Research Excellence Award, Iowa State University, 8/99
Young Scientist of the Year Award, ESRF, 2/02
Professional Progress in Engineering Award, Iowa State University 4/07

Research Interests:

Development of novel Synchrotron radiation instrumentation and techniques. grain resolved in-situ diffraction studies of fundamental materials science processes (deformation, grain growth, recrystallization, phase transformation). Development of the HXN nanoprobe beamline for NSLS-2

Synergistic Activities:

1. Beamline Scientist for the HXN project beamline of NSLS-2 with the goal of developing an instrument for nano-diffraction with a resolution of 10-30 nanometers.
2. Team member on the 4DE beamline to aid in development of the beamline to allow 3DXRD/totalcryst measurements and analysis to be done on sample at high pressure/temp
3. Designed and built a 3D high resolution detector for use at ID11, ESRF for mapping highly deformed materials as well as high temperature furnaces for diffraction at APS and ESRF.
4. LDRD currently being reviewed with provide funding for developing a conical slit that will provide a voxel resolution of 1-5 microns (currently the best conical slits achieve gauge volumes on the order of 100-200 microns.

Relevant Publications:

West, S.S., Schmidt, S., Soerensen, H.O., Winter, G., Poulsen, H.F., Margulies, L., Gundlach, C., Jensen, D.J., “Direct non-destructive observation of bulk nucleation in 30% deformed aluminum”, *Scripta Mater* (2009) 61, 875-878

Schmidt, S; Nielsen, SF; Gundlach, C; Margulies, L; Huang, X; Jensen, DJ, “Watching the growth of bulk grains during recrystallization of deformed metals,” SCIENCE, 305 (5681): 229-232 JUL 9 2004

Poulsen, HF; Margulies, L; Schmidt, S; Winther, G, “Lattice rotations of individual bulk grains - Part I: 3D X-ray characterization,” ACTA MATERIALIA, 51 (13): 3821-3830 AUG 1 2003

Margulies, L; Lorentzen, T; Poulsen, HF; Leffers, T, “Strain tensor development in a single grain in the bulk of a polycrystal under loading,” ACTA MATERIALIA, 50 (7): 1771-1779 APR 19 2002

Offerman, SE; van Dijk, NH; Sietsma, J; Grigull, S; Lauridsen, EM; Margulies, L; Poulsen, HF; Rekveldt, MT; van der Zwaag, S, “Grain nucleation and growth during phase transformations,” SCIENCE, 298 (5595): 1003-1005 NOV 1 2002

Margulies, L; Winther, G; Poulsen, HF, “In situ measurement of grain rotation during deformation of polycrystals,” SCIENCE, 291 (5512): 2392-2394 MAR 23 2001

Matthew P. Miller

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Professional Preparation: B.A., Geology, 1979, Colorado University
B.S. Mechanical Engineering, 1988, Colorado School of Mines
M.S., Mechanical Engineering, 1990, Georgia Tech.
Ph.D. Mechanical Engineering, 1993, Georgia Tech.

Appointments:
2007 - present Professor, M&AE, Cornell University
2000 - 2007 Associate Professor, M&AE, Cornell University
1994 -2000 Assistant Professor, Mechanical and Aerospace Engineering, Cornell University

Research Overview:
Miller's research focuses on the creation of tools that enable the design and selection of structural materials. Much of Miller's work is at the experiment/model interface, where he and his students have designed experiments to probe material state and behaviors on multiple size scales. A current emphasis of Miller's research is the use of high energy synchrotron x-rays and in-situ mechanical loading along to understand the crystal level mechanical state of polycrystals during deformation – including monotonic loading and fatigue. Results from these experiments – which have been conducted on copper, aluminum, beryllium and titanium alloys – are employed with crystal-based modeling formulations to improve our understanding of how micromechanical stress states evolve during plastic deformation and, eventually how damage such as a fatigue crack initiates. Miller has developed in situ mechanical loading /high energy diffraction experiments at the Cornell High Energy Synchrotron Source, where he is a member of the User's Executive Committee and the Advanced Photon Source, where he is the chair of Sector 1 Beamline Advisory group and a member of the Technical Advisory Committee on Extreme Conditions. Miller receives funding for his research from: the National Science Foundation, The Air Force Office of Scientific Research, the Office of Naval Research, The Defense Advanced Research Projects Agency and The Air Force Research Laboratory at Wright Patterson Air Force Base.

Honors:
- Cornell M&AE Shepherd Teaching Prize, 1996
- NSF CAREER Award, 1997
- National Academy of Engineering, Frontiers of Engineering, 1999
- Cornell College of Engineering , James and Mary Tien Excellence in Teaching Award, 2004
- James M. & Marsha D. McCormick Award for Excellence in Advising First Year Students, 2006
- ASM Henry Marion Howe Medal 2009 for best paper in Met. & Mat. Trans. 2008

Organizations:
- American Society of Mechanical Engineers - Member
- American Society of Engineering Education
- American Academy of Mechanics - Member
- ASM and TMS – Member

Professional Activities:
- Editorial Board, International Journal of Fatigue, 2006-
- Associate Editor ASME Journal of Engineering Materials and Technology 2002-2009
- Reviewer for journals, proposals, as well as tenure and promotion cases.

BIOGRAPHICAL SKETCH

Dr. Job Rijssenbeek, a Senior Chemist in the Chemical Energy Systems Lab at GE Global Research, has spent the last seven years conducting research in energy-related areas, including solid-state hydrogen storage, thermo-chemical energy recovery and, presently, high temperature batteries. He is currently a task leader on GE's advanced sodium metal halide (NaMx) battery program. He leads a global team of scientists and engineers that is developing fundamental understanding of the degradation mechanisms and the operational conditions that affect NaMx battery performance over life under application specific duty cycles. He is a key member of the team that developed the in-situ x-ray diffraction technique at NSLS. His familiarity with cell components, duty cycles, performance metrics, and cycle life requirements will provide guidance for commercially relevant testing.

Previously, he has performed detailed studies of the reaction pathways of hydrogen storage materials and developed new catalysts to lower the hydrogen desorption temperature of $NaAlH_4$. In 2009, Dr. Rijssenbeek was awarded GE Global Research's Albert W. Hull Award for early-career researchers who exhibit outstanding technical achievement and positive influence on their fellow technologists. He received a B.A. in Chemistry from Princeton University and a Ph.D. in Inorganic Chemistry from Northwestern University. He has authored or co-authored 17 peer-reviewed publications, and has two issued and four pending patents.

Selected Publications - *First author on 9 of 17 total publications in peer reviewed journals*

1) Crystal structure determination and reaction pathway of amide-hydride mixtures. Rijssenbeek, J; Gao, Y; Hanson, J; Huang, Q; Jones, C.; Toby, B. *J. Alloys Compounds* (2008), 454(1-2), 233-244.
2) Effect of Explicit Cationic Size and Valence Constraints on the Phase Stability of 1:2 B-Site-Ordered Perovskite Ruthenates. Rijssenbeek, J. T.; Saito, T.; Malo, S.; Azuma, M.; Takano, M.; Poeppelmeier, K. R. *J. Amer. Chem. Soc.* (2005), 127(2), 675-681.
3) Synthesis and characterization of the first 1:2 ordered perovskite ruthenate. Rijssenbeek, J.; Malo, S.; Saito, T.; Caignaert, V.; Azuma, M.; Takano, M.; Poeppelmeier, K. R. *Mater. Res. Soc. Symp. Proc.* (2002), 718(Perovskite Materials), 3-8.
4) Site and Oxidation-State Specificity Yielding Dimensional Control in Perovskite Ruthenates. Rijssenbeek, J. T.; Malo, Sylvie; Caignaert, Vincent; Poeppelmeier, Kenneth R. *J. Amer. Chem. Soc.* (2002), 124(10), 2090-2091.
5) Electrical and magnetic properties of $Ru_{1-x}M_xSr_2GdCu_2O_8$ (M = Ti, V and Nb). Rijssenbeek, J. T.; Mansourian-Hadavi, N.; Malo, S.; Ko, D.; Washburn, C.; Maignan, A.; Pelloquin, D.; Mason, T. O.; Poeppelmeier, K. R. *Physica C* (2000), 341-348, 481-482.
6) The Crystal Structure of $Ba_3CuRu_2O_9$ and Comparison to $Ba_3MRu_2O_9$ (M = In, Co, Ni, and Fe). Rijssenbeek, J. T.; Huang, Q.; Erwin, R. W.; Zandbergen, H. W.; Cava, R. J. *J. Solid State Chem.* (1999), 146(1), 65-72.
7) Electrical and magnetic properties of the two crystallographic forms of $BaRuO_3$. Rijssenbeek, J. T.; Jin, R.; Zadorozhny, Y.; Liu, Y.; Batlogg, B.; Cava, R. J. *Phys. Rev. B* (1999), 59(7), 4561-4564.
8) Electrical and magnetic properties of a series of ternary barium metal ruthenates: $Ba_3MRu_2O_9$ (M = Fe, Co, Ni, Cu, and In). Rijssenbeek, J. T.; Matl, P.; Batlogg, B.; Ong, N. P.; Cava, R. J. *Phys. Rev. B* (1998), 58(16), 10315-10318.
9) Novel cluster of transition metals and main group oxides in the alkylamine/oxovanadium/borate system. Rijssenbeek, J. T.; Rose, D. J.; Haushalter, R. C.; Zubieta, J. *Angew. Chem., Int. Ed. Eng.* (1997), 36(9), 1008-1010.

Rosa Robert - Biographical Sketch

Postdoctoral Research Associate, Department of Chemistry; Stony Brook University
Stony Brook, NY 11794-3400
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(a) Education and Training:

University of Barcelona	Chemistry	Llicenciatura degree in Chemistry, 2003
University of Barcelona	Chemistry	Master's degree, 2004
University of Augsburg	Chemistry	Dr. rer. nat. 2007, Magna cum laude

(b) Research and Professional Experience:

Postdoctoral Research Associate, Department of Chemistry, Stony Brook University, (Apr. 2009-present).
Scientist, Laboratory for Solid State Chemistry and Catalysis, Empa- Materials Science and Technology, Dübendorf (Switzerland), (March 2008- Apr. 2009).
Post-doctoral Fellow , Diffraction Group of Juan Rodríguez-Carvajal, Institute Laue-Langevin ILL, Grenoble (France), (Nov. 2007 - Febr. 2008).

(d) Honors and Awards:

Beatriu de Pinós Post-doctoral Fellow (2010); Swiss National Foundation Post-doctoral Fellow (2007); Poster Award (2005), Poster elected as outstanding example of a good scientific poster. Sócrates-Erasmus Fellowship, University of Barcelona (2003).

