

A Proposal submitted to the U.S. Department of Energy

**EXACT BRAGG BACKSCATTERING (EBB)
X-RAY BEAM FACILITY**

*A New Research Capability at the Advanced Photon Source
Argonne National Laboratory*

DOE Program: **LAB 03-03 – Enhanced Research Capabilities at DOE
X-ray and Neutron Facilities**

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Proposal submitted to the US Department of Energy
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EXACT BRAGG BACKSCATTERING X-RAY BEAM FACILITY

A New Research Capability at the Advanced Photon Source

1. Executive Summary

We propose to develop a user facility for exploiting the science based on an exact Bragg backscattering (EBB) x-ray beam at the Advanced Photon Source (APS). The EBB x-ray beam at the APS is unique in the world, in that it diffracts the monochromatic radiation back exactly at 180 degrees through the storage ring to emerge on the opposite side of the storage ring. The concept has been implemented on a test station called the normal incidence diffraction (NID) station. The NID test station, built on Sector 1-ID of the APS, provided an opportunity for developing backscattering techniques, and it showed the potential for forefront science based on the unusual properties of this beam. We now propose to fully exploit the scientific potential of an EBB x-rays with an appropriate end station and experimental equipment for user science. The proposed research program takes advantage of two well-known features of the EBB x-ray beam: a) small energy bandpass (meV) with very high efficiency, and b) very large angular acceptance (mrad). Our successful development of sapphire monochromating crystals provides a large energy range, 5-70 keV, with meV resolution. Sapphire also permits essentially full spectrum coverage by combining an intrinsically high density of available Bragg reflections with temperature dependence.

The planned areas of research are **inelastic x-ray scattering at low energies, coherent imaging, nuclear resonant scattering at high energies, x-ray metrology and high-precision measurements, and x-ray pulse accumulation.** These research programs are based on the unique nature of the EBB beam and would otherwise be difficult or impossible to pursue on conventional beamlines at the APS. The development of the required instruments builds upon the expertise from long-standing research efforts of the SRI-CAT at the APS and other researchers using the APS, ESRF, Spring-8 and HASYLAB.

The proposed backscattering facility would include an experimental station and research instruments. We plan to make use of the existing sector 1-ID straight section, which will be configured to simultaneously serve the existing scientific program on ID-1 beamline by adding a second undulator. The proposal includes a transparent monochromator to deliver EBB beam to the new station without undue interference with the scientific activities on the sector 1-ID beamline. Figures 1 and 2 show how this simultaneous use will be achieved. In addition, the budget request includes a new undulator, tailored to meet the EBB science, and timing electronics, millidegree temperature controllers, a beam tracking and alignment system, goniometers, mirrors, motion controllers, and gated detectors. Since the capability to extract the EBB beam is in place, the investment in the EBB beam facility requested in this proposal will lead to new and unique capabilities at the APS at a cost substantially less than that for a new beamline.

The scientific program at the EBB beam facility is based on the unique characteristics of the EBB x-ray beam and sapphire monochromating crystals, namely, (1) ultra high energy resolution over a broad energy range (5-70 keV), and (2) three orders-of-magnitude increase in the angular acceptance of the monochromator over conventional geometries. The resulting beam has a high intensity (generally greater than 10^{10} photons/second) and a coherence volume that is three orders of magnitude larger than a conventional beamline at the APS. This unique capability has stimulated broad interest in various scientific areas from condensed matter physics to biochemistry and offers opportunities to develop new synchrotron techniques. Indeed, the potential to perform many specialized experiments beyond the capabilities of existing beamlines will enhance many on-going scientific research areas at the APS. We summarize below the proposed scientific program in four areas. A significant user community for an EBB beam facility has been identified and will increase as the impact of the new capabilities is demonstrated. Towards this goal a set of scientific workshops will be organized in each proposed area during the construction period.

1.1. Inelastic X-ray Scattering in the 6-12 keV range

Inelastic x-ray scattering is a powerful tool to investigate collective excitations in condensed matter. Understanding the dynamics of systems is crucial in areas from hard-condensed matter to biological molecules. It is urgent that APS take advantage of a unique opportunity to augment its inelastic x-ray scattering facilities. Currently there is a beamline at the APS used part time for inelastic x-ray scattering with meV resolution, and another beamline (IXS) is under construction to provide meV resolution at 25 keV incident energies and medium energy resolution (100-200 meV) at lower energies. The existing capabilities, however, do not address the need for a facility with high energy resolution ($\Delta E=2-10$ meV) at moderately low energy (6-12 keV), and with large momentum transfer. The EBB facility will provide this capability and complement existing beamlines. This will allow a number of exciting new opportunities to be explored, including:

- a. copper K-edge (8.98 keV) resonant inelastic x-ray scattering experiments to be performed with ~ 20 meV resolution in highly correlated electron systems,
- b. the study of low-Z and organic compounds with high-resolution and with penetration depth matched to the sample, and
- c. the study of phonons with relaxed resolution, which is better suited for the study of weak high-energy modes.

In Section 3.1, we provide several examples of each of these opportunities. The advantage an EBB beam brings is related to the both monochromatization and analysis of the scattered radiation, critical to inelastic scattering research. Current high-resolution monochromators, based on channel-cut crystals with an energy-dispersive geometry, produce the required energy bandpass, but their efficiencies are relatively low, at the 20-30% level. More importantly, there are no analyzers that work in the low energy range (6-12 keV) with the required resolution of ~ 20 meV for resonant inelastic x-ray scattering (RIXS) research and 2-5 meV for nonresonant inelastic x-ray scattering (IXS) research.

Scientific interest in RIXS is growing, and this technique is particularly useful in studying electron excitations in highly correlated electron systems. For example, recent theoretical work on high-temperature superconductors has indicated the existence of a novel, new set of collective electronic excitations in the superconducting state at energy transfers of about 50-100 meV. The electronic excitations can be distinguished from phonon scattering using the RIXS technique. Furthermore, RIXS also provides significant signal enhancement at the level of two orders of magnitude. In Section 3.1.1 the proposed research program is described in more detail.

Another significant advantage of the EBB energy range occurs when small samples of low-Z materials are of interest (e.g., single crystals of superconductors such as MgB_2 , organic conductors, etc.). The EBB x-rays will have a larger scattering cross-section because of its lower energy and excellent energy resolution even at these lower energies due to proposed implementation of novel optics based on sapphire crystals. Such IXS experiments open new doors to investigations, that are otherwise not possible (see Section 3.1.2) such as, (1) studies of fundamental collective excitations in organic conductors, (2) use of the dynamics of protein molecules to extract static structure information on membrane proteins, and (3) a novel suggestion to study electron-hole pair excitations in optically active biopolymers. The EBB beam facility will compliment the ongoing and proposed research effort at the APS in these areas either through improved energy resolution or lower x-ray energy capabilities.

To achieve high resolution at low energy, we propose to use dislocation-free sapphire crystals. For example, the Al_2O_3 (1 2 17) reflection at 9.035 keV has an energy bandpass of 4.6 meV and a reflectivity of 45 % at room temperature. This reflection has an extinction length of 48 microns and an angular acceptance of 2 milliradians. These are to be compared with the best possible reflection from silicon at 9.343 keV, Si (3 3 7) with 18 meV resolution, used in conventional inelastic scattering facilities. We also propose to develop new analyzer optics using sapphire as curved crystal analyzer, which is described in Section 3.2.

1.2. Coherent Imaging

The NID beamline has the longest path length between the undulator source and the sample at the APS (\approx 100-150 m). In the proposed energy range, the transverse coherence length can be as large as 100 x 600 μm in the horizontal and vertical directions, respectively. In addition, the intrinsic high energy resolution of the EBB beam increases the longitudinal coherence by many orders of magnitude. For example, with a resolution of 2 meV at 9 keV, one would expect a longitudinal coherence length of 620 μm . We expect that the resulting three order-of-magnitude increase in coherence volume of the EBB x-rays will open opportunities for exploring new science at the APS.

There are attempts to develop a novel imaging method, a kind of hybrid of microscopy and diffraction, which can reveal the 3D arrangement of atoms of local structures without the need for crystals. The method first records diffraction patterns from finite samples by using coherent x-rays or electrons, and then directly converts the

diffraction patterns to images by using the oversampling phasing method. We plan continued development of atomic resolution 3D x-ray diffraction microscopy. Since x-ray wavelengths are on the order of the size of atoms, scientists have long dreamed of atomic resolution x-ray microscopes that could visualize arrangement of atoms in three dimensions. However, x-rays are much more difficult to focus than electrons. The smallest x-ray focal spot currently achievable is around 30 nm. This limitation can be overcome by using coherent x-ray diffraction and the oversampling method.

1.3. Nuclear Resonant Scattering at High Energies

The availability of bright hard x-rays from undulator sources at the third generation synchrotron radiation facilities along with new high-resolution monochromators has made it possible to develop nuclear resonant scattering into a powerful tool to study lattice vibrations and elastic properties of materials. Since its first demonstration in 1984 using the ^{57}Fe resonance and its subsequent applications to magnetism, electronic structure studies of high spin low-spin transitions, as a function of temperature and pressure, the technique has become even more popular with the development of nuclear resonant inelastic x-ray scattering, NRIXS, in 1995. Thermodynamic properties like vibrational density of states, specific heat, entropy, average force constant, mode specific vibrational amplitudes, Gruneisen constant, and aggregate speed of sound can all be measured in ways that were not even considered possible before. Today, materials containing ^{83}Kr , ^{151}Eu , ^{119}Sn , and ^{161}Dy can be studied. The energy resolution has been reduced to under a millielectronvolt. This, in turn, has enabled new types of measurements like Debye velocity of sound, as well as the study of origins of non-Debye behavior in presence of other low-energy excitations. The effect of atomic disorder on phonon density of states has been studied in detail. The flux increase due to the improved x-ray sources, crystal monochromators, and time-resolved detectors has been exploited for reducing sample sizes to nanograms levels, or using samples with dilute resonant nuclei like myoglobin, or even monolayers. Incorporation of micro-focusing optics to the existing experimental setup enables experiments under high pressure using diamond-anvil cells to investigate nuclear resonant scattering (the Mössbauer effect) with transition energies in the range 6-26 keV. However, there are many higher energy nuclear transitions in the range 26-100 keV in atoms with s-p, d- and f-shell configurations with broad applications in condensed matter physics and materials science. X-rays in this energy range with ultrahigh energy-resolution can be delivered by the EBB x-ray beam facility through proper choice of backscattering crystal reflections. In particular, we plan to apply the well-developed applications of the coherent forward scattering and inelastic nuclear resonant scattering to magnetic and superconducting systems based on d- and f-shell atoms. The microscopic information that can be generated through these studies will be exclusive to the EBB beam facility.

Among the most interesting nuclear resonances to be examined first are ^{61}Ni , ^{129}I , ^{121}Sb , ^{125}Te and ^{237}Np . The nuclear resonance in ^{61}Ni at 67.419 keV presents a challenge to monochromator design and it might be possible to go down to sub-meV resolution with backscattering. Nickel resonance is of great interest from the point-of-view of metalloproteins, as well as from a magnetism perspective. Nickel atoms are

found at the active sites of many enzymes that are critical in biology and with respect to the environment. Among others, these reactions include: H₂ uptake and evolution, which is accomplished by the enzyme hydrogenase (H₂ase), CO oxidation and CO₂ reduction by carbon monoxide dehydrogenase (CODH), acetyl-CoA synthesis and cleavage by a multienzyme complex designated acetyl-CoA decarbonylase/synthase (ACDS), and the last step in methane production by methanogenic bacteria, the reduction of methyl-coenzyme M (CH₃-S-CoM) with coenzyme B (H-S-CoB) by methyl-coenzyme M reductase (MCR). If ⁶¹Ni nuclear resonance vibrational spectroscopy (NRVS or NRIXS) were available, this technique could help solve important issues with these enzymes. Recent work on myoglobin and model porphyrin is elaborated in Section 3.3. The case for ¹²¹Sb resonance at 37 keV is also interesting from the point of view its application to the understanding of modern battery and semiconductor materials. The resonance in ¹²⁹I is at 27.77 keV. The unique potential of nuclear resonance using a synchrotron radiation beam coupled with its sensitivity to local structure, chemical configuration, and dynamics will permit us to address a broad spectrum of problems of current interest in materials such as intercalated nanotubes and organic superconductors. This is presented in Section 3.3.

1.4 X-ray metrology and high precision measurements

This work aims toward determining fundamental physical constants and precise tests of physical theory, an area normally referred to as metrology. This is a new area at any synchrotron facility and can now be exploited because of distinctive capabilities of the EBB beam facility. In x-ray metrology, there are two specific outputs: crystals whose lattice spacing is currently measured with respect to optical standards, and x-ray and gamma-ray wavelengths, which are also calibrated against an optical scale (and hence that of frequency). Using nuclear resonant scattering we have demonstrated our ability to define a wavelength standard to a precision of better than 1 part in 10⁷ at 14.4 keV. The Bragg law simplifies to $\lambda=2d$ with the EBB condition (with a small index-of-refraction correction), and, if the wavelength can be independently determined (using nuclear resonant scattering), one can measure lattice constants with a resolution of 1 part in 10⁸. We have tested this concept by measuring the differing expansion coefficients of Ge single crystals made up of different enriched isotopes of Ge as a function of temperature. Most of the crystal measurements involve nearly perfect large single crystals, but studies can be performed where the single-crystal information can be transferred to standard powder diffraction samples widely used in industrial processes and quality control. In addition, the metrology community would like to replace the artifact kilogram standard with an absolute standard for the Avogadro constant. This involves developing metrological tools to measure x-ray crystal density, an area in which an EBB x-ray beam would have a major impact. The plan is to explore the new area of x-ray metrology at the EBB beam facility in which institutions like NIST (USA), PTB (Germany), CSIRO (Australia), and NRLM (Italy) that specialize in metrology could potentially form a new user community.