(d) 10 Recent Relevant Publications:

1. "Photoelectrochemical water-splitting with mesoporous hematite prepared by a solution-based colloidal approach", K. Sivula, R. Zboril, F. Le Formal, R. Robert, A. Weidenkaff, J. Frydrych, J. Tucek, M. Graetzel, J. Am. Chem. Soc., 2010, *132* (21), pp 7436–7444.
2. "Crystal structure, morphology and physical properties of LaCo1−xTixO3±δ perovskites prepared by a citric acid assisted soft chemistry synthesis", R. Robert, D. Logvinovich, M. H. Aguirre, S. G. Ebbinghaus, L. Bocher, P. Tomeš, and A. Weidenkaff, Acta Mater., 58 (2), 680-691, 2010.
3. "High-temperature stability, structure and thermoelectric properties of CaMn1-xNbxO3 phases ", L. Bocher, M. H. Aguirre, R. Robert, D. Logvinovich, S. Bakardjieva, J. Hejtmanek, and A. Weidenkaff, Acta Mater., 57 (19), 5667-5680, 2009.
4. "CaMn1-x NbxO3 (x < 0.08) perovskite-type phases as promising new high-temperature n-type thermoelectric materials", L. Bocher, M. H. Aguirre, D. Logvinovich, A. Shkabko, R. Robert, M. Trottmann, A. Weidenkaff. Inorg. Chem. 47 (18), 8077-8085, 2008.
5. "Structure, microstructure, and high-temperature transport properties of La1-xCaxMnO3-d thin films and polycrystalline bulk materials", M H. Aguirre, S. Canulescu, R. Robert, N. Homazava, D. Logvinovich, L. Bocher, Th. Lippert, and A. Weidenkaff. J. Appl. Phys., 103, 013703, 2008.
6. "Doped semiconductors as half-metallic materials: Experiments and first-principles calculations of CoTi1-xMxSb (M = Sc, V, Cr, Mn, Fe)", B. Balke, G. H. Fecher, A. Gloskovskii, J. Barth, K. Kroth, C. Felser, R. Robert, and A. Weidenkaff. Phys. Rev. B, 77 (4), 045209, 2008.
7. "High-temperature thermoelectric properties of Ln(Co, Ni)O3 (Ln = La, Pr, Nd, Sm, Gd and Dy) compounds", R. Robert, M.H. Aguirre, P. Hug, A. Reller, and A. Weidenkaff. Acta Mater., 55 (15), 4965-4972, 2007.
8. "The effect of the fluence on the properties of La-Ca-Mn-O thin films prepared by pulsed laser deposition", S. Canulescu, Th. Lippert, A. Wokaun, M. Döbeli, A. Weidenkaff, R. Robert, and D. Logvinovich. Appl. Surf. Sci., 253 (19), 8174-8178, 2007.
9. "Synthesis, crystal structure, and microstructure analysis of perovskite-type compounds LnCo0.95Ni0.05O3 (Ln = La, Pr, Nd, Sm, Gd, and Dy)", M. H. Aguirre, R. Robert, D. Logvinovich, and A. Weidenkaff. Inorg. Chem., 46 (7), 2744-2750, 2007.
10. "Ni-doped cobaltates as po-tential materials for high temperature solar thermoelectric converters", R. Robert, L. Bocher, B. Sipos, M. Döbeli, and A. Weidenkaff. Prog. Solid State Chem, 35(2-4), 447-455, 2007.

BIOGRAPHICAL SKETCH

Esther S. Takeuchi SUNY Distinguished Professor, University at Buffalo

EDUCATION/TRAINING

University of Pennsylvania, BA, 1975, Chemistry, History
The Ohio State University,,PhD,1981,Chemistry
University of North Carolina at Chapel Hill, Postdoc, 982-1983, Electrochemistry
University at Buffalo, SUNY, Postdoc, 1983-1984, Electrochemistry

RESEARCH AND PROFESSIONAL EXPERIENCE:

Previous Employment

1981-1982	Senior Chemist, Research and Development, Union Carbide Corporation
1984 - 1986	Senior Chemist, Research and Development, Wilson Greatbatch Ltd.
1986 - 1990	Group Manager of Research and Development, Wilson Greatbatch Ltd.
1990 – 1991	Associate Director of Research and Development, Wilson Greatbatch Ltd.
1991 - 1998	Director of Electrochemical Research, Wilson Greatbatch Ltd.
1999 - 2006	Executive Director, Battery Research and Development, Center of Excellence, Greatbatch Inc.
2006 - 2007	Chief Scientist, Greatbatch Inc.
2007 – 2010	Professor, Department of Chemical and Biological Engineering, Department of Electrical Engineering, Department of Chemistry, University at Buffalo (SUNY)
2010 –present	SUNY Distinguished Professor, Department of Chemical and Biological Engineering, Department of Electrical Engineering, Department of Chemistry, University at Buffalo (SUNY)

Notable Honors

National Medal of Technology and Innovation, October 7, 2009. For her seminal development of the silver vanadium oxide battery that powers the majority of the world's lifesaving implantable cardiac defibrillators.

National Academy of Engineering, Inducted 2004. For successfully developing silver vanadium oxide batteries for implantable cardiac defibrillators and lithium/carbon monofluoride cells to power implantable pacemakers.

Relevant Publications (48 total refereed publications)

1. Marschilok, A. C., Takeuchi, K. J., Takeuchi, E. S. (2009). "Preparation and Electrochemistry of Silver Vanadium Phopshorous Oxide." *Electrochemical and Solid State Letters, 12*, A5-A9.

2. Takeuchi, E. S., Marschilok, A. C., Tanzil, K., Kozarsky, E. S., Zhu, S., and Takeuchi. K. J., (2009) "Electrochemical Reduction of Silver Vanadium Phosphorus Oxide, Ag2VO2PO4: The Formation of Electrically Conductive Metallic Silver Nanoparticles." *Chemistry of Materials*, *21*, 4934-4939.

Oleg CHUBAR (alternative spelling: **TCHOUBAR**)
Staff Scientist, NSLSII, BNL 817, (631) 344-4525, chubar@bnl.gov
Physicist, scientific software developer, Ph.D.

Work experience

Jan. 2009-present: X-ray source scientist, Photon Division, Photon Sciences Directorate, Brookhaven National Lab., USA.
Parametric optimization of insertion devices for the National Synchrotron Light Source II (NSLS-II) project beamlines; calculation of emission characteristics (spectral-angular and intensity distributions, brightness, flux, power density distributions / heat load on optical elements) for all NSLS-II radiation sources; knowledge transfer on properties of different kinds of synchrotron radiation to beamline scientists. Development of general physical optics based simulation methods for partially-coherent synchrotron radiation wavefront propagation; implementation of these methods in the SRW computer code and application of this code for performance evaluation and optimization of NSLS-II beamlines. Support and further development of Radia magnetostatics code.

2002 - 2009: "Physicien du rayonnement" (<synchrotron> radiation physicist), Division of Accelerators and Sources, Synchrotron SOLEIL, France.
Design and optimization of insertion devices for Synchrotron SOLEIL (responsible for first SOLEIL APPLE-II type undulators); calculation of synchrotron emission and wavefront propagation through optical beamlines; participation in optimization of infra-red and some X-ray beamlines; physical optics simulations and extraction scheme optimizations for femtosecond slicing project; automation of magnetic measurements; undulator commissioning; electron beam optical diagnostics. Development of genetic algorithm based computer code for sorting and shimming of insertion device magnets; support and further development of SRW and Radia codes. Transfer of knowledge on magnetostatics and SR calculation to SOLEIL scientists and engineers.

2000 - 2002: Developer of scientific software, ESRF, Grenoble, France.
Support and extension of SRW and Radia computer codes; analysis and development of the ESRF Scientific MIS project. Synchrotron emission calculations; participation in optimization and construction of the infrared beamline based on Edge Radiation.

1996 - 2000: Scientific collaborator, group of Insertion Devices, European Synchrotron Radiation Facility, Grenoble, France.
Development of “Radia” – a 3D magnetostatics computer code optimized for insertion devices, and a code for high-accuracy computation of synchrotron emission and wavefront propagation – “Synchrotron Radiation Workshop” (SRW). These codes are currently used in large number of laboratories dealing with synchrotron radiation worldwide. Web: http://www.esrf.eu/Accelerators/Groups/InsertionDevices/Software.

1992 - 1996: Scientific collaborator, Kurchatov Synchrotron Radiation Source, RRC Kurchatov Institute, Moscow.
Development of accurate calculation methods for synchrotron radiation generated by relativistic electrons in magnetic fields of arbitrary configuration, in near-field observation region; theoretical and experimental studies of "Edge Radiation" - a special kind of synchrotron radiation with properties similar to the Transition Radiation. Development of Synchrotron Radiation interference-based methods of electron beam diagnostics. Participation in design and optimization of insertion devices for synchrotron radiation sources.

1991 - 1992: Teacher assistant, Department of Nuclear Physics, Moscow Engineering Physics Institute, Russia.

Degree

Dec. 1995: Candidate of Physical and Mathematical Sciences (= Ph.D), held in Moscow Engineering Physics Institute.
Thesis: “Computation methods for synchrotron radiation; applications to electron beam diagnostics”.

Education

1992 - 1995: Post-graduate courses in Moscow Engineering Physics Institute, Russia. Qualified as researcher.

1983 - 1991: Moscow Engineering Physics Institute (Technical University), USSR. Diploma with honors. Qualified as engineer-physicist specialized in nuclear physics.

THOMAS TSAKALAKOS

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School of Engineering; Rutgers University 607 Taylor Road; Piscataway NJ 08854
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Education

Ph.D., 1977, Northwestern Univ., Evanston, Illinois: Materials Science and Engineering. Thesis Advisor Prof. John Hilliard, "Interdiffusion & Enhanced Modulus Effect in Composition Modulated Copper-Nickel Thin Foils"

M.S., 1974, Northwestern Univ., Evanston, Illinois, Materials Science and Engineering

BS. 1972, Physics, Univ. of Athens, Greece

Areas of Research

Nanostructured materials, Nanotechnology in Medicine and Magnetic Storage, Nanostructured Coatings and Films , Processing and Advaced Characterization of Nanoparticles, Strain and Phase Mapping of Engineering Materials and Structures by Light Source Synchrotron Radiation, Residual Stress Measurements by Energy Dispersive X-Ray Diffraction, Life Prediction of Fatigue Crack Growth Damage of Engineering Structures, Welding, Shot and Laser Peening, Micromechanics Modeling, Mechanical Behavior, Phase Transformation in Solids, Spinodal Alloys, Diffusion in Solids.

Prof. Tsakalakos has worked in the field of Nanostructured Materials and Technology. As Co-founder and Editor-in-Chief of the Nanostructured Materials Journal for over ten years, he published 12 volumes of scientific work in Nanomaterials Research. Prof. Tsakalakos participated in the Bio NanoTechnology Initiative (NNI) and continues to work in the field of Mechanical Properties of Nanostructured Materials. Most recently, his work on 3D strain mapping of internal stresses by synchrotron probe at the nanoscale level has been recognized by Defense University Research Initiative on Nanotechnology as innovative approach to the new field of nanomechanics. Industrial applications include pharmaceutical, chemical, communications, manufacturing, defense, transportation, energy, and gas turbine; offshore and polar, aircraft and airspace.

Professional Work Experience

July/94 - Present Rutgers Univ., Dept. of Materials Science and Engineering; Professor II
Sept/90-Dec/00 Pergamon Press/Elsevier Publishing Co/Acta Metallurgica Inc., J. Nanostructured Materials; Editor
Sept/91-Present Comm. Sc & Tech New Jersey, Laboratory for Nanostructured Materials Research; Director
July/77-June/94 Rutgers Univ., Dept. of Mechanics and Materials Science; Assistant./Associate / Full Professor
1972-1977 Northwestern University, Research Assistant

Recent Publications Publications

"Stress Gradient Induced Strain Localization in Metals: High Resolution Strain Cross Sectioning via Synchrotron X-Ray Diffraction" M. Croft, N. Jisrawi, Z. Zhong, R. Holtz, M. Shepard, M. Lakshmipathy, K. Sadananda, J. Skaritka, V. Sukla, R. Sadangi and T. Tsakalakos, Engineering Materials and Technology, 130, 021005 (2008)

"Fatigue history and in-situ loading studies of the overload effect using high resolution x-ray strain profiling", M. Croft, N. M. Jisrawi,Z. Zhong, R. Holtz, K. Sadananda, J. Skaritka, and T. Tsakalakos International Journal of Fatigue 29 (issues 9-11) 1726-1736 (2007)

"Measurement of Residual Stress Distributions by Energy Dispersive X-ray Diffraction Synchrotron Radiation"
T. Tsakalakos , M. Croft, N.. Jisrawi, RL. Holtz, and Z. Zhong, International Journal of Offshore and Polar Engineering,
Vol 16, 358-366, (2006)

"Cold drawn steel wires—processing, residual stresses and ductility—part I: metallography and finite element analyses"
A. Phelippeau, S. Pommier, T. Tsakalakos, M. Clavel and C. Prioul, Fatigue Fract Engng Mater Struct 29, 243–253, (2006)

"Cold drawn steel wires—processing, residual stresses and ductility Part II: Synchrotron and neutron diffraction"
A. Phelippeau, S. Pommier, I. Zakharchenko, R. Levy_Tubiana, T. Tsakalakos, M. Clavel, M. Croft, Z. Zhong and C. Prioul
Fatigue Fract Engng Mater Struct 29, 255–265, (2006)

"Strain profiling of fatigue crack overload effects using energy dispersive X-ray diffraction" Croft M, Zhong Z, Jisrawi N, Zakharchenko I, Holtz RL, Skaritka J, Fast T, Sadananda K, Lakshmipathy M, and **Tsakalakos T** International Journal of Fatigue, 27 (10-12): 1408-1419, (2005)

"Strain field and scattered intensity profiling with energy dispersive x-ray scattering" Croft M, Zakharchenko I, Zhong Z, Gurlak Y, Hastings J, Hu J, Holtz R, DaSilva M, **Tsakalakos T**, Journal of Applied Physics 92 (1): 578-586 (2002)

"On the Mechanical Stability of Nanostructured Coatings by Synchrotron Radiation" T. Tsakalakos, M. Croft, I. Zakharchenko, Z. Zhong , Y. Gulak, M. Desilva, R. Holtz, AIAA-2002-1314

"Methodology of Synchrotron EDXRD Strain Profiling" I. Zakharchenko, Y. Gulak, Z. Zhong, M. Croft, and T. Tsakalakos, X-ray Analysis, Vol. 46 (2002)

"Application of Synchrotron EDXRD Strain Profiling in Shot Peened Materials", I. Zakharchenko, Y. Gulak, Z. Zhong, M. Croft, and T. Tsakalakos, Advances in X-ray Analysis, Vol. 46 (2002)

"XRD strain and stress determination in nanostructured films and coatings" T.Tsakalakos and M. Croft , NATO Science series Vol 78 Nanostructured films and coatings,223-230, 2000

Dr. Zhong Zhong
Physicist – x-ray optics
National Synchrotron Light Source — Ph: 631 344 2117
Brookhaven National Laboratory — Fax: 631 344 3238
Upton, NY 11973 — Email: zhong@bnl.gov

Dr. Zhong specializes in materials characterization using high-energy, synchrotron-generated x-rays. He pioneered the method of using EDXD for strain mapping at the X17B1 and introduced the battery term at GE to adopt this method for battery research. He has 15 years experience in synchrotron radiation instrumentation, x-ray crystal optics, high-energy x-ray monochromator design, high-resolution x-ray single-crystal and powder scattering, and strain mapping with energy-dispersive x-ray scattering. He currently leads X17B1 beamline for materials science, and the X15A beamline for Diffraction Enhanced Imaging (DEI) programs at the National Synchrotron Light Source. Dr. Zhong is the inventor of the now-popular DEI phase contrast imaging method, and the R&D100 winner sagittal focusing Laue monochromator. Dr. Zhong holds 90 refereed publications, 7 patents, and over 40 conference proceedings.

Education

September 1992 - December 1996, Ph.D. Physics, SUNY at Stony Brook, Stony Brook, New York

September 1990 - August 1992, M.S. Applied Physics, Michigan Technological University, Houghton, Michigan

September 1986 - July 1990, B.S. Physics, Beijing University, Beijing

Research & Professional Experience

October 1998 – Present: Physicist, National Synchrotron Light Source, Upton, New York.
November 2001 – Present: Assistant Professor, Biomedical Engineering Department, SUNY at Stony Brook, Stony Brook, New York
May 2005 – Present: Assistant Professor of Research Radiology, Department of Radiology, School of Medicine, SUNY at Stony Brook, Stony Brook, New York.

Selected peer-reviewed publications and presentations

1. Z. Zhong, D. Chapman, R. Menk, J. Richardson, S. Theophanis, and W. Thomlinson, "Monochromatic Energy-Subtraction Radiography Using a Rotating Anode Source and a Bent Laue Monochromator". *Phys. Med. Biol.*, **42** (1997) 1751-1762.

2. Z. Zhong, D. Chapman, W. Thomlinson, F. Arfelli and R. Menk, "Bent Laue Crystal Monochromator for Producing a Large Area X-ray Beam". *Nucl. Instrum. Meth. in Phys. Res. A* **399** (1997) 489-498.

3. Z. Zhong, W. Thomlinson, D. Chapman and D. Sayers, "Implementation of Diffraction Enhanced Imaging Experiments: at the NSLS and APS", *Nucl. Instrum. Meth. in Phys. Res. A.* **450** (2000) 556-567.

4. Z. Zhong, "Using a Prism to Reject or Select Harmonic Reflections in an X-ray Monochromator", *J. Appl. Cryst.* **33** (2000) 1082-1087.

5. B. Noheda, D.E. Cox, G. Shirane, E.S. Park, L.E. Cross and Z. Zhong, "Polarization rotation via a monoclinic phase in the piezoelectric 92%PbZn1/3Nb2/3O3-8%PbTiO3", *Phys. Rev. Lett.* **86** (2001) 3891-3894.

6. Z. Zhong, C.C. Kao, D.P. Siddons and J. B. Hastings, "Sagittal focussing of high-energy synchrotron x-rays with asymmetric Laue crystals, I: theoretical considerations", *J. Appl. Cryst*. **34** (2001) 504-509.

7. Z. Zhong, C.C. Kao, D.P. Siddons and J. B. Hastings, "Sagittal focussing of high-energy synchrotron x-rays with asymmetric Laue crystals, II: experimental studies", *J. Appl. Cryst*., **34** (2001) 646-653.

8. Z. Zhong, F. A. Dilmanian, T. Bacarian, N. Zhong, D. Chapman, B. Ren, X. Y. Wu and H. J. Weinmann, "Producing parallel x rays with a bent-crystal monochromator and an x-ray tube", *Med. Phys.* **28** (2001) 1931-1936.

9. Z. Zhong, C. Kao, D.P. Siddons, H. Zhong, and J.B. Hastings, "A lamellar model for the x-ray rocking curves of sagittally bent Laue crystals", *Acta. Cryst.* A **59** (2003) 1-6.

Appendix IV Letters of Support

GE Global Research

Mark M Little
Senior Vice President
Director

One Research Circle
Niskayuna, NY 12309
USA

T +1 518 387 7770
F +1 518 387 6633

July 8, 2011

Photon Sciences Scientific Advisory Committee:

I hereby express General Electric's strong support for the HEX beamline proposal at NSLS-II. The proposed beamline will create a world-class facility for studying advanced engineering and energy storage materials. This beamline will be unique in the United States and ensures that New York, the Northeast, and our nation as a whole, will remain competitive in these vital materials development areas. GE has long been a user and strong supporter of synchrotron techniques, and this beamline's suite of capabilities will provide continued benefits for both academic and industrial research.

High performance **materials for energy storage** are critical to solving the world's energy-related challenges. The ability to study such materials in real systems, under real use conditions, and in real time yields fundamental insight into the complex processes that take place during use, while speeding commercial application because the results come from relevant systems in a relevant timeframe. GE has benefited from this capability at NSLS-I during the development of its sodium metal halide battery technology. This technology is now being commercialized and its immediate economic impacts are reflected in the over $100 million dollar battery factory being built in Upstate New York that will create 350 new jobs by 2015. The proposed beamline will not only benefit current and emerging battery technologies, but will also accelerate GE's and the nation's development of next generation materials and processes.

The proposed beamline will also enable us to study the microstructure of important **engineering ceramics and alloys**, critical to areas such as gas turbine development, under stress and temperature conditions resembling their real application environment. The development of next-generation thermal barrier coatings and Ni-based superalloys by GE Energy and GE Aviation, for example, is largely dependent upon our ability to understand materials' performance and their underpinning microstructures. In this regard, GE has benefited greatly from its access to the NSLS-I. Maintaining uninterrupted access to an advanced characterization facility like the one proposed here, especially one located in the U.S., is essential to our global technological competitiveness in energy and aviation industries.

In closing, I enthusiastically support the proposed HEX beamline at NSLS-II. This beamline's unique combination of high energy x-ray techniques will accelerate government, university and industry collaborations and provide capabilities essential for U.S. technical and economic leadership.

Sincerely,

Mark Little
Senior Vice President and Director
GE Global Research

DEPARTMENT OF THE NAVY
OFFICE OF NAVAL RESEARCH
875 NORTH RANDOLPH STREET
SUITE 1425
ARLINGTON VA 22203-1995

IN REPLY REFER TO:

10 June 2010

NSLS-II Committee:

It is with great deal of pleasure to provide to support the Rutgers Group's Beamline Development Proposal (BDP) for the National Synchrotron Light Source II (NSLS-II). I believe the research conducted by the Rutgers Group on *nanomaterials under high temperature pressure* using the X17-B beamline has great promise to shed light to the microstructural evolution of such materials, which is of fundamental scientific importance while being of technological relevance.

The transition of X17-B1, NSLS-I to NSLS-II will enable the further growth of the advancement of nanostructure materials research under high pressure and temperature which has great promise in the future. As such, we believe that the establishment of a high energy beamline at NSLS-II is indeed justifable for the said reasons.

Sincerely,

Proto Mfg. Inc.
1980 East Michigan Ave.
Ypsilanti, Michigan, 48198-6010
Tel: 313-965-2900

11 June 2010

Re: High energy x-ray scattering beamline at NSLS-II for strain/stress field mapping in engineering materials

To Whom It May Concern,

The purpose of this letter is to support the proposed superconducting wiggler beamline proposal for NSLS-II. This beamline will enable residual (and under load) strain/stress field mapping in materials crucial to the technological competitiveness of this country.