The observation of a standing wave between crystals reflecting x-rays at EBB geometry was recently observed. This demonstration could lead to a new class of

experiments in the field of phase-amplitude contrast and phase-sensitive interferometry. The ability to perform phase-contrast imaging using high-energy x-rays will be unique at the EBB facility and will allow us to perform exploratory experiments in this field. The impact is discussed in Section 3.4.

1.5 X-ray pulse accumulation

In the hard x-ray range, the third generation synchrotron radiation facilities are fully meeting expectations by supporting a broad spectrum of scientific research requiring high-brilliance beams. The limitations of these storage-ring-based sources have recently become apparent in the forefront research area of temporal science experiments. Most of these experiments require either x-ray pulses of very high intensity and/or those with subpicosecond duration. Delivering such pulses has limitations that are intrinsic to the physics of the storage rings. In all pump-probe experiments, the pump laser has a repeat frequency of 100 Hz to 1 kHz, which is many of orders of magnitude smaller than bunch frequency in a storage ring. The ideas presented to overcome these limitations are strategic to this section of the proposal and will provide new directions in performing a unique set of time domain experiments in the hard x-ray range, which otherwise would not be possible. The essence of this proposal includes development of a x-ray optical cavity, which would perform x-ray pulse accumulation. As a result the program will generate unique tools for performing a new class of x-ray pulse experiments in various areas of science. While we focus here on the development of techniques and instrumentation for advanced x-ray pulse physics, the research addresses many exciting problems, such as the seeding physics for the conceptualization of the x-ray free-electron laser (FEL), storage and distribution of x-ray pulses from an FEL to different beamlines, dynamical x-ray diffraction at normal incidence, and a Fabry-Perot interferometer in the hard x-ray range.

1.6 Relation to U.S. Department of Energy Programs

The EBB x-ray beam facility is expected to enhance our knowledge of materials at the atomic level and fully capture the capabilities of the APS. The capability will support existing BES programs and nucleate new directions of research and development both at the APS and at the future fourth-generation sources (LCLS and/or ERL).

1.7 Organization and Budget

The EBB x-ray beam facility will operate as part of the group of APS operated beamlines. Since full development of the capabilities of the EBB beam is still emerging, the scientific applications and experiments have to be developed in synergy with the instruments and techniques. An initial compliment of the core research group will consist of APS staff developing the facility and a principal user group that is being formed. The core research group will construct the facility over three years of funding. In the first year after the completion of facility construction, the core research group will commission the facility and perform early experiments. In future years, the core research group will use 25% of the available beam time, the priorities of research being identified through an

internal review process to allocate beam time. The remaining 75% beam time will be allocated to APS users based on the peer-reviewed process established under the General User Program of the APS.

The EBB facility manager will oversee the design and construction of the EBB x-ray beam facility with full support from the high-resolution x-ray scattering group and the APS divisions. The summary of construction cost for the EBB x-ray beam facility is given in Table 1. The break down is provided over the project duration of 3 years, separated between labor and equipment costs. The costs include both APS and ANL overheads distributed per current rates to specific categories.

Table 1. Development costs for the EBB x-ray beam facility at the APS in K\$. Escalation is calculated based on DOE provided rates for various categories.

| | FY 2003 | FY 2004 | FY 2005 |
|----------------------|------------|-------------|-------------|
| Personnel | 149 | 285 | 399 |
| Materials & Services | 125 | 186 | 259 |
| Capital Equipment | 100 | 600 | 350 |
| Indirect Costs | 71 | 170 | 189 |
| Total | 445 | 1241 | 1197 |

2. Properties of Exact Bragg Backscattered X-rays

X-ray diffraction with Bragg angles at *exact* $\pi/2$ from perfect crystals has two unique characteristics: One can obtain the smallest possible energy bandwidth of any Bragg reflection at a given energy, and the angular width of backscattered radiation is three orders of magnitude greater than at ordinary diffraction angles. The backscattering of x-rays *at or near* normal incidence was proposed as a method of monochromatization [1] and analysis of inelastically scattered x-rays from collective excitation in condensed matter, which were later realized [2-8]. However, geometrical separation of incident beam from diffracted beam continues to be problematic for a variety of reasons that are of either practical or principal in nature. In spite of this difficulty, many high-energy-resolution beamlines for performing inelastic x-ray scattering have been proposed or built at the third-generation hard x-ray synchrotron facilities.

The unusual properties of exact Bragg backscattered (EBB) x-rays have many new applications, such as high-precision measurements of radiation wavelengths, crystal lattice constants, thermal expansion coefficients and elastic constants, studies of hyperfine interactions and applications to phonon spectroscopy, use of very large coherent phase space volume, possibilities for x-ray storage cavity, and an x-ray Fabry-Perot resonator. Some of the theoretical and experimental aspects of EBB x-rays were given earlier [9-10]. However, a lack of transparent x-ray source, which could provide EBB at $\pi/2$, hindered further developments of the applications, despite the fact that such a possibility was discussed explicitly for a bending magnet source [11].

Recently, a unique normal incidence diffraction (NID) beamline, based on a transparent undulator source has been commissioned at the Advanced Photon Source (APS) [12], and the use of high-resolution monochromators and semitransparent, time-resolved detectors has allowed more detailed studies of the physics of backreflection [13-16]. It is now known that the multiple-beam diffraction suppresses the reflectivity in the back reflection channel to down to a few percent level for cubic crystals such as silicon [13]. On the other hand, in crystals with symmetry, one can avoid the problems of simultaneous-multiple scattering. (This is usually known as the n-beam case in the dynamical diffraction theory of x-rays). For instance, sapphire, a crystal with a rhombohedral lattice, allows exact Bragg backscattering with high reflectivity for x-rays over a broad spectral range [14]. These characteristics span a broad energy range of the electromagnetic spectrum with $4 < E < 60$ keV.

In this proposal, we discuss the opportunities to develop special applications that would benefit from the unique properties of EBB x-rays. The proposed development will be included in an experiment station at the APS, and we hasten to point out, this would be the only beamline with the capability of EBB x-ray beam in the world. The current test station, the NID at the APS uses the radiation from an undulator, normally delivering x-rays to the beamline in Sector 1-ID. The elevation and plan view of the proposed modification of the present setup is given in Figures 1 and 2. The beamline includes a

high-heat load-monochromator on beamline 1-ID that delivers the monochromatic beam to the backscattering optics. The backscattered x-rays then retrace the incident path through the undulator, travel through the storage ring vacuum chamber to a reverse beam pipe feeding the temporary enclosure NID-X.

The beamline geometry shown in Figures 1 is used to evaluate the feasibility of exact Bragg backscattering. The x-ray beam, after being monochromatized by a pair of cryogenically cooled Si (111) crystal, is incident onto a sapphire, silicon or germanium crystal, which is placed in 1-ID-C or 1-ID-B station to reflect the beam back. The beam incident onto this crystal has an energy width of 1.1 (3.3) eV at 8 (24) keV. This particular arrangement puts an effective vertical angular slit proportional to the angular acceptance (or Darwin width) of the Si (111) crystal at a given energy. In the energy range between 8 and 25 keV, this width is between 36 and 11 μrad . In the horizontal direction, the limiting aperture is the width of the white beam slits in front of the Si (111) monochromator, which is typically kept at 2 or 3 mm. Thus, the angular deviation from exact backscattering is limited to 36 and 10 μrad vertically and 70-100 μrad horizontally in the mentioned energy range. There is no access to the beam between NID-X and 1-ID-B stations, which is enclosed by the storage ring tunnel. The necessary modifications to the magnets and vacuum chamber were carried out as a part of the construction project of the APS, making the undulator source fully transparent to backscattered x-rays. The backscattering sapphire crystal is oriented in the (0 0 1) direction, and mounted in the center of an Euler cradle. A high-resolution monochromator was installed in the NID-X station to perform energy analysis. In all experiments, the temperature of the backscattering crystals has to be stabilized within 5 mK. The layout given in Figure 1 provided a practical way to test several concepts regarding the peak reflectivity of the silicon and sapphire crystals, their energy resolution, and mechanical and thermal stability of x-ray beams over large distances. The length of path traveled by the x-rays from the undulator to the NID-X enclosure is approximately 120 m and represents the longest beamline at the APS. The lengths of other beamlines are limited to 60-70 m.

The reflectivity of a thick, semi-infinite crystal is given by dynamical diffraction theory. The intrinsic reflectivity of sapphire can only be measured if the incident beam has an energy bandpass lower than that of the sapphire reflection being measured. We have used a 1.2 meV-resolution-analyzer at 21.6306 keV to measure the reflectivity and energy width of Al_2O_3 (1 1 45) reflection. The calculated and measured reflectivity is shown in Figure 3. This result demonstrates that reflectivity of sapphire is adequate to perform research applications, and energy widths approaching theoretical values can be attained using perfect sapphire crystals. Further evaluation of this sapphire crystal showed a direct correlation between dislocation density and reflection width [16]. The flux obtained typically at the NID beamline from various sapphire reflections with energy resolution ranging from 2 meV to 35 meV are 2×10^9 photons/s to 10^{11} photons/s, adequate to perform experiments discussed in this proposal.

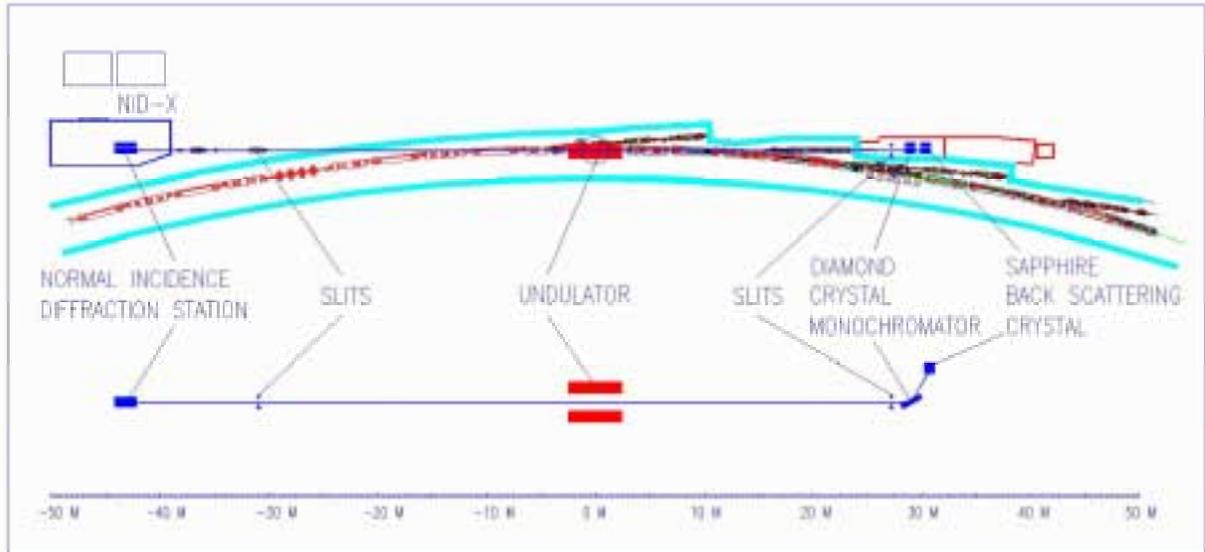


Figure 1. The schematic layout of the proposed exact Bragg backscattering beamline to be placed at Sector 1-ID. The light blue partial circle represents the walls of the storage ring tunnel. The proposed modification allows simultaneous operations with the 1-ID beamline.

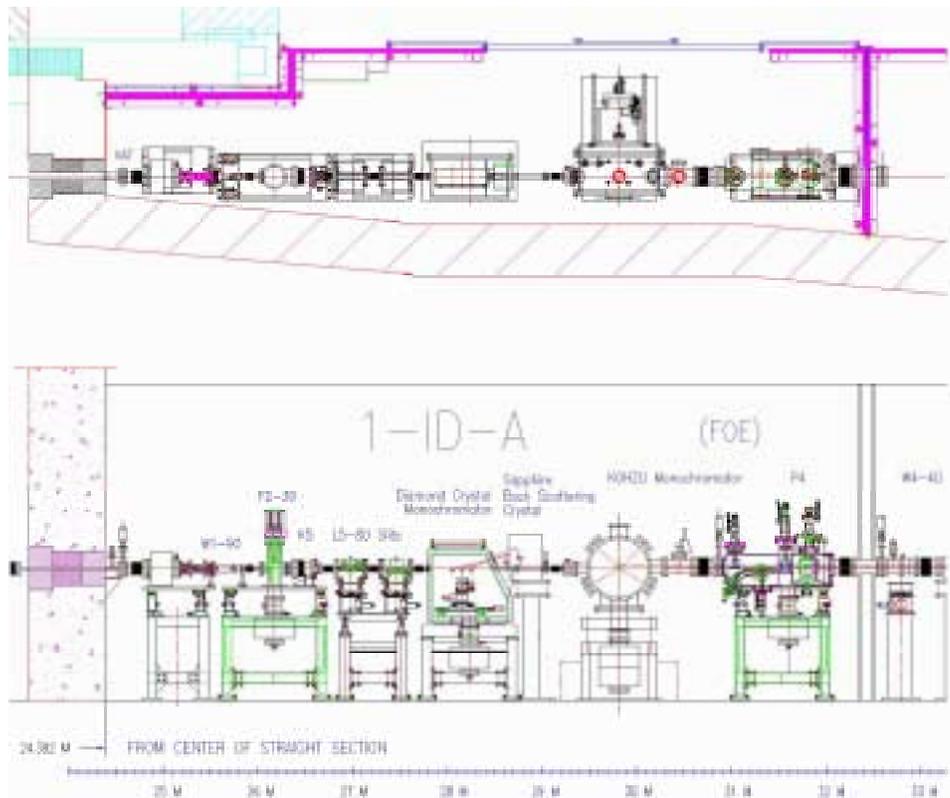


Figure 2. The top and side view of the 1-ID-A side of the proposed beamline. The modifications made involve the white beam (L5-80) slits, diamond crystal monochromator and sapphire back-scattering crystal. The L5-80 slits are ready to install. The diamond crystal monochromator is being acquired as part of the feasibility project and will be available in May 2003.

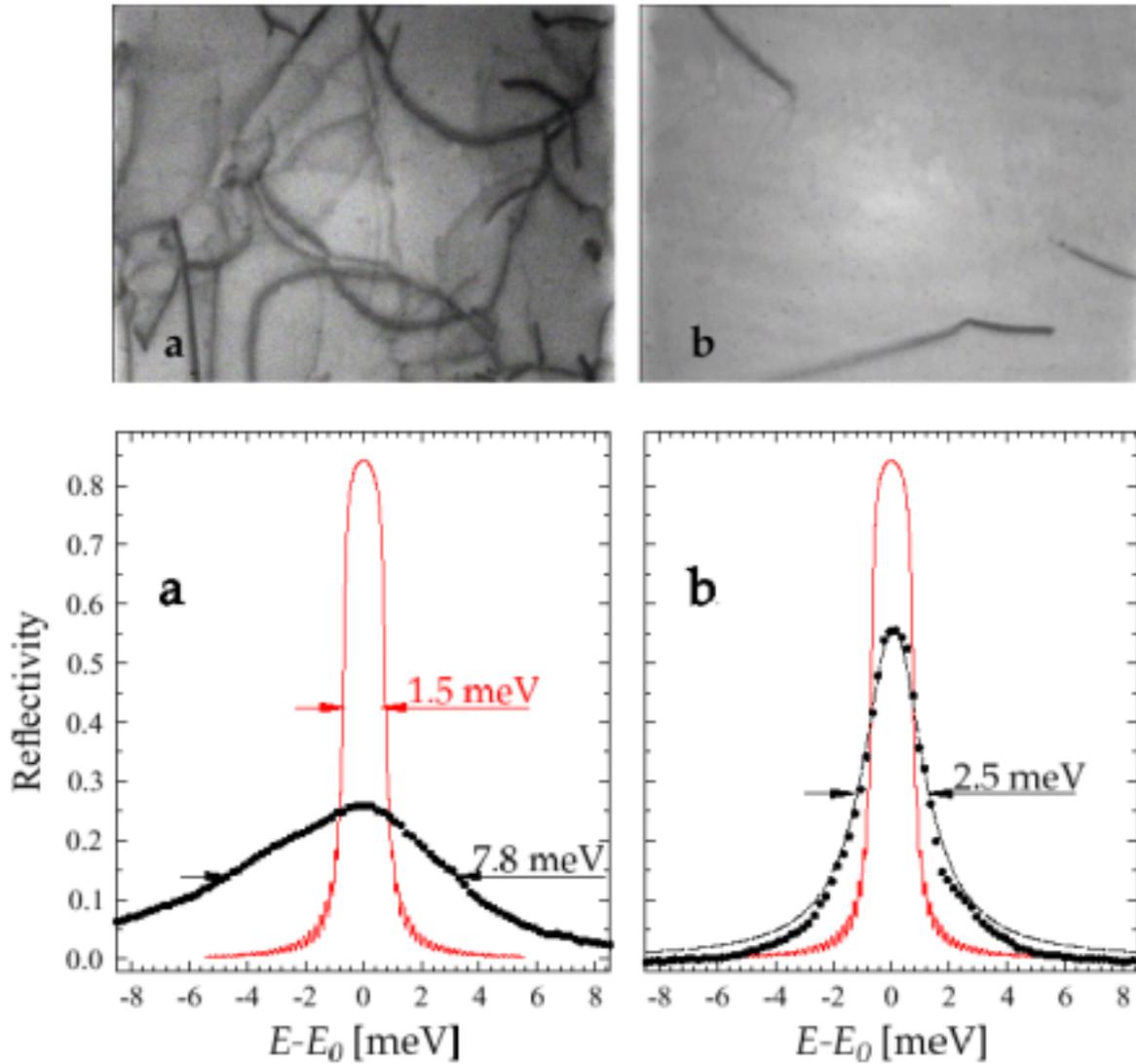


Figure 3. Top: Back-reflection topography of sapphire wafers (grown by heat exchange, HEMEX, method cut from different boules show different dislocation densities: (a) $10^3/\text{cm}^2$, (b) much lower dislocation density. The sample area illuminated by x rays is 2.1 x 1.7 mm. **Bottom:** Reflectivity of sapphire crystals for x rays measured at normal incidence to the sapphire (1 1 -2 45) planes at 21.629 keV. (a) HEMEX standard-dislocation-density sapphire, and (b) HEMEX low-dislocation-density sapphire, circles are measured values; the solid line is the calculated profile from the dynamical theory of diffraction for perfect crystals. The dashed line in (b) is a fit with a Lorentzian [17]. Reflectivity data taken at the APS, topography at HASYLAB.

Another important feature of the EBB beam in the NID-X enclosure is its coherent properties. For the APS low-emittance lattice, the undulator source dimensions are 254 μm horizontally and 12 μm vertically. Using the incoherent source approximation, the coherence lengths for 1 \AA x-rays at the sample located in NID-X is approximately 10 μm x 219 μm . This should be compared with typical number of 3 μm x 66 μm for a 50-m-long source-to-sample distance at a typical APS beamline. The longitudinal coherence is also dramatically more because of the very high degree of monochromaticity of the EBB x-ray beam, $\lambda/\Delta\lambda$ being 10^6 - 10^8 . Assuming $\lambda/\Delta\lambda$ of 10^7 for 1 \AA radiation, the longitudinal coherence length is 1000 μm , making the coherence volume for the EBB beam in the NID-X enclosure to be over $2 \times 10^6 \mu\text{m}^3$. This is at least three orders of magnitude larger than that typically available at most of the beamlines at third generation hard x-ray synchrotron facilities, entirely due to longer distance (a factor of 3^2) and higher monochromaticity (a factor of 10^2 - 10^3).

In short, the EBB x-ray beam in the NID-X enclosure at the APS has very distinctive properties in terms of its collimation, flux, energy bandwidth, and coherence. The current proposal plans to develop x-ray techniques with potential for new applications that would use the exceptional set of capabilities of the EBB x-ray beam. These are explained in Section 3.2.

Table 2. Observed reflections and measured flux at the NID-X station.

| (h k l) | E (keV) | ΔE (meV) | Measured Flux (Hz) | Reflectivity |
|------------------------------------|---------|------------------|----------------------|--------------|
| Si | | | | |
| 7 7 7 | 13.839 | 5.1 | 6×10^9 | 10-20 % |
| 12 4 0 | 14.315 | 6.2 | | |
| 8 8 8 | 15.816 | 4.4 | 5×10^9 | |
| 9 9 9 | 17.793 | 2.0 | 7×10^8 | |
| Al₂O₃ | | | | |
| 0 0 18 | 8.589 | 35.4 | 1.1×10^{11} | |
| 1 0 22 | 10.604 | 2.5 | 1.7×10^{10} | |
| 0 0 30 | 14.310 | 13.5 | 1.6×10^{10} | 60-90% |
| 1 2 29 | 14.399 | 1.7 | 8.5×10^9 | |
| 0 0 36 | 17.716 | 2.8 | 4.8×10^9 | |
| 0 0 42 | 20.045 | 1.8 | 2.5×10^9 | |

3. Scientific Case

The planned areas of research are **inelastic x-ray scattering at low energies, coherent imaging, nuclear resonant scattering at high energies, x-ray metrology and high-precision measurements, and x-ray pulse accumulation**. These areas are chosen based on the unique nature of the EBB beam, research topics that are otherwise would be difficult to pursue for principal or practical reasons using the conventional beamlines at the APS. The required resources and know-how for the development of instruments will be provided from the present expertise at the APS and that of other researchers using the APS, ESRF, Spring-8 and HASYLAB. Preliminary characterization of the EBB beam to evaluate its potential research applications has been performed using the NID beamline in a temporary enclosure. This proposal describes the potential capabilities of the EBB beam as a user facility to perform a unique set of experiments that cannot be performed elsewhere.

3.1 Low-Energy High-Resolution Inelastic X-ray Scattering

This section is organized in two parts. In the first part, the scientific case for resonant and nonresonant inelastic x-ray scattering is discussed (**3.1.1 and 3.1.2**). In the second part, x-ray cross-sections arguments, and the optical reasoning are presented for low-energy, high-resolution inelastic x-ray scattering (**3.1.3**). The technical reasons why the EBB beam is necessary to implement this type of inelastic x-ray scattering is given along with the properties of sapphire and other potential crystals for x-ray optics.

3.1.1 Resonant inelastic x-ray scattering

The important transition metal K-edges required for resonant scattering are precisely in the range 5-12 keV of the EBB beamline. Of tremendous current interest are the cuprates and nickelates. Further, since 20 meV corresponds to energies comparable to thermal temperatures (room temperature is 25 meV), this beamline will allow studies of thermodynamically relevant energy changes in these systems. Resonant inelastic x-ray scattering (RIXS) has already proven to be a valuable technique in the study of highly correlated materials, including the high-temperature superconducting materials and their parent compounds. However, to date all studies have been performed at relatively poor resolution (0.3 – 1 eV). The ability to look at these same materials with resolutions of the order of 20 meV would be a significant advance. Further, since phonons dominate inelastic x-ray scattering spectra in the energy range of interest (10 ~ 100meV), tuning to a resonance to provide contrast between the electronic excitations and the collective lattice dynamics is necessary. A number of obvious experiments present themselves.

Spectral weight changes

When a metal undergoes a transition to the superconducting state, there is a redistribution of the spectral weight. Finite frequency excitations in the normal state are shifted into a delta function at zero frequency in the superconducting state due to the presence of loss-free response. For conventional superconductors, the noticeable changes only occur for frequencies that are less than about 6Δ where Δ is the superconducting gap energy (this is the so-called Ferrel-Glover-Tinkham sum rule). Recently, violations of this rule have been seen in a number of high- T_c superconducting compounds, with especially large effects in the Bi(2223) compound [18]. These measurements imply that there is a large energy in the superconducting pairing which seems to rule out conventional mechanisms such as phonon-based superconductivity.

In the Bi (2223) compound there are significant energy changes at wave numbers of about 500 cm^{-1} , which corresponds to about 60 meV. These changes could be studied with RIXS with an EBB beam. There are several advantages to this technique over the earlier measurements. First, surface quality would not be an issue. Second, the resonant scattering provides site selectivity (to the Cu atoms), which helps in determining the nature of the excitations probed. Third, and perhaps most importantly, we can look at different points in reciprocal space and determine any momentum dependence of the excitations. Finally, direct observation of excitations across the superconducting gap might also be possible.

New excitations

The ability to probe electronic excitations of finite momentum transfer is a unique and extremely valuable feature of RIXS. As an example of the power of this capability, consider the recent gauge field theory of Lee and Nagaosa (cond-mat/0211699) for the cuprate superconductors, which predicts a novel collective mode of order 50-100 meV that couples to x-rays. In normal superconductors, there are collective modes associated with the phase and amplitude of the pairing order parameter. But in the cuprates, which have very strong electron correlation, a new degree of freedom is introduced associated with the hopping matrix element. Predictions have been made that these modes are observable at the (π, π) position by inelastic x-ray scattering. Observation of these modes would be a direct test of these models of cuprate superconductivity. RIXS is, in practice, the only technique capable of studying such an excitation. The resonance effect will allow these electron excitations to be distinguished from phonon scattering and are also expected to provide a significant intensity increase.