Proto Manufacturing Inc. is a company that has been involved in non-destructive inspection and evaluation (NDI/E) since its inception in the late 1960s initially in support of the automotive industry. In the late 1980s, Proto turned its attention toward x-ray diffraction (XRD) technology as its foundational means of performing NDI/E and delivering useful systems and technical services. While much of its work to date has been applied toward measuring surface residual stresses (RS) for both aerospace defense and civil sectors, it has also continued to support highly technical areas of the automotive industry.

Recently, Proto has directed its attention toward measuring RS and diffraction peak full width at half maximum (FWHM) non-destructively at depth for high strength aerospace materials, such as Pyrowear 53 (X53), Al 7075-T651 and Inconel 100, using a synchrotron. So far, Proto has been successful in these measurements for material thicknesses of up to 0.25 inches using the high energy x-ray scattering beamline at NSLS-II.

Residual stresses introduced by processing and in-use duty cycling of engineering components can dramatically alter (for good or for ill) the lifetime of load bearing components. In the case of fatigue, for example, this alteration can result in simple breakage or catastrophic failure of key structural or aerospace components. In contrast, shot peening treatment can dramatically lengthen a components lifetime by introducing a crack resistant near surface compressive stress.

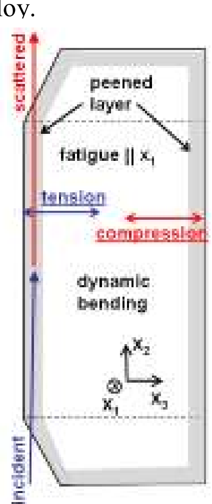
Understanding residual stress distributions and their evolution under cyclic loading and/or environmental degradation is absolutely crucial in many DOD and industrial applications. Keeping high performance aircraft, safely, in the air is a prime example of this criticality. High energy, synchrotron-based x-ray diffraction serves an essential and growing role in this field. Synchrotron results can serve as a “gold standard” for evaluating such residual stresses at the highest resolution and spanning both surface and the deep interior regions of specimens. Such synchrotron measurements can be used to both explore fundamental material properties and to absolutely calibrate other diagnostic measures used in the field to make essential decisions, such as to ground aircraft or close bridges.

Attempting to characterize the lifecycle of the ubiquitous shot peened layers in turbojet engine components provides a good example of the above. Our company was recently involved in an Air Force project regarding the characterization of fatigue degradation in such shot peened layers. Synchrotron measurements were an essential component in this project. Originally we had planned to make the required measurements at the Grenoble synchrotron. The Air Force, however, understandably required the work to be done in the US. In collaboration with Prof. Croft we made the necessary measurements at NSLS beamline X17-B1. Selected results from this study, shown below, provide specific motivation for such scientific infrastructure within the US.

The cross section of a typical specimen is shown in schematically in Figure 1. Initially our intention was to probe in the1-3 mm depth range of these large specimens. The high spatial resolution and deep penetrating power available at X17-B1 made it possible to do depth profiling through the entire thickness of the Ni aerospace alloy. Figure 2 shows the in-plane (ε_{11}) and out-of-plain (ε_{33}) strain profiles of a specimen shot peened on both surfaces. The in-plane shot peening compression and the Poisson ratio out-of- plane dilatation can clearly be seen in the figure. Moreover, the balancing residual strain throughout the interior can also be seen.

Figure 2 shows the ε_{11} strain profile of such a specimen fatigued (in a four-point bending mode) to 80% of its fatigue-failure lifetime. The degradation of the shot peening compression can be seen in the figure. Crucially however it should be noted that large, deep internal residual strains have been introduced by the bending fatigue treatment. The actual shot peening near surface compression rides on top of these deep internal strains and this becomes an important component in understanding the fatigue relaxation of the peened layer.

Figure 1 (below left) A schematic of a trapezoidal fatigue specimen used in the study of fatigue relaxation of the shot peened layer in the aerospace Ni alloy, Inconel 100. The tension and compression labels indicate the signs of the applied cyclic bending fatigue loading process. Note that the x-ray beam penetration path length required by the sample is 34 mm through high density Ni alloy.



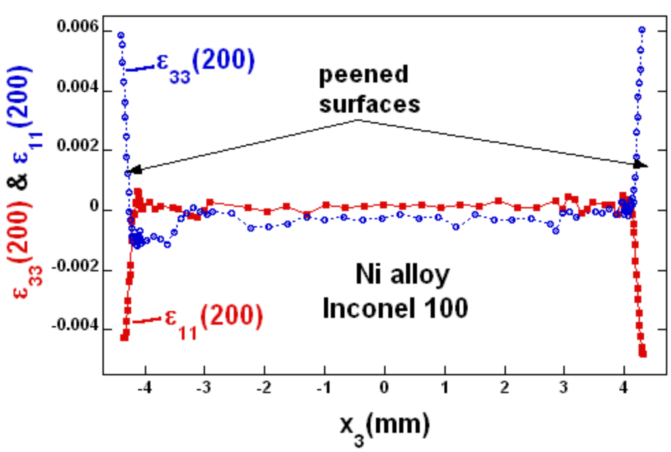


Figure 2 (above right) The 200-line ε_{11} and ε_{33} strain profiles (see previous figure for direction definitions) for a shot peened specimen. Note the near surface in-plane (ε_{11}) shot peening induced compressive strain.

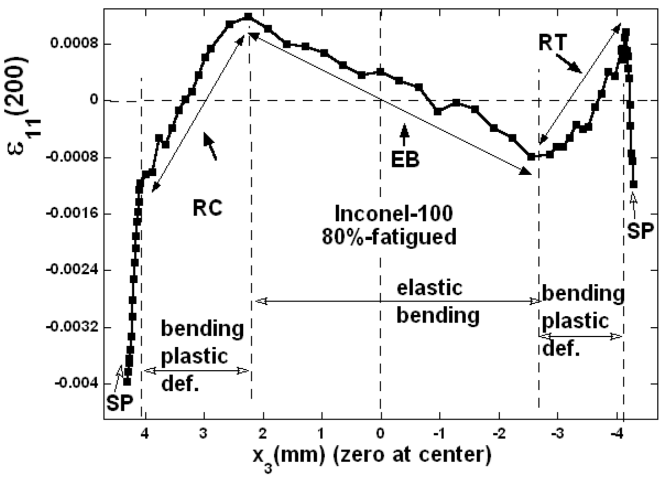


Figure 3 (left) The 200-line ε_{11} strain profile for a shot peened specimen fatigued to 80% of the fatigue failure level. The following regions should be noted: the shot peened (SP) compressions below both surfaces; and the RC (residual compression), EB (elastic bending) and RT (residual tension) regions caused by the plastic deformation introduced under the cyclic bending.

In summary, from our industrial view point and with our long-standing knowledge of the requirements of DOD aerospace component concerns the proposed wiggler beamline will play an essential role in supporting core national technologies. Conversely, the absence of such infrastructure facilities will leave a hole at the technological core of the coupled scientific and economic health of the country.

Kind Regards,

Michael Brauss, PresidentProto Mfg. Inc.
1980 East Michigan Ave.
Ypsilanti, Michigan, 48198-6010
Tel: 313-965-2900
Email: xrdlab@protoxrd.com
Web: www.protoxrd.com

Raytheon

Integrated Defense Systems

Integrated Defense Systems
Materials Engineering
350 Lowell Street
Andover, Massachusetts
01810 USA

15 June 2010

NSLS-II Committee:

This letter of endorsement is provided in support of the Rutgers Group's Beamline Development Proposal (BDP hereafter) at the National Synchrotron Light Source II (NSLS-II hereafter) to which we offer our strongest support.

In the last ten years, the Rutgers Group has developed an unprecedented energy dispersive X-ray diffraction method and metrology using high energy synchrotron radiation with which a wide range of engineering materials research challenges were addressed. Their efforts have met with substantial success which is now well documented and known among pertinent scientific and engineering communities.

Recently, Raytheon has collaborated with the Rutgers Group through a DARPA/ONR program on Nanocomposite Optical Ceramics in which the Rutgers' role was to provide crucial information on 3D residual strain in sintered materials. Their approach has been most effective thanks to the high energy X-ray facilities at the X17-B1 beamline as it enables one to use a Laue-type diffraction geometry, superceding conventional diffraction methodologies thereby.

Therefore, we feel that it is appropriate to transition the facilities at the X17-B1 beamline to NSLS-II or implement even more powerful facilities therein as the needs for high energy X-ray diffraction facilities in materials research is well known and yet neither the expertise nor the facilities are easy to locate around the world. The Rutgers-BNL partnership is most efficient and effective in this regard which leads us to wholeheartedly endorse the said BDP.

Sincerely,

C. Scott Nordahl, Ph.D.
Senior Principal Engineer
Mechanical Engineering

Corporate Research Laboratory
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Annandale, NJ 08801
908 730 3056 Telephone
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raghavan.ayer@exxonmobil.com

Raghavan Ayer
Senior Scientific Advisor
Section Head – Structural Materials

ExxonMobil
Research and
Engineering

June 15, 2010

NSLS-II Committee:

With great enthusiasm, we support the Rutgers Group's Beamline Development Proposal (BDP) for the National Synchrotron Light Source II (NSLS-II) for we believe the high synchrotron energy dispersive X-ray diffraction (S-EDXRD) research that has been ongoing at NSLS-I by the said group has been of utmost importance to the engineering community at large. Specifically, the strain mapping studies carried out on welded structured have proven to be most useful in assessing the quality of weldments in a series of critical industrial applications. To the best of our knowledge, there is no alternative methodology by which such critical assessments can be made. Therefore, we feel that it would be to the NSLS-II's interest to ensure a seamless transition of the capabilities of the X17-B1 beamline at NSLS-I to the new facility whereby this superb experimental facility can be used with even greater effectiveness in the future.

Sincerely,

Raghavan Ayer

NEI Corporation

10 June, 2010

NSLS-II Committee:

I herewith provide my strongest support to the development of a new high energy X-ray beamline at the NSLS-II –an effort led by the Rutgers Group. I am confident that a new high beamline with equal or higher capability, fashioned after the X17-B1 in NSLS-I, would ascertain that the unique energy dispersive X-ray diffraction method and metrology would continue to evolve. The ramification of such a progress would be most beneficial to advancing the frontiers in cutting-edge materials research. I must mention that NEI Corporation has greatly benefited from the expertise of the Rutgers Group in a Department of Energy funded research program which involved the use of 3D phase and strain mapping. Were it not for the capabilities at NSLS-I and the Rutgers expertise, it would have been impossible to analyze the advanced functionally gradient materials that are being developed by NEI. Therefore, I am convinced that a new high energy beamline would serve the functionally gradient materials community extremely well, which makes me endorse the Rutgers Group's BDP without any reservation.