A second example comes from Emery and Kivelson's theory of these materials, in which the low-energy charge dynamics of a cuprate superconductor are expected to be incommensurate; that is, the collective charge excitation occurs at a reciprocal space position away from (π, π) , at a wave vector corresponding to the periodicity of the so-

called stripes. Despite large amount of neutron scattering evidence for incommensurate spin fluctuations, the counterpart in the charge sector has been elusive. Recent quasi-elastic x-ray scattering by Lee and Moncton has found the first evidence of correlated charge-density fluctuations in underdoped LSCO (12% Sr) (unpublished). Clearly, studying the momentum dependence of collective charge excitations using RIXS could yield new and important information about high-temperature superconductivity. These experiments will only be possible in a EBB beamline for which the appropriate resolution can be obtained while maintaining the resonance condition.

Nickelates

Nickel systems are also of interest. The layered nickel oxides, such as La_2NiO_4 , are prototypical insulating compounds exhibiting stripe physics. Studying incommensurate charge excitations in these nickelates, in comparison with their metallic cuprate counterparts, could help our understanding of strong electron correlations in these systems.

A second nickel system of note is $\text{NiSe}_x\text{S}_{1-x}$. This is a well-known system that undergoes a metal-insulator transition (MIT) as a function of temperature and doping. It is of interest since it is a relatively simple system whose transition temperature can be tuned by altering the Se content and it does not undergo a structural phase transition along with the MIT. High-quality single crystals are available. Photoemission studies have indicated an opening of a gap in the density of states near the transition for excitations with energies on the order of 30-50 meV. With exact Bragg backscattering and RIXS we would be able to study the momentum dependence of these excitations and how they change at the MIT.

3.1.2 Nonresonant inelastic scattering in low-Z or organic compounds

For low-Z compounds, resonant scattering is not an option and it becomes especially important to match the penetration depth of the radiation to the sample volume. This requires relatively low-energy x-rays for typical samples. Further, in many organics, radiation damage can be a problem. Thus by going to very high resolution one can not only study the interesting physics of the problem, but also ameliorate the radiation damage. Below, we give a few examples experiments well matched to the EBB beamline.

MgB₂ superconductors

Development of this capability will lead to a many demonstration experiments. Here we will present an illustrative example. Superconductivity in magnesium boride (MgB_2) has been observed at temperatures higher than theories predicted. The understanding of phonons in the MgB_2 lattice is critical to describing their coupling to the electrons, which allows them to move in the lattice without any resistance. The phonon measurements have been performed using inelastic neutron scattering on powder

samples [19, 20], and enough information has been gathered to convince us that the modes permit formation of Cooper pairs. A more detailed study of phonon dispersion along various symmetry axes of the crystal requires a single crystal; such studies are hindered by the limited size of available crystals to perform inelastic scattering either using neutrons or high energy x-rays. This is a good example to demonstrate the usefulness of the low energy IXS capability proposed for development. Furthermore, many interesting aspects of superconducting behavior under high pressure can only be performed on small samples suited for the proposed instrument.

Organic conductors

Organic conductors, such as TTF-TCNQ, exhibit many attributes of a 1D metal. The physical properties of 1D metals are very different from the Fermi liquid behavior of 3D metals, and require the novel description of Luttinger liquid theory. In particular, the elementary excitations of a Luttinger liquid are collective charge and spin modes called holons and spinons, respectively, arising from the concept of spin-charge separation. Spectroscopic studies of electronic excitations using IXS and angle resolved photoemission spectroscopy, ARPES, are crucial in elucidating Luttinger liquid physics in these organic conductors. However, the downside of studying organic samples is the radiation damage from the high x-ray flux. For example, at the NSLS bending magnet beamline X22C ($\sim 10^{11}$ ph/s), the charge density wave, CDW, superlattice peak of TTF-TCNQ disappeared within a few hours of exposure. Therefore, to make most efficient use of the data acquisition time, one must maximize the signal by using low-energy radiation to match the penetration depth of organic sample and also by matching the energy resolution to the electronic excitation width. The proposed EBB beamline could uniquely provide the flexibility necessary for an IXS investigation of organic conductors.

Structure and dynamics of membrane proteins

Some 25% of gene sequences in the data bases code for expression of membrane proteins. Although structures for several thousand soluble proteins have been determined, only a handful of structures are known for membrane proteins owing to the difficulties of crystallizing proteins that are naturally stabilized by the hydrophobic environment of their surrounding lipids. Reconstruction of low-resolution electron density maps from scattering data can be obtained from samples in solution, without the need for crystallization. Traditionally, neutron scattering has been a natural way to separate the components of scattering from proteins and lipids by allowing for the use of hydrogen-deuterium contrast variation. However, neutron scattering cannot access high energy transfers at low momentum transfers and has relatively poor q-resolution even for low energy transfers.

Efforts have been made in this direction to use IXS as an alternate route to the separation of the different scattering components. The excitation spectra of lipid bilayers are qualitatively different from those of proteins. In particular the high-frequency peptide backbone bands are not expected to be manifest in the lipid bilayers, which

exhibit rather slow overdamped, or highly damped, propagating sound modes characteristic of a viscous molecular liquid. Thus one can possibly use the high-frequency energy loss/energy gain sidebands of the main elastic scattering peak to distinguish the protein contributions to the total scattering for a sample containing membrane proteins, from those of the lipids. Then a measurement of the form factor would provide the spatial distribution information.

In addition, one is naturally learning about protein dynamics at intermediate length scales. In recent work performed at ESRF, Z. Hasan (Princeton) and collaborators have had some success in extracting information on protein dynamics at intermediate length scales, and an extension of this idea to membrane proteins is underway. This type of work does not require ultra high resolution but would benefit from better flux compared to the existing phonon beamlines. Thus the lower resolution mode of the EBB line, coupled with the lower incident energy would make the EBB beamline an ideal place to perform such studies.

Pair dynamics in optical proteins

A comprehensive understanding of the dynamics of electron-hole pairs in biopolymers is an issue of major significance. Optically sensitive proteins, such as rhodopsins or the photosynthetic unit, exhibit complex delocalization behavior of charge pairs. IXS provides a natural way to study localization/ delocalization of particle-hole pairs. It has been argued that some photosynthetic units consist of light-harvesting complexes that form a quantum-mechanically coherent system. This would be reflected in the momentum-resolved dielectric function or the loss-function. By measuring the length scale associated with these coherent excitations, one can learn about the mechanism of charge/energy transports in these complex systems. The low-energy electronic excitations in insulating complexes appear at some finite energy and are typically broader than phonons. Having a branch line with medium resolution (~ 20 - 40 meV) but with higher flux than typical phonon lines again provides an ideal match to this emerging area of research.

Charge-lattice dynamics at relaxed resolution

Most of the doped Mott insulators as realized in transition metal oxides (cuprates, manganites etc.) exhibit a complex interplay of charge, spin and orbital degrees of freedom with the lattice. Understanding low-energy charge dynamics below 100 meV will allow us to probe the coupling of charge to spin and lattice dynamics. Most of these oxides do not naturally grow as large single-domain crystals making it difficult for studies with neutrons. Another remarkable property is that in many cases only one or two highest optical branches are affected by changes in the electron dynamics typically in the range of 50-90 meV. The ESRF group has reported IXS measurements on cuprates. Further, recent work by Hasan and collaborators and Egami (Tennessee) and collaborators have seen some phonon anomalies in manganites and cuprates, respectively, at beamline 3-ID at the APS (unpublished). These excitations are fairly broad (~ 20 meV) and weak. The study of such lattice dynamics anomalies does

not require ultra high resolution but is hungry for photons. An EBB configuration with a resolution of 10-20 meV would be well matched to the study of these excitations and would help further elucidate the role of the all-important electron-phonon coupling in these materials.

Electron delocalization in bacterial photosystems

The degree of electron delocalization in the light-harvesting complex (LHC) of *Rhodobacter sphaeroides* is unknown but critical to understanding its function. The LHC is a chromophore–protein complex that traverses the plasma membrane and consists of a reaction center (RC) and light-harvesting subcomplexes, LHI and LHII. The function of LHI and LHII is to absorb light and transfer the energy to a RC where it initiates the photocycle of the cell. The quantum efficiency of LHC has been estimated to be ~ 95%, in contrast to silicon photocells whose quantum efficiency cannot exceed 27%. How does LHC achieve such high efficiency?

Both LHI and LHII have circular symmetry (Fig. 4), a property conserved across many bacterial species. Hu [21] have argued that this symmetry suppresses fluorescence losses, enhancing the efficiency of the complex. For Hu's arguments to be valid, the coupling between neighboring chromophores within LHII, V_{chl} , must be large enough to coherently delocalize excited electrons around the entire ring. Attempts to measure delocalization conflict, with results ranging from complete delocalization to only over near neighbors [22]. Experimental estimates of V_{chl} differ from quantum chemistry calculations by a factor of three [23]. With nonresonant IXS, which measures $S(\mathbf{q},\omega)$, it is a straight forward matter to resolve this issue. The light harvesting states of LHII appear at ~ 1.2 eV in $S(\mathbf{q},\omega)$, and their width in \mathbf{k} space, Δk , is related to the quantum coherence length or mean free path $\xi = 2\pi/\Delta k$. Experiments of this sort are ideally matched to the EBB line at APS since they are flux driven, requiring $\sim 10^{11}$ photons/sec, and medium energy resolution ~ 80 meV. The latter requirement comes from the need to discriminate from the elastic line since amorphous specimens diffract strongly everywhere in reciprocal space.

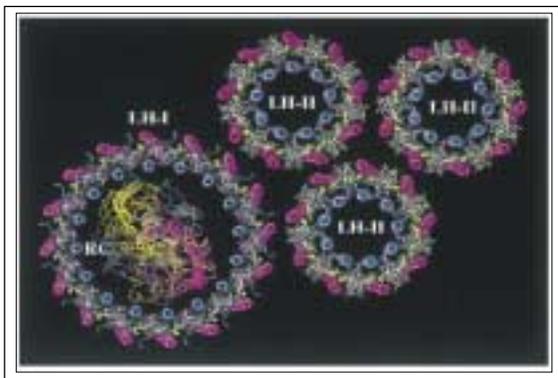


Figure 4 Light-harvesting center from *Rhodobacter sphaeroides* (courtesy of the Theoretical Biophysics Group at the University of Illinois)

Photoisomerization reactions: Bacteriorhodopsin, green fluorescent protein, stilbene

There is a mystery concerning the behavior of the retinal in Bacteriorhodopsin (bR), which bR is another light-harvesting protein that exists in the plasma membrane of halobacteria. It is a 26 kDa transmembrane barrel containing one retinal molecule noncovalently bound (to Lys216) by a protonated Schiff base. In its ground state, the retinal is *all trans* and, upon absorbing a photon, undergoes a photoisomerization to 13-*cis*, initiating a series of structural changes which translocates a proton to periplasm. The resulting potential is used as an energy source for phosphorylation.

Strangely, the properties of the retinal in bR are completely different from free retinal Schiff base (RSB) in solution. *All trans* RSB has an absorption band in the red (1.9 eV) and, when struck with a photon, decays to several photoproducts, 9-, 11- and 13- *cis*, with a combined quantum efficiency of 20%. In bR the retinal absorbs in the green (2.2 eV), where sunlight is maximum, and decays only to 13-*cis* with an efficiency of 60%. Somehow the protein environment tunes the retinal perfectly for its purpose. It is not known how this is accomplished.

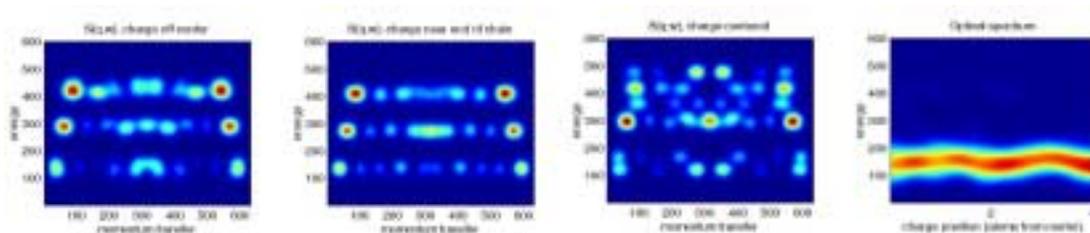


Figure 5 – (first three frames) False color plots of the IXS cross section from a toy model of retinal in the presence of a point charge held at fixed distance and various locations along the chain. (fourth frame) The optical absorption spectrum for many charge locations.

IXS turns out to be extremely sensitive to such environment effects. To see how, consider a model of retinal, represented as a π -bonded chain of sp^2 carbon atoms. The lowest excited states are $\pi \rightarrow \pi^*$ transitions, and environment effects can be represented as a shift in the vacuum level of one carbon atom compared to another. The optical absorption and IXS cross sections for this model in the presence of a point charge held at fixed distance from the chain is shown in Fig. 5. The message to take from Fig. 5 is that environment effects, which produce only slight changes in the optical absorption spectrum of the molecule, can have dramatic effects on the IXS cross section. This is because in quantum mechanics perturbations influence eigenvectors in first order, but *eigenvalues* only in second order. Because IXS couples to the entire eigenvector, it provides a relatively direct measure of the influence of the geometric environment around the molecule.

Similar issues exist for the chromophore in Green fluorescent protein (GFP), other photoactive proteins, and simple model systems, such as olephins like stilbene. The requirements to perform studies like this are similar to studying LHC and so are ideally suited to the EBB FACILITY at the APS.

3.1.3 Special properties of the EBB beam for resonant and nonresonant IXS

At an increasing rate, IXS with very high resolution is used to study collective excitations in solids and liquids at an increasing rate. The number of beamlines performing inelastic scattering at the APS, ESRF, and SPring-8 exemplifies this. At the APS there is a new proposal to build a dedicated beamline (IXS Collaborative Access Team) for this research. However, we are proposing to pursue some aspects of inelastic scattering that no other current beamline intends to do. Scientific applications were discussed in Sections 3.1.1 and 3.1.2. Here, we will explain the details of choice of energy and optics for high-resolution inelastic x-ray scattering at lower energies. First, we will explain the advantage of using x-rays with 8-15 keV for study of collective excitations. Second, we will discuss the choice of optics for RIXS.

The intensity of scattered radiation from phonons can be estimated as follows:

$$I = I_0 \frac{r_e^2 \hbar^2 c^2 (\delta Q)^2}{2eE_i^2} Z^2 \cdot \rho \cdot l_{abs} \frac{k_B T}{M v^2}$$

Here, I_0 is the incident intensity, r_e is the classical electron radius, δQ is the solid angle or the size of the analyzer, ρ is the density of the material, l_{abs} is the absorption length, v is the speed of sound, M is atomic mass, and E_i is the incident energy. When plotted for pure elements at different energies, it becomes clear that there is not a single incident energy optimal for every material, but rather different energies may be optimal for different materials. This is demonstrated in Figure 6, in which three different incident energies are compared for elemental materials as samples. Scattering power per atom near the center of the Brillouin zone where phonon frequencies are very low is estimated at different energies based on the formula given above. This variation of scattering power is mostly related to the absorption length difference below and above the absorption edge of an element [7]. For those elements in the range of $30 < Z < 42$, a spectrometer working at 9 or 14 keV is clearly more efficient than one working at 21 keV. The problem is that there is no Si back-reflection energy with sufficient resolution in this energy range. Figure 7 shows all possible reflections of Si and Al_2O_3 in this energy range. While there are a number of reflections with an energy bandpass of less than 5 meV for Al_2O_3 , one needs to go above 15 keV to reach 5 meV or better, as shown in Figure 8.

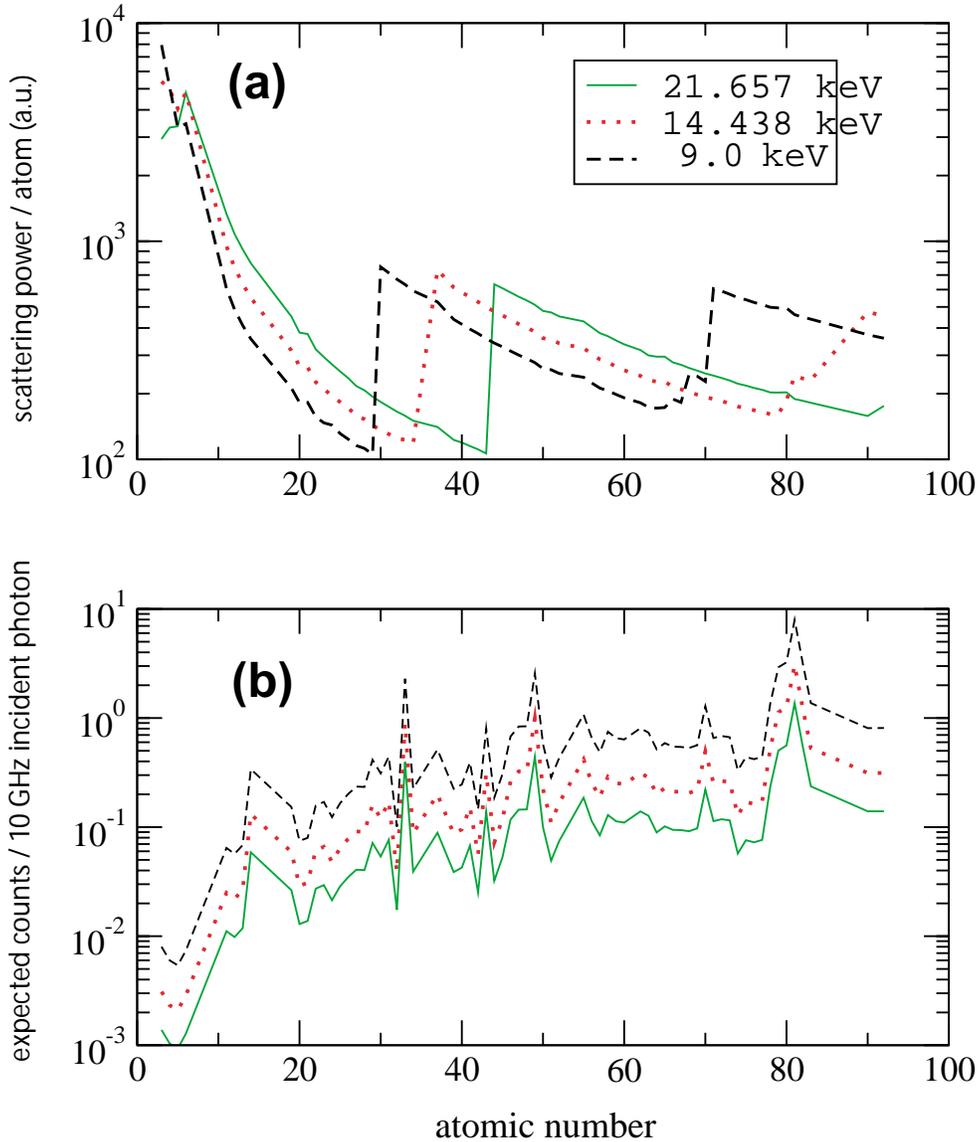


Figure 6. The advantage of having different incident energies for high IXS is shown. (a) The scattering power, which is defined as the scattered intensity per unit volume, is plotted for different elements at two different energies. For elements with $34 < Z < 42$, a spectrometer with 14.4 keV works 5 times better than a spectrometer of 21.657 keV. This variation is mostly related to the absorption length difference below and above the absorption edge of an element [7]. Similarly, for element 30, a spectrometer working at 9 keV is more desirable. This calculation assumes sample thickness is a few absorption length. In reality, an IXS spectrometer can only intercept a small physical source size to obtain high resolution. (b) Assuming a finite thickness (0.1 micron) for each element, expected count rates in the detector are plotted as a function of Z for three different incident photon energies. The irregular nature of the graph is related to differing values of the speed of sound in the equation on p. 22.

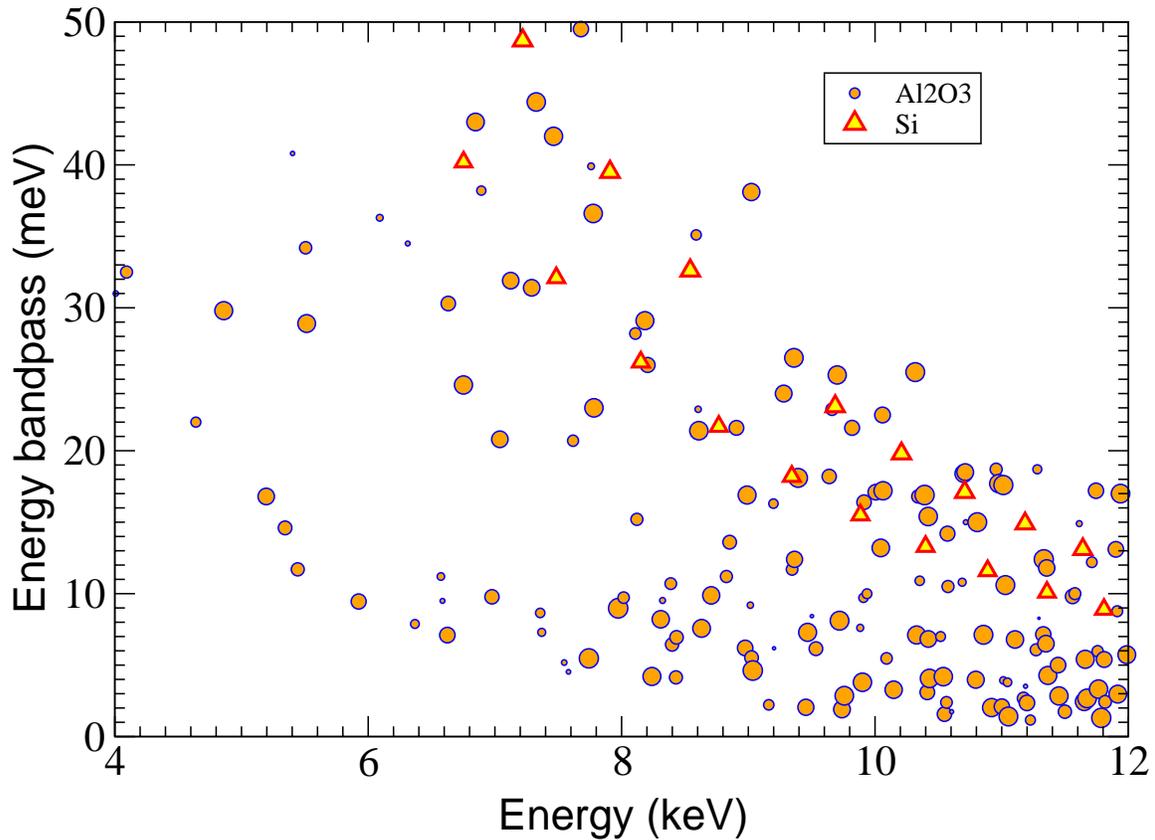


Figure 7. The energy bandpass of sapphire (circles) and silicon (triangles) backreflections in the low-energy region. The size of the circles is proportional to the reflectivity, the larger ones with above 90% and smallest ones above 10%. There are no reflections for Si that will yield better than 10 meV in this energy range, while one can reach 2 meV levels at 9 keV using sapphire.

Optics considerations for resonant inelastic x-ray scattering

What we plan to do at the EBB beamline is to explore ways to overcome the current difficulty encountered in silicon-based optics, which dictates the choice of energy. The method of choice for monochromatization of incident beam varies at each of the beamlines, but the achieved energy resolutions are similar. The instruments at ESRF and SPring-8 use a backscattering Si crystal as a monochromator and as an analyzer and achieve tuning by changing the temperature of the monochromator. The APS spectrometer uses an “in-line” tunable monochromator and a bent Si analyzer to achieve a similar performance. Here, Si backreflection dictates the choice of energy. However, these choices are limited due to the high symmetry and monatomic nature of Si. On the other hand, a crystal like sapphire, Al₂O₃, does not have these restrictions. A comparison of allowable backreflections in silicon and sapphire is shown in Figures 7 and 8.

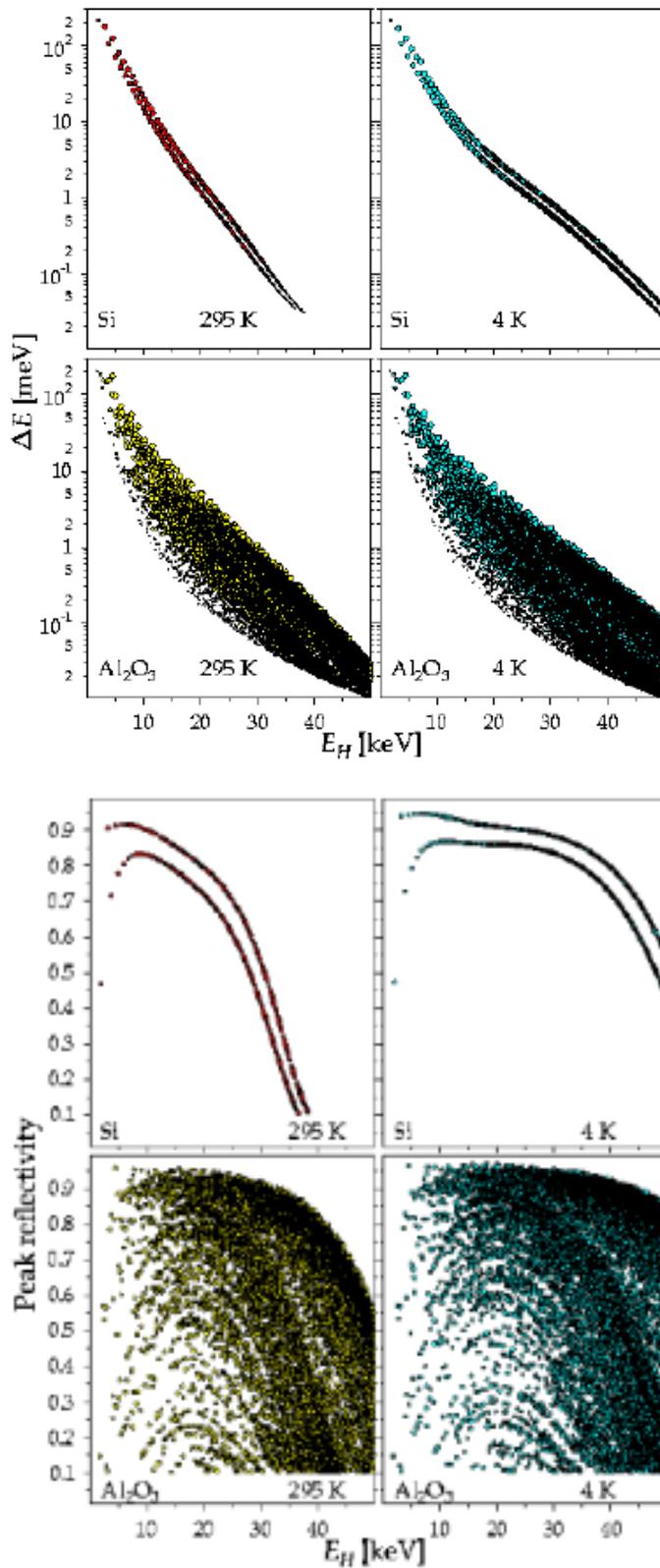


Figure 8. Energy bandpass and peak reflectivity of sapphire and silicon at room temperature and at 4K. The number of possibilities for exact Bragg back reflection can further be enhanced by temperature tuning and mixing sapphire with another oxide. Similar potential exists for $LiNbO_3$, $YAlO_3$, SiO_2 , and many other crystals not considered here [17].