With best regards

Dr. Ganesh Skandan, CEO

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10 June 2010

NSLS-II Committee:

It is with great deal of pleasure that Perpetual Technologies offers its strongest support and endorsement to the development of a new high energy X-ray beamline at the NSLS-II –an effort led by the Rutgers Group. We are certain that a new high beamline with equal or higher capability, fashioned after the X17-B1 in NSLS-I, would ascertain that the unique energy dispersive X-ray diffraction method and metrology would continue to evolve. The consequences of such a progress would be most beneficial to advancing the frontiers in cutting-edge materials research on nanostructured thermal spray coatings which are extremely complex materials that are subjected to very harsh environmental conditions. One should note that the high energy X-ray diffraction method and metrology, as developed by the Rutgers Group, is ideally suited for analyzing such complex materials while conventional diffraction methods are of limited use at best. Therefore, we believe that the establishment of a high energy diffraction beamline at the NSLS-II, which is fashioned after the X17-B1 in NSLS-I, is a natural progression in the evolution of the 3D phase and strain mapping methods and metrology that has been created by the Rutgers Group. The said envisioned transition would ensure continued development which would have a profound impact on various lines of materials research, especially on the mechanical behavior of nanostructured engineering materials.

It is with the aforementioned rational that we provide our strongest support and endorsement to the Rutgers Group's BDP without any reservation.

Sincerely,

METALLIZING
PLASMA COATINGS
HVOF COATINGS
PTA COATINGS
HARD SURFACING
ELECTRIC ARC

A&A COMPANY INC.

FUSED COATINGS
HEAT RESISTANT COATINGS
CORROSION RESISTANT COATINGS
WEAR RESISTANT COATINGS
CERAMIC COATINGS
CARBIDE COATINGS

RESPONSIVE COATING TECHNOLOGY

ESTABLISHED 1944

10 June 2010

NSLS-II Committee:

A&A Company, Inc., which is a U.S. Navy certified thermal spray coating company, herewith, offers its strong support to the Rutgers Group's Beamline Development Proposal (BDP hereafter) at the National Synchrotron Light Source II (NSLS-II hereafter).

A&A Company, Inc. has a long standing and productive working relationship with the Rutgers Group through a series of Office of Naval Research funded research programs wherein the Rutgers team has carried out comprehensive and graoundbreaking studies on the mechanical behavior of nanostructured thermal barrier coating using synchrotron energy dispersive X-ray diffraction –a methodology and metrology pioneered by them. Were it not for the Rutgers Group's innovative approach in 3D phase and strain mapping, our current understanding on the mechanical behavior of such technologically critical coatings would not be where it is now. The work carried by the Rutgers Group decisively aided in optimizing the properties of such nanostructured coatings which are used in a wide range of U.S. Navy missions.

Besides its importance for the reasons explained above, A&A Company, Inc. believes that the use of the Rutgers Group's method and metrology can be used in applications such as experimental fracture mechanics, study of the behavior under harsh environmental conditions, energy materials research to name but a few. Hence, A&A Company, Inc. believes that it would be to this nation's interest to transition or to upgrade the high energy X-ray diffraction facilities at X17-B1 in NSLA-I to NSLS-II which is why we wholeheartedly offer our strongest support and endorsement.

Sincerely,

R. Stewart Brunhouse, Jr.
President

2700 South Clinton Avenue • South Plainfield, NJ, 07080 • (908) 561-2378 Fax (908) 561-4201

DEPARTMENT OF CHEMISTRY
Clare P. Grey
Professor of Chemistry
Director,
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June 14, 2010

To Whom It May Concern,

The purpose of this letter is to support the proposed high-energy x-ray scattering beamline for NSLS-II whose partial focus will be on battery studies. This beamline will enable unique and essential in situ characterization of advanced batteries under cycling conditions. Such *in situ* probes on real electrochemical cells are important to achieving the significant advances in this field that are required for national scientific and economic interests.

The thermal stability, long operation life, non-toxicity, abundant Fe resources and overcharging/discharging tolerance have made $LiFePO_4$ one of the more important and commercially viable cathode materials for Li-ion batteries for transportation and grid-storage applications. Many important advances concerning the fundamental origin of the kinetic limitations and failure in the $LiFePO_4$ systems must still be made. Despite much work on this system, the mechanism by which this material functions is still unclear. The functionality of $LiFePO_4$ suffers from an intrinsically low electrical conductivity. Tailoring $LiFePO_4$ cathode crystallite size and morphology is a promising route toward significantly enhancing cell electrochemistry, but this seems to alter the deintercalation mechanism.

The microstructure of the electrode is key to its performance in batteries. Ex-situ measurements are performed on recovered electrode powders after scraping the powder off the current collector, which leads to sample alteration. Previous lower energy synchrotron studies had to be on small, specially designed, windowed cells which usually results in battery failure and/or lower performances. The coin cell geometry, on the other hand, makes direct connection with commercial battery geometry and provides good pressure across the electrode. Therefore, temporal in situ EDXRD measurements carried out on functioning coin cells has the potential of characterizing how the electrode reaction proceeds and the results can be taken as representative and not due to a battery designed for low energy x-ray transparency. Moreover, it should be noted that proof of principle in situ EDXRD results have already been obtained on a full sized commercial video camera battery and measurements on a portable computer 18650 cell appear eminently feasible.

Recent, potentially landmark work by our group at X17-B1 [R. Robert et al] on $LiFePO_4$ based coin cells has clearly demonstrated the ability to perform high spatial resolution profiling (20 μm on a ~ 100 μm thick electrode) across this cathode under in situ cycling conditions. Here it important to emphasize that not only time-resolution but spatial-resolution results, which were beyond our initial expectations, within the cathode in the charge/discharge process were obtained. These results underscore the potential power that such a high-energy x-ray scattering characterization tool can bring to battery research. In order to concretely emphasize the power and feasibility of this technique selected preliminary results from this recent work are briefly discussed below.

Electrochemical and EDXRD data were collected simultaneously. Figure 1 shows the voltage vs. time, during the first charge/discharge, for a $LiFePO_4/Li$ coin cell cycled at 16.7 mA/g during the in situ EDXRD measurements. The EDXRD patterns in Figure 2 show the transformation, as a function of position in the cathode film, between the two phases of Li_xFePO_4 at the state of charge E5 (see Fig. 1), in situ. Here the cathode thickness was less than 100 μm. In Figure 3 the spatial variation in the fractional the x=1 phase content, (obtained by fitting EDXRD patterns collected during in situ cycling) is shown for a sequence of cell charge states. These first preliminary results clearly show that in situ profiling of the electrochemistry in the cathode, both as a function of space and time (charged state), is eminently feasible in real functioning coin cells. This last statement is provided that high energy x-ray scattering facilities of the type proposed here are available.

In summary high-energy x-ray scattering constitutes an important new tool for in situ studies of real batteries under operating conditions. We are excited by the possibilities that the new NSLS-II instrument will offer and look forward to working with the beam-line scientists to develop the technologies and instruments to enable research on battery systems.

Sincerely Yours

Clare Grey

Rosa Robert

Figures

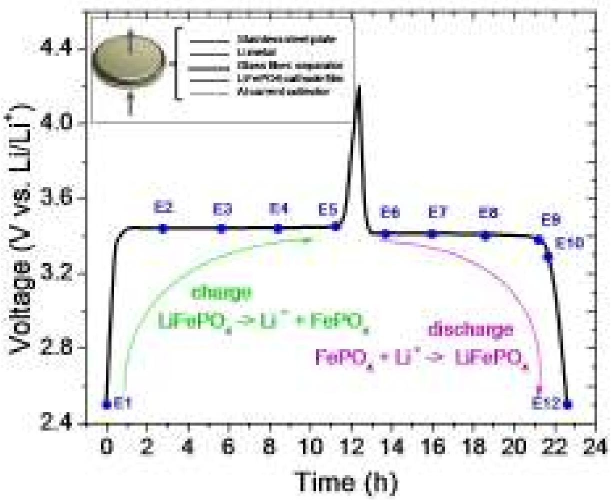
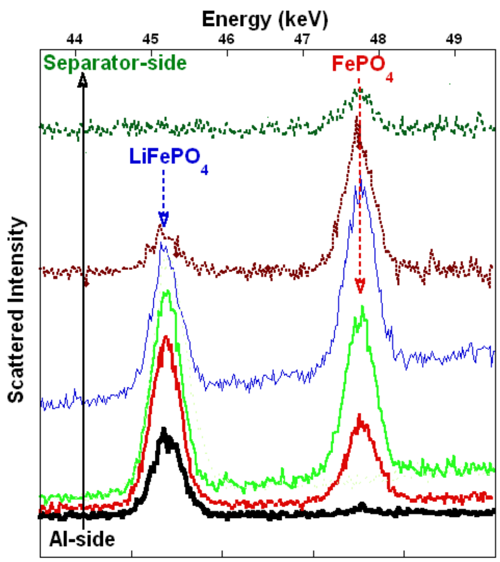


Figure 1. (left) voltage vs. time, during the first charge/discharge, for a $LiFePO_4$/Li coin cell cycled during the in situ EDXRD measurements. The inset picture displays schematically the parts of the coin cell and the arrows indicate the direction of the EDXRD profile.

Figure 3 (below). The spatial variation across the cathode of the x=1 fractional phase content across the cathode in various states during charge. Here phase fractions were obtained by fitting the (002) Bragg line intensities is patterns as shown in Figure 2. The curves with decreasing $LiFePO_4$ content correspond to the steps E1 to E5 during charge (see Fig. 1).



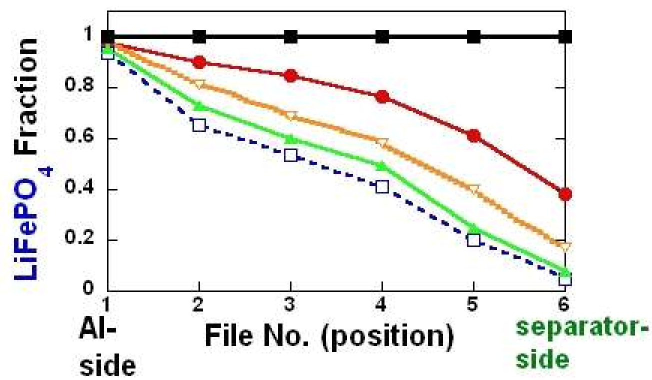


Figure 2. (above left) EDXDR in situ (002) Bragg line patterns taken at various depths in a thin Li_xFePO_4 cathode in a coin cell in the state of charged E5 in the electrochemistry profile (Fig. 1). The separator is the interface with the Li-reservoir and the Al-side is the electron current collector.

University at Buffalo The State University of New York

Esther S. Takeuchi
SUNY Distinguished Professor

To whom it may concern

I am writing this letter in support of the proposal for a high energy x-ray scattering beamline on NSLS-II at Brookhaven National Laboratory. I would also like to be a Proposal Team Member for this beamline which will be partially devoted to battery studies. I am quite enthused about the type of data collected in proof of principle studies conducted at X17B1 on our groups bimetallic vanadium based batteries. The high energy of NSLS II allows direct in-situ interrogation of electrochemical systems. This eliminates any risk of modifying the materials during a disassembly process.

By way of further justification, I would like to highlight my area of work. I conduct research in energy storage. The critical aspect of energy storage systems is that they are dynamic and change with use and patterns of use. The opportunity for our research at NSLS II is to probe the energy storage materials in-situ within an active cell. The cell can then be charged or discharged further to track the material changes during the oxidation or reduction process. My particular area of interest is on bimetallic materials including transition metals Fe, Mn and V. These materials allow us to tune desired functional properties. However, in order to do this successfully, we need to understand how the structure is affected by state of discharge. The use of NSLS II is highly suited for this type of interrogation.