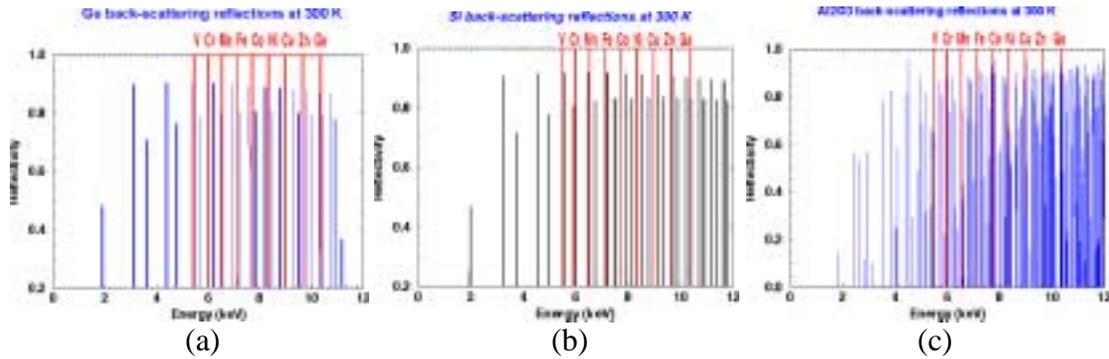


Figure 9. All possible backreflections of Ge, Si, and Al_2O_3 around the transition metal K-absorption edge energies. Clearly crystals like Al_2O_3 provide better alternatives to simpler structures like Ge or Si.

We had mentioned that the method of choice for monochromatization of incident beam varies at each of the beamlines. On the other hand, the preferred method for analyzing the scattered radiation from the sample is uniformly similar, where one uses spherically bent analyzers working very near the normal incidence. This geometry dictates a very narrow energy range. Figure 9 compares possible backreflections of Ge, Si and sapphire as a potential analyzer for transition metal element containing materials like manganites, nickelates and cuprates. Using crystals of lower symmetry like sapphire, YAlO_3 , LiNbO_3 , SiO_2 and SiC , we expect to prepare efficient analyzers RIXS spectroscopy. These investigations are critical for the realization of new opportunities using IXS technique and they will benefit IXS-CAT. In addition, many third generation synchrotron radiation sources with 3 GeV particle energy have peak performance around 5-10 keV, and an IXS spectrometer in this energy range would be very attractive.

3.2 Coherent Beam Imaging

In Section 2, we described the unique coherent properties of the EBB beam from the NID beamline. The large size of both the transverse and longitudinal lengths opens opportunities for exploring new science at the APS. Much of this capability is derived from the fact that the effective distance between the source and the sample is 2-3 times that at any other beamline, and that the EBB geometry provides very high energy resolution.

The transverse and longitudinal coherence for electromagnetic radiation is described by the following:

$$l_{x,y} = \frac{\lambda D}{2\sqrt{\pi}\sigma_{x,y}}, \quad l_z = \frac{\lambda^2}{\Delta\lambda},$$

where λ is the wavelength, $\Delta\lambda$ is the bandpass, D is the total distance traveled between the undulator, back-reflecting crystal and detector in the EBB station, and $\sigma_{x,y}$ is the source size.

It is clear that while the transverse coherence length, $l_{x,y}$ is proportional to the source size, $\sigma_{x,y}$, the longitudinal l_z is proportional to the degree of monochromaticity. For the APS ring, source size is 145 μm horizontally and 23 μm vertically. With a degree of monochromaticity between $\lambda/\Delta\lambda=10^6$ - 10^8 , the coherent volume may exceed $4 \times 10^6 \mu\text{m}^3$, thus providing an opportunity for coherent imaging. While the longitudinal coherence length may exceed a mm, the transverse coherence length is between 20-100 μm and 60-600 μm , in the horizontal and vertical directions, respectively. Table 3 summarizes available coherence lengths and volumes at various energies.

Table 3. Calculated coherence length at different energies for a realistic EBB beamline with a total length of D = 110 m.

| E (keV) | ΔE (meV) | λ (Å) | λ_x (μm) | λ_y (μm) | λ_z (μm) |
|---------|------------------|---------------|-------------------------------|-------------------------------|-------------------------------|
| 5 | 25 | 2.47 | 333 | 53 | 50 |
| 10 | 2 | 1.24 | 166 | 26 | 620 |
| 15 | 2 | 0.83 | 111 | 18 | 465 |
| 20 | 1 | 0.62 | 83 | 13 | 1240 |
| 25 | 0.5 | 0.49 | 66 | 10 | 1960 |

The large coherent volume of the beam allows coherent illumination of larger samples using the EBB beam. In a scattering experiment, the longitudinal coherence length should be larger than the maximum path length difference (PLD) in the sample, which will give an opportunity to perform coherent x-ray diffraction experiments at high x-ray energies.

An unusual application of the large transverse coherence of the beam will be to measure the correlations in a Bose-Einstein condensate [24]. While the experiment is in no way simple, it will give direct information on the density-density correlation.

The observation of a standing wave between crystals reflecting x-rays at EBB geometry has been observed [25]. This is the first inference on a contentious suggestion by Dirac that a photon only interferes with itself. There will be ample opportunity to retest this idea using the EBB x-ray beam. The demonstration can lead to new class of experiments in the field of phase-amplitude contrast experiments [26] and phase-sensitive interferometry [27]. The ability to perform phase-contrast imaging using high-energy x-rays will be unique at the EBB facility and will allow us to perform exploratory experiments in this field.

The main research interests lie in the interplay of physics, nanoscience and biology. We are especially interested in developing new physical methods for quantitatively imaging nanostructured materials, nanoparticles, complex materials and biological structures at the atomic or near atomic level in three dimensions. There are already a few ways of visualizing atomic structure, but each has its limitations. Scanning probe microscopes are limited to imaging atomic structures at the surface. Transmission electron microscopes can resolve individual atoms but only for samples thinner than ~ 30 nm. Crystallography can reveal the globally averaged 3D atomic structure based on the diffraction phenomenon but requires crystals.

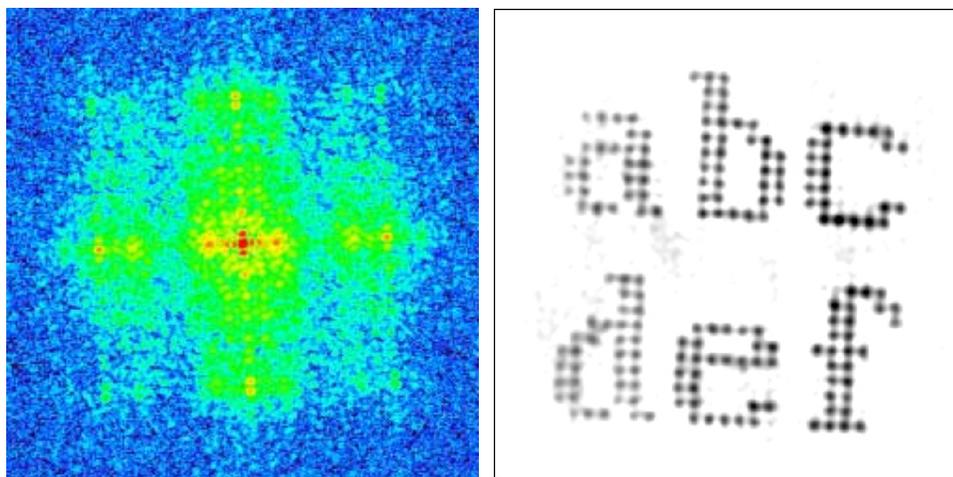


Figure 10. A coherent x-ray diffraction pattern (left) and a reconstructed image (right)

Miao et al (Stanford) have been developing a novel imaging method, a kind of hybrid of microscopy and diffraction, which can in principle reveal the 3D arrangement of atoms of local structures without the need for crystals. The method first records diffraction patterns from finite samples by using coherent x-rays or electrons and then directly converts the diffraction patterns to images by using the oversampling phasing method [28] as shown in figure 10 (a). The theory of the oversampling method can be

briefly summarized as follows. When a finite specimen is illuminated by a coherent wave, the scattered waves form a continuous diffraction pattern in the far field. This continuous diffraction pattern can be sampled at a spacing finer than the Nyquist frequency (i.e., the inverse of the specimen size), which corresponds to surrounding the electron density of the specimen with a no-density region. The higher the sampling frequency, the larger the no-density region. When the no-density region is larger than the electron density region, the phase information is available inside the diffraction pattern itself and can be directly retrieved by using an iterative algorithm.

The seminal experiment of x-ray crystallography without crystals was carried out in 1999 [29]. Since then, we have been continuously improving the method and also pursuing its applications in physics, nanoscience and structural biology. Below we outline several scientific areas we have been working on and plan to continue.

3.2.1 Towards atomic resolution x-ray diffraction microscopy

Due to the fact that x-ray wavelengths are on the order of the size of atoms, scientists have long dreamed of atomic resolution x-ray microscopes that could visualize arrangement of atoms in three dimensions. However, X-rays are much more difficult to focus than electrons. The smallest x-ray focal spot currently achievable is around 30 nm. This limitation can be overcome by using coherent x-ray diffraction and the oversampling method. We have recently carried out an experiment to image a buried nanostructure at 8 nm in two dimensions and 50 nm in three dimensions (Figure 10 (b)) using coherent x-rays [30]. The 2D and 3D imaging resolution is currently limited by the exposure time and the computing power, while the ultimate resolution is limited by the X-ray

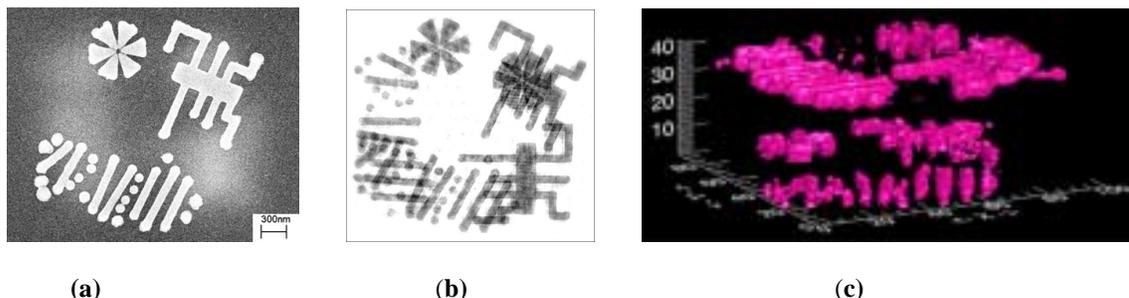


Figure 10 (a) A SEM image of a buried nanostructure. (b) An image obtained from the x-ray diffraction microscope. (c) A 3D image of the nanostructure

wavelengths. Moreover, by calibrating both the incident x-ray flux and the diffraction pattern, we have experimentally demonstrated that the *absolute* electron density of nanostructured materials can be directly determined [31].

We propose to further improve the resolution of this form of microscopy. Specifically, we will attempt to record diffraction patterns at better than 1 nm resolution. We will first determine the 3D electron density of nanostructured particles of MCM-48 (mesoporous materials consisting of 3D platinum rod hexagonal frameworks) as a test example, due to its high-Z materials and scientific importance. Looking forward, we

expect atomic resolution 3D x-ray diffraction microscopy will have a significant impact in condensed matter physics, nanoscience.

This section describes the work of J. Miao (Stanford) regarding coherent imaging. The electron diffraction part does not request support from DOE within the context of this proposal. However, it is included here to explain the connection between the x-ray work and electron diffraction. Electron lens aberration is one of the major barriers limiting the resolution of electron microscopy. The traditional approach to overcome the barrier is to use holography [32]. However, holography not only requires reference waves but also is primarily useful for 2D imaging. We have recently proposed a novel form of 3D electron diffraction microscopy based on coherent electron diffraction and the oversampling method, which requires neither high-resolution electron lenses nor reference waves. By using computer simulation (Figure 11), we have shown that the 3D structure of a nanocrystal can be determined *ab initio* at a resolution of 1 Å from twenty-nine simulated noisy diffraction patterns [33]. The resolution of this form of microscopy, only limited by the quality of sample diffraction, can in principle reach the subatomic level. Figures 12 and 13 provide examples of x-ray images, and tomographic reconstruction.

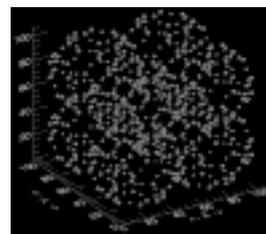


Figure 11. A reconstructed 3D structure of a nanocrystal made of Al, Si and O atoms



Figure 12. *E. coli* bacterium images from the x-ray diffraction microscope. The dense regions inside the bacteria are the distribution of yellow fluorescent proteins labeled with KMnO_4 . The semitransparent regions are devoid of proteins.

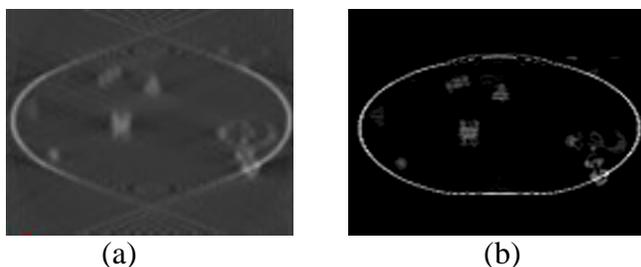


Figure 13 (a) One slice of a 3D artificial vesicle reconstructed from 47 projections using tomography. (the artifacts are due to the limited number of projections). (b) The same slice of the 3D reconstructed vesicle using the oversampling method.

We propose a series of experiments to verify this form of diffraction microscopy, including (i) imaging a gold nanoparticle (~ 3 nm in diameter) at 1 Å resolution in two dimensions, (ii) imaging the nanoparticle at 1 Å resolution in three dimensions, and (iii) imaging a single carbon nanotube at atomic resolution in three dimensions. We anticipate that 3D electron diffraction microscopy will find important applications in physics, nanoscience, and materials science.

3.2.2 Imaging biological cells, cellular structures and viruses using coherent x-rays and electrons

We have recently carried out the first experiment of recording and reconstructing the diffraction pattern from intact *E. coli* bacteria at 30 nm resolution using coherent X-rays [34]. The distribution of proteins inside the bacteria labeled with manganese oxide has been identified and this distribution confirmed by fluorescence microscopy images. By using heavy metal labeling of fluorescently tagged (yellow fluorescent protein and other short peptides) and histidine-tagged protein constructs, we propose to conduct correlated studies of proteins in living cells using fluorescence microscopy followed by high-resolution structural analyses with x-ray diffraction microscopy. To reduce radiation damage and improve the resolution, we plan to use cryogenic technologies to freeze the biological samples at liquid nitrogen temperatures.

Compared with lens-based electron microscopy, electron diffraction microscopy imposes relatively lower sample charging and less sample drift and can achieve better resolution for a given amount of radiation dose [35]. We propose to image cellular structures and viruses using cryoelectron diffraction microscopy, which can achieve better resolution than cryotransmission electron microscopy. Moreover, preliminary studies suggest that the 3D reconstruction using the oversampling method can get better quality images than conventional tomography.

Potential of determining the 3D structure of single biomolecules at or near atomic resolution

X-ray protein crystallography is currently the primary method used for determining the 3D structure of protein molecules at near-atomic or atomic resolution (the other being NMR). However, typically around 20% - 40% of all of the protein molecules, including most of the important membrane proteins, are difficult or impossible to crystallize, and hence their structures have not been accessible by crystallography. Also, NMR has limitations on the size of the molecules that can be structurally characterized. With the prospects of the x-ray free- electron lasers (X-FEL) providing ultrashort and extremely intense coherent pulses, a completely new approach to molecular imaging may become feasible. Theoretical studies showed that when a pulse is short enough, a diffraction

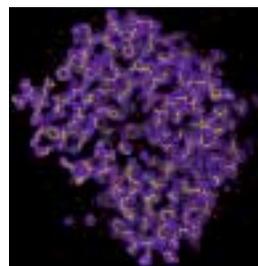


Figure 14. A 3D electron density map of a rubisco protein molecule reconstructed from simulated diffraction patterns.

pattern can be recorded before a molecule is destroyed [36,37]. By using the oversampling method, we have shown that a simulated molecular diffraction pattern at 2.5 Å resolution (Figure 14) accumulated from multiple copies of single rubisco biomolecules each generated by a femtosecond-level X-FEL pulse can be successfully phased and transformed into an accurate electron density map comparable to that obtained by more conventional methods [38].

The experiments proposed here will pave the way for next-generation experiments that can be conducted on X-FEL. Since the first X-FEL will be available around 2008 [39], we hope to begin of imaging nanoparticles and nanoclusters due to their relatively larger scattering cross section. These experiments can then be extended to imaging viruses and single protein molecules. If this project is successful, the impact on molecular biology and a number of other fields where non-crystalline materials play significant roles would be tremendous.

3.3 Nuclear Resonant Scattering at High Energies

The availability of hard x-rays from undulator sources at third generation sources along with high-resolution monochromators has made it possible to investigate nuclear resonant scattering (the Mössbauer effect). In particular, coherent forward scattering and inelastic nuclear resonant scattering have added many new capabilities that were not possible via the traditional Mössbauer effect [40]. Especially applications to samples under extreme conditions like high pressure, low/high temperature, high external magnetic field, confined geometries or tiny samples especially benefit from the outstanding properties of synchrotron radiation.

Besides basic and fundamental research, nuclear resonant scattering applications may be roughly divided into hyperfine spectroscopy and vibrational dynamics. Using hyperfine spectroscopy, poly- and single crystalline samples and amorphous specimens can be investigated by nuclear forward scattering. Surfaces, buried interfaces and multilayers have been investigated using nuclear reflectometry. Single crystal studies have also allowed determination of the electric and magnetic structure by nuclear Bragg diffraction. Magnetic and electric domains, and domains with roughness have been mapped by nuclear small angle scattering. In studying the structural dynamics, the density of phonon states has been probed in amorphous solids and biomolecules by nuclear resonant inelastic x-ray scattering. Nuclear quasi-elastic scattering lends itself to the study of diffusion in the ns time domain.

Currently, the isotopes with nuclear transitions between 6 and 25 keV have been employed in such studies using synchrotron radiation. However, there are many higher energy nuclear transitions in atoms with s-p, d- and f-shell configurations with broad applications in condensed matter physics and material science. In order to extend the energy range, high-resolution monochromators have to be developed. The angular acceptance of higher order Si reflections drop below 1 μ rad levels in the forward scattering geometry (with nested monochromator) making it unsuitable for this application.

We propose to explore EBB geometry, which provides both natural collimation and very high resolution for x-ray beams. Si crystals allow backscattering in a limited region of the x-ray energies with loss of reflectivity at the EBB condition and mostly far from Mössbauer transitions. Furthermore, the Mössbauer transition energies cannot be reached by changing the Si lattice spacing (by heating), the required heating being impractical. On the other hand, sapphire provides lattice reflections at EBB geometry with excellent reflectivity at energy values with about 15 eV intervals in the 10-25 keV range and even closer at higher energies.

We propose to investigate nuclear resonant transitions with energies above the current capabilities of 25 keV using a synchrotron radiation source. A list of potential candidates is given in Table 4 along with the properties of nuclear resonant transitions and sapphire reflections.

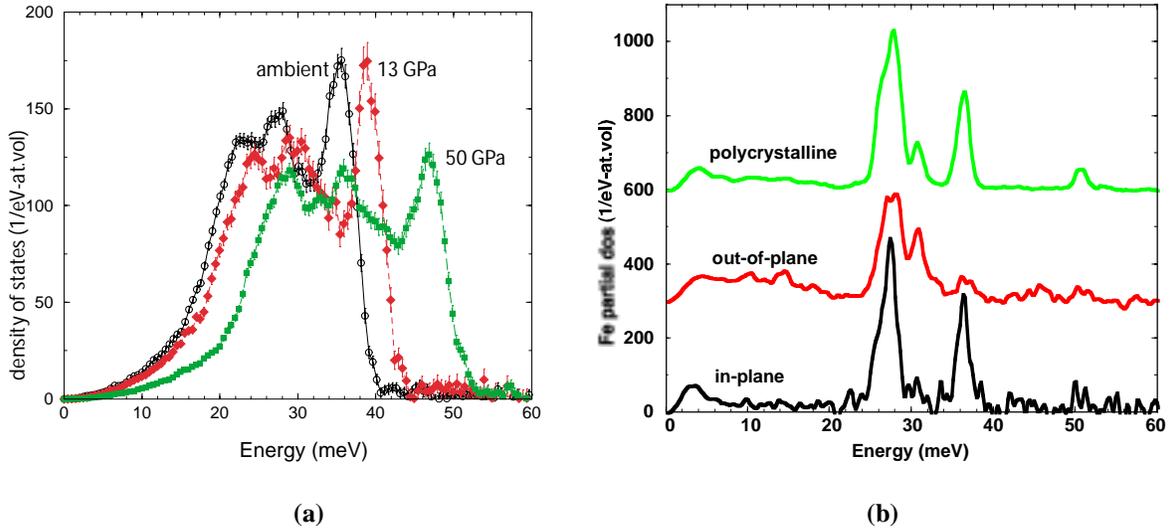


Figure 15. Two recent applications of nuclear resonant inelastic x-ray scattering, NRIXS, to geology, and biophysics: (a) High-pressure density of states of iron in a diamond-anvil cell. Note that there is a structural phase transition between 13 and 20 GPa, during which iron transforms from a body-centered cubic phase to a hexagonal close-packed structure. (b) Fe-partial density of states for [Fe(TPP)(2-MeIm)], (2-methylimidazole) (tetraphenylporphyrinato) iron(II). The single crystal whose porphyrin plane was oriented either parallel or perpendicular to the x-ray propagation axis helped unambiguous identification of in-plane and out-of-plane vibrations.

Table 4. Potential candidates for the study of nuclear resonant scattering studies using EBB capabilities planned to be developed on the NID beamline at the APS. The isotopes that have been highlighted (bold face) will be the focus of this proposal.

| Isotope | Isotopic Abundance (%) | Nuclear Transition Energy (keV) | Half Life (ns) | Transition I_{gd} I_{ex} | Resonant Cross-Section (10^{-20}cm^2) | Al_2O_3 -back reflection (hkil) | Reflectivity |
|-------------------|------------------------|---------------------------------|----------------|------------------------------|--|---|--------------|
| ^{161}Dy | 18.88 | 25.6513 | 28.2 | 5/2 – 5/2 | 95.3 | (5 10 <u>15</u> 34) | 0.92 |
| ^{129}I | 0.0 | 27.77 | 16.8 | 7/2 – 5/2 | 39.0 | (7 13 <u>20</u> 18) | 0.91 |
| ^{40}K | 0.012 | 29.834 | 4.25 | 4 – 3 | 28.7 | (16 5 <u>21</u> <u>16</u>) | 0.88 |
| ^{201}Hg | 13.22 | 32.138 | 0.20 | 3/2 – 1/2 | 0.95 | (5 18 <u>23</u> 14) | 0.89 |
| ^{125}Te | 6.99 | 35.499 | 1.48 | 1/2 – 3/2 | 26.5 | (3 13 <u>16</u> <u>58</u>) | 0.89 |
| ^{189}Os | 16.10 | 36.22 | 0.50 | 3/2 – 1/2 | 1.15 | (7 8 <u>15</u> <u>64</u>) | 0.87 |
| ^{121}Sb | 57.25 | 37.15 | 3.50 | 5/2 – 7/2 | 19.5 | (16 12 <u>28</u> 14) | 0.84 |
| ^{129}Xe | 26.44 | 39.58 | 1.01 | 1/2 – 3/2 | 23.5 | (21 8 <u>29</u> 14) | 0.83 |
| ^{238}U | 99.27 | 44.915 | 0.23 | 0 – 2 | 0.92 | (15 19 <u>34</u> 14) | 0.72 |
| ^{183}W | 14.40 | 46.4837 | 0.18 | 1/2 – 3/2 | 5.52 | (17 17 <u>34</u> <u>30</u>) | 0.64 |
| ^{159}Tb | 100.00 | 57.995 | 0.11 | 3/2 – 5/2 | 10.53 | (20 20 <u>40</u> 54) | 0.20 |
| ^{237}Np | 0.0 | 59.537 | 68.3 | 5/2 – 5/2 | 30.6 | (20 20 <u>40</u> 60) | 0.09 |
| ^{61}Ni | 1.14 | 67.419 | 7.6 | 5/2-3/2 | 70.1 | (0 36 <u>36</u> 84) | 0.32 |

The development of both the coherent forward scattering and inelastic nuclear resonant scattering for each of these isotopes has the potential to initiate new programs in many fields, such as material science, condensed matter physics, chemical physics and environmental science. Two examples are provided in Figure 15, which are related to high-pressure and protein applications. In the present proposal, we intend to pick only a few candidates with an intent to have maximum potential for broad applications. Hence, the highest priority will be given to the study of ^{61}Ni , ^{129}I , ^{125}Te , ^{121}Sb , and ^{237}Np . Table 4 summarizes their characteristics, as well as potential sapphire reflections to be studied.. Selected demonstrations of applications would include study of phonons under high pressure, chemical characterization, diffusion, and lattice and magnetic behavior of correlated electron systems. The community which is currently using the nuclear resonance scattering techniques with Kr, Fe, Sn, and Eu will have to be acquainted with the potential of new resonances, and new users have to be educated and attracted through demonstration experiments and community outreach activities. In strengthening the scientific case for the EBB facility, we will present below a small set currently conceived demonstration experiments using various nuclear resonances in a few selected areas.