I would also like to take a moment to introduce my background and the work that I have done in energy storage related to this proposal. I am currently a SUNY Distinguished Professor in the Departments of Chemical and Electrical Engineering and Chemistry at the University of Buffalo. I began this position in September 2007 after a 22 year industrial career with Greatbatch, Inc. While at Greatbatch, I was active in the research and development of power sources for medical devices. In fact, for the majority of those years, I led the Battery R&D group of up to 40 individuals. My work has been widely recognized and with more than 140 patents, am noted to be the most prolific living female inventor (*USA Today*, 12/13/05). I have received local, national, and international recognition from the premier scientific societies and technical organizations, including the Electrochemical Society (Battery Division Technology Award), the American Chemical Society (Jacob Schoellkopf Medal, Astellas Award), and the American Institute for Medical and Biological Engineering (fellow). In 2004, I was inducted into the National Academy of Engineering (NAE). I was also honored by the Achievement in Health Care Award from D'Youville College and as a Pioneer of Science by the Hauptman-Woodward Medical Research Institute. Most recently, I received the National Medal of Technology and Innovation from President Obama. Therefore, I am well qualified to judge the potential impact of the work that is being proposed.

I am highly supportive of the proposed work and hope to be an active user of this facility. collaborate. This would enable investigation of energy storage materials which are consistent with the overall mission of Brookhaven National Laboratory.

Sincerely,

Esther S. Takeuchi, Ph. D.

SUNY Distinguished Professor
Greatbatch Professor

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June 14, 2010

Professor Mark Croft
Beamline Development Proposal Team
Department of Physics and Astronomy
Rutgers, The State University of New Jersey
136 Frelinghuysen Road
Piscataway, NJ 08853-8019

Subject: *Support for the Beamline Development Proposal for a High-Energy X-Ray Micro-Mapping of Materials for Advanced Energy and Structural Engineering Applications*

Dear Professor Croft:

This letter is written in support of the beamline development proposal for a high-energy x-ray micro-mapping of materials for advanced energy and structural engineering applications. The beamline is essential for several research areas that greatly enhance our understanding of materials for advanced nuclear energy systems. It aligns well with the laboratory mission to use synchrotron techniques (a core competency) to develop energy technologies (a laboratory initiative) and the white paper on Materials in Extreme Environments. Research preformed at the beamline would also respond directly to recommendations from the DOE that synchrotrons and other large user facilities be used to develop applied technologies for advanced energy systems.

New materials capable of withstanding extreme environments are important to virtually every energy technology. New high-temperature, radiation resistant structural materials are crucial for advanced reactors. The proposed beamline can be used to characterize new structural materials and irradiation damage in materials. It will be capable of mapping strains in the material and therefore, the local elastic material properties. By combining the structural characterization with the ability to perform strain mapping to determine the material properties in the samples, it will be possible to directly relate the environmental conditions (dpa and annealing temperature) to microstructural features (dislocation structures, point defects, segregation of solutes) to mechanical properties (elastic modulus and yield strength). This increase in understanding of material process will allow new materials to be designed far more quickly and efficiently than was previously possible. It is critical to realizing the full potential of new classes of radiation resistant materials, such as nanostructured ferritic alloys.

Computational materials modeling of nuclear fuel and materials offer the potential to reduce high-cost nuclear testing and predict performance. Rather than continuing with time-consuming irradiation of prototypical samples and environmental conditions, materials and performance could be optimized. Accident scenarios, such as reactivity and power transients, that create off-nominal conditions that are difficult to duplicate experimentally could be better investigated. However, developing and verifying the computational models is difficult because fundamental understanding of radiation damage processes is lacking and the environmental conditions for most irradiation experiments are dictated by other priorities, such as establishing fuel performance. The modeler is frequently required to try to decipher complicated and path-dependent material processes from very few data points for macroscopic material properties at the end of long irradiation exposures. Research performed at the proposed beamline will be used to develop and verify materials models and will enable the advances in computational materials science to have a near-term and greater influence in materials design and performance estimates.

The beamline aligns directly with the Brookhaven National Laboratory Mission and Vision. It leverages BNL's core competency in synchrotron science. The new materials designed and characterized at the beamline will include new nano materials for energy technologies such as oxide dispersion strengthened steel and nanostructured ferritic alloys. In addition, it will strengthen the major laboratory initiatives in photon sciences and energy. A white paper "Materials in Extreme Environments" further describes the development of a core program on advanced materials for energy applications that this beamline supports.

The proposal directly addresses science requested by the DOE. The DOE report "New Science for a Secure and Sustainable Energy Future" summarizes the results of eleven BES Basic Research Needs workshops and describes the research required for advanced nuclear energy systems as beneficial to other technologies. The report states "understanding how materials respond to radiation, very high temperatures, and a wide variety of corrosive substances is important not just for nuclear energy systems but for many other industrial processes such as high performance turbines. And it is clear that the ability to characterize and control the structure of materials at the nanoscale will be crucial to finding solutions, as well as new computational tools that can model the resulting complexity so as to provide predictive tools for engineers. These research efforts will use advanced synchrotron X-ray sources, neutron sources, and supercomputers to transform the scientific understanding that underpins technology development for advanced nuclear energy systems."

The proposed beamline will attract an active user community, produce new material science and directly impact advanced energy technologies, including materials for high temperature, structural applications in nuclear systems. I strongly support the beamline development proposal.

Sincerely,

A40

Ly[illegible] E. Ecker
Scientist, Advanced Nuclear Technologies

LE/jf

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Managed by Brookhaven Science Associates
for the U.S. Department of Energy

June 17, 2010

Professor M. Croft
Department of Physics
Rutgers University

RE: **High-energy x-ray micro-mapping of materials for advanced energy and structural engineering applications**

Dear Prof. Croft,

The purpose of this letter is to express strong commitment of support to the proposal on "**High-energy x-ray micro-mapping of materials for advanced energy and structural engineering applications"** that is being submitted aiming at a beamline with high spatial resolution and 3-D mapping capabilities that will allow the characterization of engineering materials during thermo-mechanical cycling via in-situ strain mapping.

The need to understand the microstructural behavior of materials under extreme loading accompanying a number of novel concepts of next generation energy and in particular nuclear energy is crucial if we were to develop materials that will be able to operate at the extreme environments that characterize the next generation energy concepts. While we have reached a point where the effects of extreme environments can be observed macroscopically on the next generation materials such as super-alloys and composites and we can attribute the changes and or limitations to phase or lattice transformations that occur, we have no means of assessing or tracing the exact path within the phase diagram that transformation in these complex lattice structures occur. And since the phase transformations and thus the macroscopic changes prompted by external loading are path dependent without a clear understanding of these processes we are not in a position to influence or redesign/optimize the lattice structure. The proposed beamline with the capabilities on phase and strain mapping with high resolution can provide the means for understanding the phase transformation or transition paths that occur as a result of combined extreme environments. Especially in nuclear energy related materials and more so in complex materials that are to support the next generation fission and fusion reactors where extreme fluxes of fast neutrons, primarily, are combined with high temperatures and aggressively corrosive environments, the ability to shed light on the changes induced will be a crucial step towards the design of materials that can support the next generation nuclear energy. Further, the capabilities offered with the proposed beamline will enhance the on-going work at BNL on irradiation damage of new materials under the combination of fast neutron spectra, high temperatures and corrosive environments.

Sincerely,

Nicholas Simos, PhD, PE
Scientist
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June 17, 2010

RE: Letter of support for the new High Energy Beamline at NSLS II

Dear Mark:

I write this letter of support with extreme enthusiasm for a new High Energy x-ray beamline at NSLS-II. This is a pivotal time for the development of high energy x-ray capabilities in the US. The recent development of user-friendly experimental methods and data reduction software has made high energy diffraction available to non-experts and has shifted the new science from the x-ray to the material. While the transitioning of high energy methods from "heroic effort" into real experimental **capabilities** is enabling unprecedented gains in the area of 3D materials characterization, many of the US high energy beamlines are becoming seriously oversubscribed. The only way US research will remain competitive in this area is by the development of facilities like the beamline you are proposing at NSLS II. Perhaps the most important reason for expanding our current high energy capabilities is the new generation of users that our research is creating. My mechanical engineering graduate students are "growing up" at the beamline. The important discoveries that they will make in their careers will only happen if enough high energy beam time is available. With the lead time that is common for the development of such facilities, it is imperative that construction begins as soon as possible. As examples of the potential of high energy x-rays for characterization of engineering materials, I briefly describe in this letter some of the high energy x-ray experiments that we are working on as well as some of the other experiments that I have seen lately at the beamline. I also include a short list of references.

As you might recall, we came to high energy x-ray diffraction from the area of mechanical testing and micromechanical model validation. You and I met several years ago when my group in mechanical engineering had just ventured into the area of x-rays in 2002 or 2003 for the purpose of characterizing elastic-plastic deformation of metallic polycrystals. Your *in situ* experiments have served as a motivation for us and I think we have come a long way. Since we first met, my group has developed a new diffractometer / close-loop control loading system [1] that we use primarily at the Cornell High Energy Synchrotron Source (CHESS) for measuring distributions of lattice strains during loading. Figure 1 below depicts a photo of our system within the A2 hutch at CHESS. The lattice Strain Pole Figure (SPF) experiments we conduct using this system have become a standard characterization experiment for us [1-4]. In addition to enabling new understanding of micromechanical processes such as crystallographic slip in HCP titanium alloys [5], these data are also ideal for comparison to crystal-scale modeling results [6]. In fact, validation of multiscale modeling is the application that first brought us to high energy x-rays. Figure 2 below shows a comparison between the stress distribution determined from the SPF experiments and a finite element simulation of a copper specimen during tensile loading[6]. As can be seen, the comparison is remarkable.

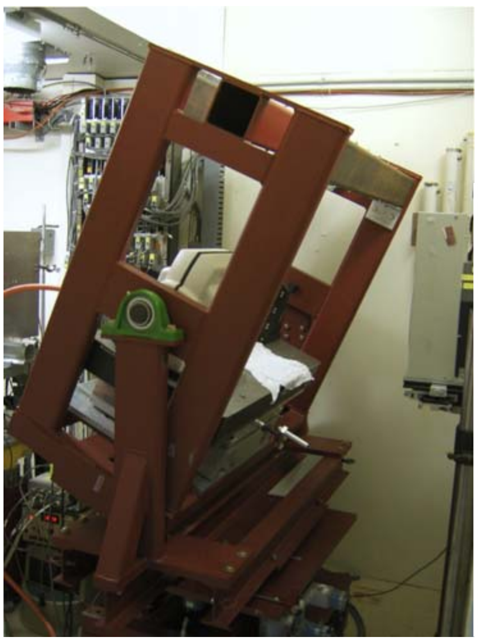
We also currently have a significant experimental effort at the Advanced Photon Source 1-ID-C conducting High Energy Diffraction Microscopy (HEDM) stress measurement experiments. The sector 1 beamline scientist, Ulrich Lienert, has significant experience in this area [7,8]. We have upgraded the mechanical testing capabilities at sector 1. Figure 3 depicts the small loadframe that our group redesigned installed within the six circle diffractometer at APS 1-IDC. In these experiments, we are able to track the evolving stress state within individual crystals within a polycrystalline aggregate. Figure 4 depicts the macroscopic stress strain curves of an HCP titanium alloy, Ti-7Al, in two states [9]. In the air cooled (AC) state, short range order forms within the unit cell resulting in a different strengthening mechanism than the ice water quenched (IWQ) structure. Also shown in Figure 4 are the stress states from crystals within each specimen. The things to note are the difference from the macroscopic uniaxial stress state and the different stress directions at the various points in the stress-strain curve. The differences in the plasticity processes exhibited by the AC and the IWQ material are evident in Figure 5 – high resolution images of diffraction spots from each specimen. The short range order in the AC specimen – which results in planar slip – produces a diffraction spot that is much more broad than the IWQ specimen. Basically the AC grain is decomposed into regions that can support different mechanical states. These data are examples of how the HEDM experiment can be employed to quantify stress state and then to study resulting deformation processes on the grain scale and below.

Others who are working on developing HEDM methods at APS 1-ID-C include Professor Bob Suter from Carnegie Mellon University who is building 3D grain maps - basically non-destructive serial sectioned EBSD maps[10,11]. These data are invaluable for understanding complicated 3D structural artifacts like titanium lathes. A group at Lawrence Livermore – including my former student Joel Bernier – is using HEDM methods to investigate phenomena like twinning and yield asymmetry in Magnesium alloys [12].

Mark, I give this proposal my strongest support. Please let me know if there is anything else I can do to support it. It is crucial that we secure high energy x-ray beam sources for the next generation of users working on the next generation of important research problems.

Regards,

Matthew P. Miller



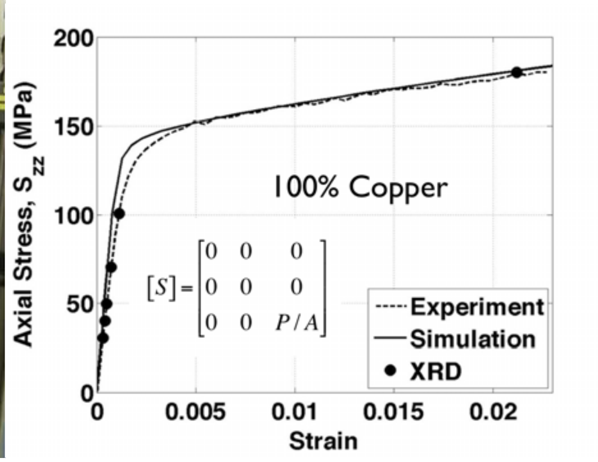


Figure 1. (Left) Diffractometer / in-situ loading system shown within the A2 experimental station at CHESS. (Right) Macroscopic stress-strain curve for copper specimen showing the fit to the finite element model and the points where diffraction experiments were conducted.

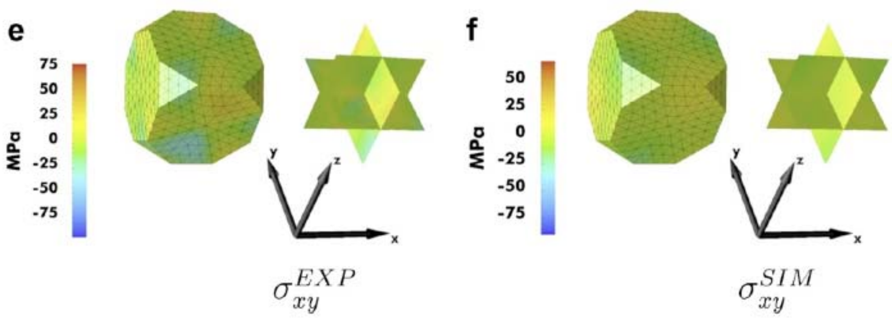


Figure 2. Distribution of the σ_{xy} shear stress component over orientation space for a uniaxial copper specimen loaded in the z direction to Szz = 100 MPa (shown in Figure 1).

The experimental data (EXP) are derived from strain pole figures measured during in situ loading at the A2 experimental station at CHESS. The simulation results (SIM) are from a crystal-based finite element simulation containing 2916 crystals [6].

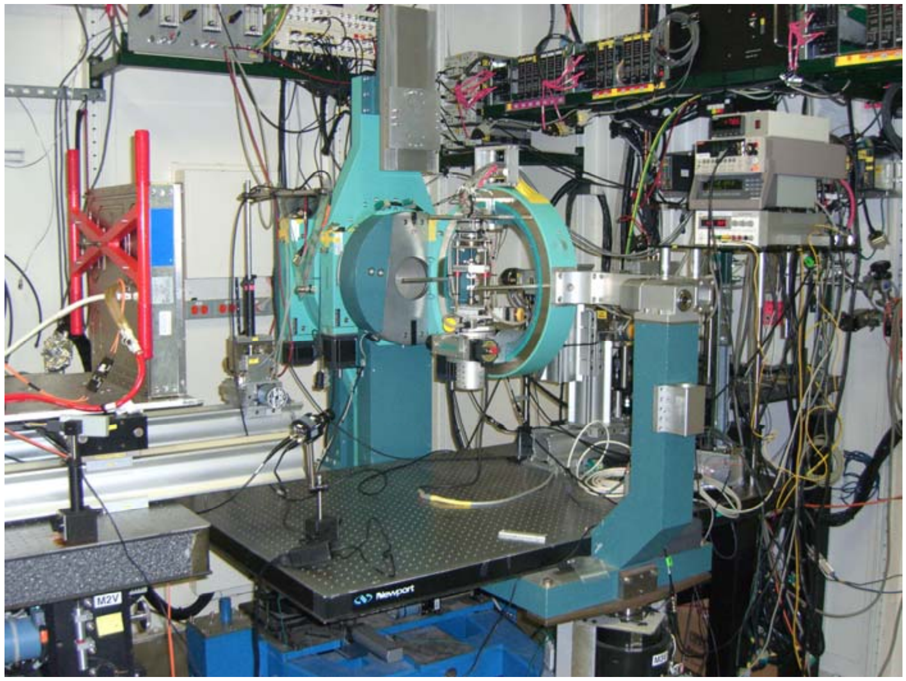
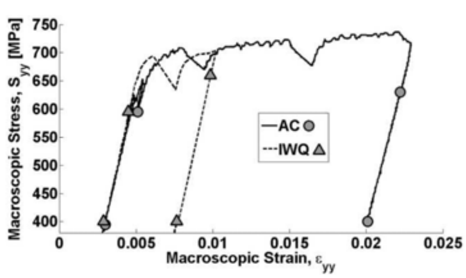


Figure 3. Cornell-designed in situ loadframe mounted within a six circle diffractometer at APS beamline 1-ID-C. With this small apparatus, we are able to track individual grains within a deforming polycrystalline aggregate.



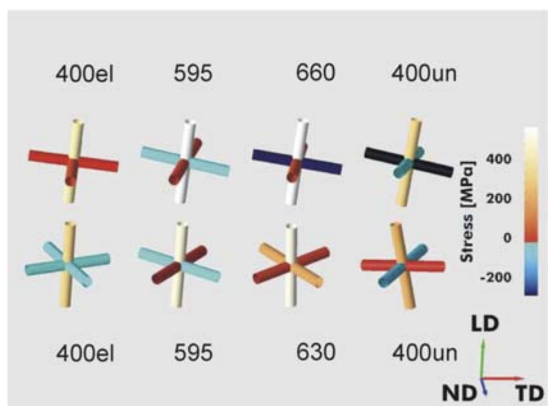


Figure 4. (Left) Macroscopic loading curves for the Ti-7Al AC and IWQ specimens. The loads at which diffraction measurements were taken are indicated. (Right) Principal axis "jacks" depicting the orientation of the principal stress state at the four indicated macroscopic stress levels (in MPa) for the IWQ (top) and AC (bottom) specimen.

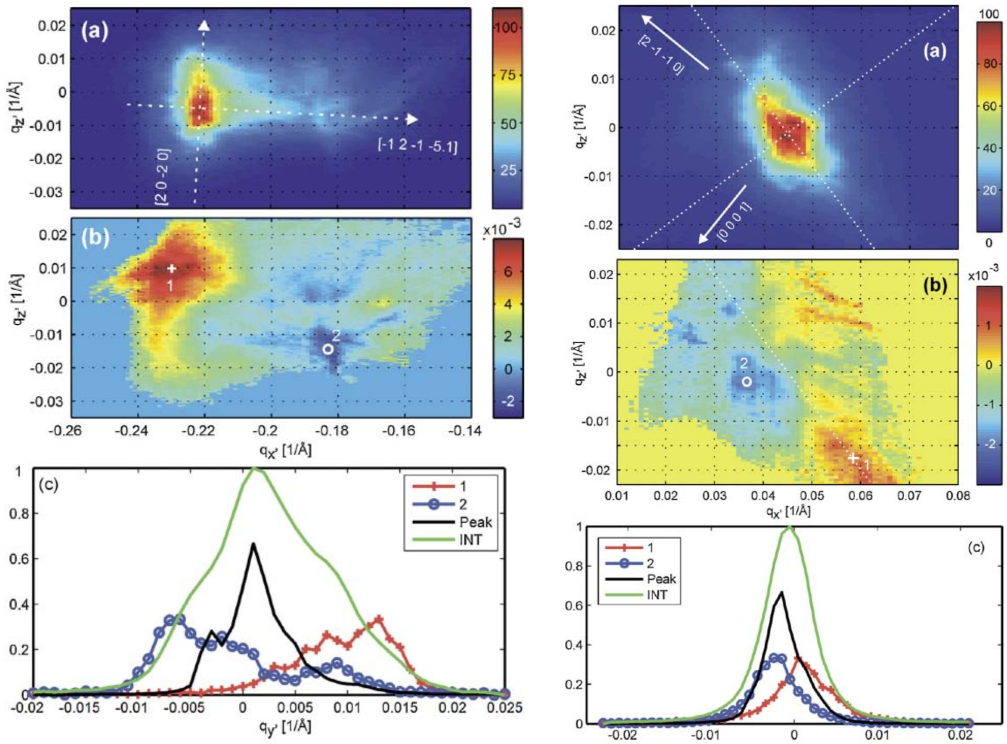


Figure 5. (Left) Representations of the (1 2 1 2) AC reference grain in reciprocal space map unloaded to 400 MPa. (a) Azimuthal intensity projection. The dashed lines indicate the directions of the narrowest and widest widths at half maximum. (b) Center-of- mass positions of radial profiles. (c) Selected radial profiles with arbitrary intensity scale for better visibility: azimuthal positions '1' and '2' are indicated in (b), at the azimuthal peak intensity (intersection of dashed lines in (a)), and azimuthally integrated. (Right) Representations of the (0 2 2 0) IWQ reference grain reciprocal space map at 660 MPa. (a) Azimuthal intensity projection. The dashed lines indicate the directions of the narrowest and widest widths at half maximum. (b) Center-of-mass positions of radial profiles. (c) Selected radial profiles with arbitrary intensity scale for better visibility: azimuthal positions '1' and '2' are indicated in (b), at the azimuthal peak intensity [intersection of dashed lines in (a)], and azimuthally integrated.

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Re: HEX NSLS-II Beamline Development proposal Review Panel

As the principal scientists with long years of experience running the established high-energy beamline at ESRF we wish to provide our perspective in this letter of support for the proposed HEX beamline at an NSLS-II.

The evolution of the beamtime request in the past years shows that the engineering/industrial community as a whole should be recognized as a new major user community for synchrotron radiation science. This community produces important scientific output – although its publication pathway often differs from the typical synchrotron radiation physics/chemistry community – and that contribution to the economic comptetiveness of the science-based industrial nation (nations) which supports the synchrotron, which in turn supports the engineering/industrial community, must strongly be considered.

A striking example in the rapidity of science to commercialization is the recent General Electric/Brookhaven/Rutgers collaboration at X17B at NSLS. The detailed characterization of the GE sodium-metal hydride electrochemical cell could only have been done using high-energy x-ray diffraction at synchrotron source due to the length and time scales requirements. As noted in the DOE Discovery & Innovation release (see http://science.energy.gov/stories-of-discovery-and-innovation/127017/), the collaboration helped substantially in the creation of new industrial facility and the jobs which accompany it.

In the case of the X17B beamline suite only one of four hutches is even partially dedicated to engineering/industrial experiments. This lack of availability and facilities prevents the engineering/industrial community to realistically incorporate experiments into their thinking. This is analogous to the situation at when ESRF started operation. At that time the engineering community was not yet recogniced as a potential synchrotron radiation user and beamlines were predominantly distributed among the established classical physics and chemistry user groups. As a consequent it took long time to the engineering/industrial community to "get a foot into the door".

At a present Europe is at an inflection point in which engineering/industrial materials research is playing an increasing role in synchrotron science. One recent example is the Joint Engineering, Environmental and Processing beamline at the UK's Diamond Light Source where engineering applications are heavily emphasized (see http://www.diamond.ac.uk/Home/Beamlines/I12.html). A second recent example is the High Energy Materials Science beamline at PETRA III in Germany (see http://www.hzg.de/central_departments/genf/branch/desy/004478/index_0004478.html).

Synchrotron radiation is thusly now ready to make a real contribution to science in the engineering/industrial/economic sector. The purpose of this letter of support is to urge that the necessary investments be made to similar position US synchrotron-based engineering/industrial research.

Sincerely Yours

Veijo Honkimäki

Thomas Buslaps

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Eric M. Johnson
Staff Engineer
Materials Engineering

26 May 2011

Dr. Mark Croft
Department of Physics and Astronomy Rutgers University
136 Frelinghuysen Road
Piscataway, NJ 08854-8019

Dear Dr. Croft,

I am writing to lend you my support in the effort to add NLSL-II beam line to the Brookhaven Synchrotron. A beam line to support industrial use is very much needed to move applied research forward. Currently, the beam lines that are available at U.S. facilities are focused on basic science. This makes it very difficult to obtain time, since industrial work is much closer to the application and not typically down at the basic research level.

The drive for cleaner more productive machines in our industry is pushing our materials to new limits. In order to achieve these objectives, a better understanding of the mechanical response of the material at the microstructural scale is needed. This information will be used to increase the accuracy of the durability predictions of our products, which will lead to more efficient machines. The synchrotron provides the spatial resolution and depth of penetration to gain this information to validate and develop these material models. A dedicated beam line will allow industry to implement the models in the design process faster, which leads to increase speed to market for machines and technology, and increases the competitiveness of U.S. companies.

I appreciate your efforts in leading this much needed project.

Sincerely,

Eric Johnson

Eric Johnson
Staff Engineer
Materials Engineering – John Deere

Carnegie Mellon

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July 20, 2011

Professor Matthew Miller
Sibley School of Mechanical and Aerospace Engineering
Cornell University
Ithaca, NY 14853

Dear Matt,

I am writing to express enthusiastic support for the high energy beamline at NSLS-II being proposed by Mark Croft and collaborators. I am a heavy user of APS 1-ID and have helped develop capabilities for mapping crystal orientation fields in polycrystals. I am also currently the chair of the "Scattering – Applied Materials" beam time proposal review panel at the APS and this panel receives many proposals for high energy measurements at, for example, 1-ID and 11-ID beamlines. The oversubscription rate at the APS high energy beamlines appears to get worse with each proposal cycle. There is a clear need for additional capabilities as well as simply more beamlines where the work can be done. It's important to note the diverse origins of this demand: users come from all categories of institution: academic, industrial, the DOE labs, and DOD labs. Much of the work is technologically and application oriented, thus giving a somewhat distinct flavor to the work and distinct potential economic and societal impacts.

Taking the High Energy Diffraction Microscopy (HEDM) microstructure mapping method as an example, it is clear that demand for beam time is going to continue to increase as new capabilities come forth. This technique is essentially a non-destructive version of the standard tool of microstructural science, electron backscatter diffraction (EBSD). There are somewhere around 1500 EBSD systems in use around the world (according to Stuart Wright of TSL, Inc.); there are three existing or under construction beamlines with HEDM mapping capability in the world, to the best of my knowledge. EBSD is done in a scanning electron microscope and is therefore a surface probe; to gain three dimensional information, material must be sectioned away which means destroying the previously measured surface. Thus, no studies of the evolution of a given ensemble or volume of material can be done. Conclusions are based only on statistical inference. Using the penetration power of high energy x-rays, HEDM maps can be done deep inside of bulk materials and responses to stimuli (thermal, mechanical, or other fields) can be tracked directly. Given that the measurements measure parameters that go into computational models of materials response, this tracking ability yields a new and direct method for testing model predictions and generating validated, trusted computational codes. A number of proposed projects aim to tightly integrate modeling with analysis of measurements. Furthermore, HEDM does not require polished surfaces (in contrast to EBSD), so complex near surface microstructures, such as occur at fracture surfaces, can be studied. It is a little frightening to think about the potential demand for these measurements from all sectors of the materials community–academic, industrial, national laboratories, and defense. We already have on-going or nascent collaborations with LANL, LLNL, General Electric, Army Research Laboratory, Wright-Patterson Air Force, Arizona State, two groups at Cornell, and another group at Carnegie Mellon. The list of interested parties will grow rapidly as HEDM capabilities become better known through publications such as the recent Journal of Materials special issue (Lienert, et al, July 2011).

It would appear to be quite foolish to allow a *reduction* in high energy capacity that would occur without this new beamline. The case for going ahead with the project is extremely strong. The APS scientific advisory committee recently came to a similar conclusion in recently giving the scientific case for a high energy upgrade the top priority rating.

Sincerely yours,

Robert M. Suter
Professor of Physics and Materials Science and Engineering

Pratt & Whitney
400 Main Street
East Hartford, CT 06108

Pratt & Whitney
A United Technologies Company

July 22, 2011

NSLS-II Committee:

Pratt & Whitney supports the HEX beamline proposal at NSLS-II. The HEX beamline will have state-of-the-art characterization capabilities, which will help both academic and industrial development of advanced materials for aerospace applications.

Pratt & Whitney is a leader in the development and production of gas turbine and rocket engines for the commercial, military, space, and stationary power markets. Pratt & Whitney is actively developing new alloys and composite materials and is working on new processes to improve the mechanical and thermal properties of these materials. The capability of the proposed beam line is important for our strategy to develop new materials and processes that will enable more efficient engines. In particular, strain field profiling/ mapping of local strain field gradients in non-ambient conditions is essential for understanding the mechanical properties of materials. Strain/phase and microstructure profiling of ceramic coatings on metals at ambient and non-ambient conditions will help drive the development of next-generation coatings for jet engine applications. In addition x-ray imaging techniques will be an important tool to help understand the role of defects and morphology in alloy and composite behavior.

We support the proposal for a beam line facility and we are looking forward to utilizing the facility to help us improve our products.

Dr. Francis R. Preli
Chief Engineer
Materials and Processes Engineering
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Ulrich Lienert, PhD
Physicist

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23 July 2011

Letter in support of a beamline for **high-energy x-ray micro-mapping of materials for advanced energy and structural engineering applications.**

As responsible scientist I have developed the high-energy diffraction microscopy (HEDM) program at the APS 1-ID beamline. Exploiting the outstanding brilliance of high-energy x-rays produced by APS undulators, the characterization of polycrystalline materials is pushed down to the grain and sub-grain length scales. I am convinced that the HEDM program should also in future focus on applications that are only possible at the APS. This necessarily leaves a large and very fruitful area of applications of high energy synchrotron radiation diffraction in materials engineering and science that would not be covered at all, or only insufficiently, within the US. I therefore want to express my strong support for the proposed HEX beamline at the NSLS II. While the capabilities of the proposed HEX beamline and HEDM program are almost completely complementary, I would expect strong synergies between the programs. Scientifically, true multi-lengthscale characterizations from the component to dislocation structure will be feasible by combining experimental results from both beamlines. The capabilities and capacity provided by the proposed HEX beamline are absolutely required for competitiveness to the European community. Second, realization of the HEX beamline will help reaching critical mass to tackle common challenges from the development of custom high-energy detectors to coupling diffraction data and materials modeling.

Sincerely,

(Ulrich Lienert)

Pratt & Whitney
A United Technologies Company

400 Main Street
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Materials & Processes Engineering

July 22, 2011

Mark Croft
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Re: Letter of support for the for the HEX beamline proposal at NSLS-II

Dear Prof. Croft and the NSLS-II Committee:

This letter is intended to express a very strong interest in the HEX beamline proposal at NSLS-II. The HEX beamline as proposed would have stat-of-the-art characterization capabilities which will help both academic and industrial development of new advanced materials for aerospace and general industrial applications.

Pratt & Whitney is a world leading manufacturer of turbine engines and propulsion systems for aerospace and general industrial energy applications. Pratt & Whitney develops and implements advanced materials required for the demanding applications within gas and wind turbine, and liquid fueled rocket engines for the commercial, military, space, and land-based power markets. Development and characterization of new materials, such as metallic alloys, ceramics and CMCs, and organic-based materials and OMC is critical to the continued success and advancement of these power systems.

The capability of the proposed beam line could directly support our quest to develop new materials and processes that will create superior energy and propulsion systems for the future. In particular strain field profiling/ mapping of local strain field gradients in non-ambient (temperature, load, gasses, etc) conditions is essential for understanding of mechanical properties of materials on length scales down to the microns level. Strain/phase and microstructure profiling of ceramic coatings on metals at ambient and non-ambient condition will help drive the design the next generation coatings for jet engine applications. Besides the structural and microstructural information given by X-ray diffraction, using micro-CT would be an excellent tool for the understanding of morphological features of intended phases and potential anomalies, such as voids and inclusions. Characterization of anomalies as a function of material processing or in-service application environment is critical for a more complete understanding of a material's capabilities in various product forms.

Pratt & Whitney
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Materials & Processes Engineering

We would again like to provide note our strong interest in the proposed facilities and capabilities. The resultant capabilities will be truly unique and will enable greater understanding of a wide range of materials. We would very much like to stay involved with this proposal effort and would like to determine how we might interact and utilize these facilities when they become available.

If you would like to review our needs and potential applications, or if you need any other information relative to our interest in your proposed effort, please contact Iuliana Cernatescu at Iuliana.Cernatescu@pw.utc.com or (860)557-2528. We look forward to working further with you on this new center.

Sincerely,

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