3.3.1 Advanced electrode materials

The interest in portable power is ever increasing, with demand for batteries in a wide variety of transportable electronic applications. Advanced lithium rechargeable batteries have taken center stage because of their portability. There is major research effort on lithium electrode materials because of the low electronegativity and high electron/atom ratio for lithium. The enhancements in lithium battery performance are hindered by limitations in the electrode materials. Improvements of the electrode materials demand higher capacity for lithium uptake, higher lithium diffusivity, and greater chemical and structural stability. While a whole class of tools is being used in the development and characterization of electrode materials, nuclear resonance scattering offers some unique capabilities for *in situ* investigation of chemical behavior of electrode materials. With this goal, we have selected two classes of electrode materials that have drawn great attention during recent years, viz., intermetallic compounds [41] and nickelates [42]

Intermetallic Electrodes

In recent years there has been a renewed interest in intermetallic negative electrodes as alternatives to graphite for lithium-ion batteries because of the inherent safety hazards of those carbon-based cells, particularly when subject to abuse or overcharge. The choice of new materials includes ternary systems in which a strong structural relationship exists between a parent binary intermetallic electrode, AB, in which A and B are different metal atoms, and a lithiated LiAB product [43].

Studies of the copper-antimonide system, notably Cu_2Sb , have shown significantly superior electrochemical properties. The excellent cycling behavior of these cells is shown in Figure 16, in which it can be seen that, after one conditioning cycle, the Cu_2Sb electrode provides a steady rechargeable capacity of approximately 300 mAh/g;

this practical specific capacity compares favorably with the theoretical capacity of graphite (372 mAh/g). With respect to volumetric capacity, the Cu₂Sb electrode provides 1914 mAh/ml (based on an average electrode density of 6.6 g/ml), which is significantly superior to the theoretical volumetric capacity of graphite (818 mAh/ml). *In situ* x-ray diffraction data obtained during the operation of Li/ Cu₂Sb cells have provided structural information about the reaction mechanism that occurs at the Cu₂Sb electrode (Fig. 17).

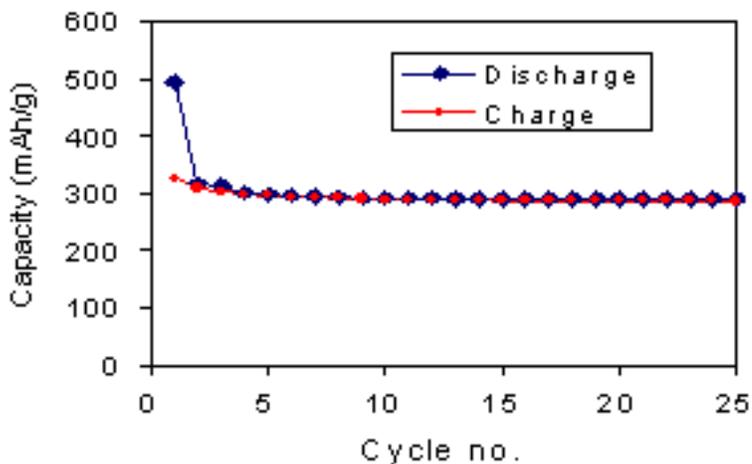


Figure 16. Plot of capacity vs. cycle number for a Li/Cu₂Sb cell.

In situ x-ray diffraction data obtained during the operation of Li/ Cu₂Sb cells have provided structural information about the reaction mechanism that occurs at the Cu₂Sb electrode (Fig. 17). Analysis of the data has shown that lithium is inserted into Cu₂Sb with a concomitant extrusion of copper, which initiates a phase transition to a lithiated zinc-blend-type structure, Li_xCu_{2-y}Sb for 0 < x ≤ 2 and 0 ≤ y ≤ 1, yielding Li₂CuSb at x=2, y=1. Further lithiation results in displacement of the remaining copper to yield Li_{2+z}Cu_{1-z}Sb compositions (0 < z ≤ 1) with the end member Li₃Sb [43].

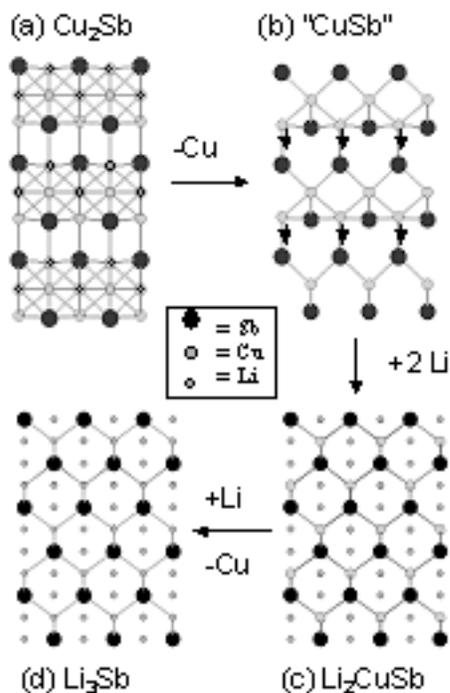


Figure 17. Schematic illustrations of the structures formed during the electrochemical transformation of the Cu_2Sb to Li_3Sb : (a) Cu_2Sb [010] projection, (b) A CuSb component of Cu_2Sb , (c) Li_2CuSb [110] projection, and (d) Li_3Sb [110] projection [43].

The excellent electrochemical performance obtained from Cu_2Sb electrodes is attributed to the retention of a face-centered cubic Sb array throughout discharge and charge, despite a 42% expansion/contraction of the array that occurs during electrochemical cycling. Other factors that contribute to the good electrochemical properties of Cu_2Sb electrodes are the fast diffusion of both lithium and copper within the Sb array and the apparent lack of exaggerated crystal growth of the extruded copper.

There is a whole class of questions, however, concerning the chemical processes responsible for the performance of the battery electrodes. For example, how is the charge neutrality maintained in the cell? What are the electronic charge distributions in the cell? How does the antimony structure remain stable through the charge-discharge cycle? Are there phase transitions and major changes in the atomic dynamics as the structures change?

The proposed development of high resolution optics for nuclear resonance in ^{121}Sb would allow us to address some of the above questions. For example, it is easy to evaluate the Sb charge state, its local symmetry and phonon dynamics from elastic and inelastic nuclear resonance measurements. *In situ* measurements will give us insight into the phase transitions in these interesting electrode material.

Role of nickel oxide based anode and cathode materials

Lithium-ion battery systems, based on the use of layered $\text{LiNi}_{0.8}\text{Co}_{0.2}\text{O}_2$ as the positive electrode material, have high energy density compared with other secondary batteries. However, this cathode material exhibits significant capacity fade because of its high surface reactivity with the nonaqueous electrolytes, which affects the ability to cycle [44]. It is speculated that the displaced divalent nickel causes rapid capacity fade by blocking the path for lithium ions, preventing them from shuttling into and out of the cathode and resulting in a corresponding large, irreversible capacity loss. Alternatively, a new layered material, based on $\text{LiNi}_{1-x}\text{Ti}_x\text{O}_2$, with titanium substitution is considered to be an excellent cathode. Figure 18 shows the cycle performance of $\text{LiNi}_{0.95}\text{Ti}_{0.05}\text{O}_2$.

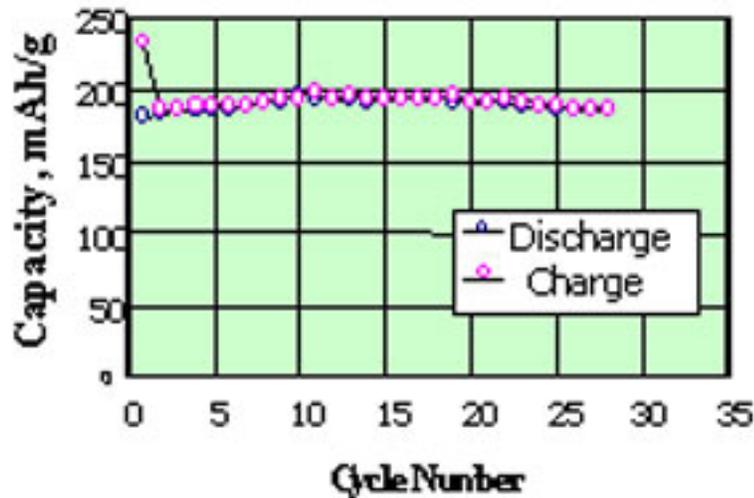


Figure 18. Capacity as a function of cycles for a cell with $\text{LiNi}_{0.95}\text{Ti}_{0.05}\text{O}_2$ cathode material [45].

The material exhibits high capacity densities (almost 200 mAh/g) and outstanding cycleability, with no fade for almost 30 cycles. The success of this material as compared to $\text{LiNi}_{0.8}\text{Co}_{0.2}\text{O}_2$ is associated with nickel ions that keep the lithium channels open.

While the structure of these oxides consists of NiO_2 slabs made of edge-sharing NiO_6 octahedra, the charge balance requires Ni atoms to have different valence states. The microscopic nature of chemical balance in these materials is governed by valence on nickel atoms and could be both 2+ and 3+. Evaluation of the valence can be performed in situ as the battery is charge cycled using the nuclear resonance of ^{61}Ni . We expect such measurements to make a major contribution in developing electrode materials with improved composition.

In addition, one expects Jahn-Teller distortion of the $\text{Ni}^{\text{III}}\text{O}_6$ octahedra with Ni in the low-spin state. While there is no evidence for cooperative Jahn-Teller distortion of the lattice, locally NiO_6 octahedra are distorted [44]. The ^{61}Ni nuclear resonant scattering will provide direct evidence for such distortions and provide diagnostics for the absence of such material distortion expected in materials where Ni atoms are partially replaced by Co or Ti atoms.

3.3.2 Chemical and dynamic structure of iodine chains in carbon nanotubes

Single-walled carbon nanotubes (SWNTs) have been doped with a variety of atoms and molecules to change their electrical properties [46,47]. High-resolution electron microscopy has revealed that the iodine in SWNTs forms helical polyiodide [48]. In Fig. 19, the structural model for the iodine chains intercalated in SWNTs based on high-resolution electron microscopy is shown. This observation has been corroborated by Raman scattering work[49]; however, the behavior under pressure suggests that the iodine chains might reside both in the interstitial channels and inside the pores of the SWNTs.

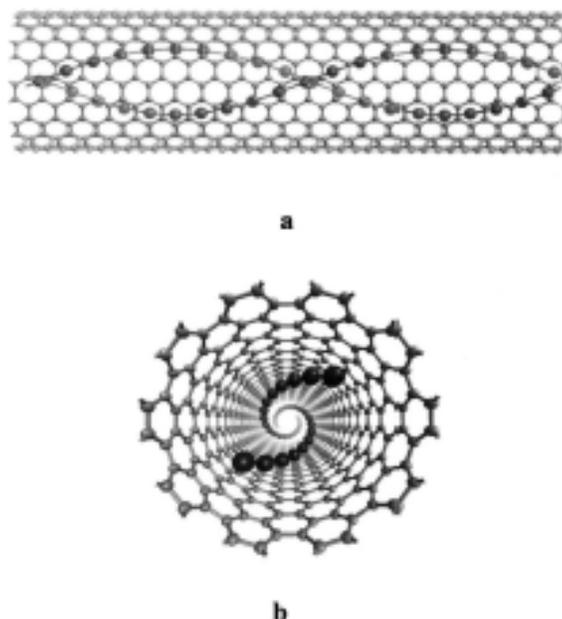


Figure 19. Structural model of I-SWANT based on high-resolution electron microscopy. The figures show the (a) sideview and the (b) top view of the 5 nm helical polyiodide chain in SWNT.

There are many questions still to be addressed regarding the chemical nature of iodine atoms in I-SWNTs. What is the intercalation mechanism? Is there a charge transfer between SWNT walls and the end atoms in a chain? What is the charge on iodine in the chain? Are the iodine chains residing in the interstitial channels different in structure from those occupying the pores? How does the confinement of iodine chain influence its dynamics?

The resolution of nuclear resonance of ^{129}I would permit us to investigate the local symmetries of iodine atoms and their phonon dynamics. A close comparison of these measurements with accumulated data should give us an opportunity to address some of the above questions.

3.3.3 Extraordinary magnetoresistance (EMR) in inhomogeneous semiconductors

Materials that have a large magnetoresistance are useful in a wide variety of applications, and have drawn major research interest. The best examples are the “giant magnetoresistance materials” (GMR), which exhibit 25% increase in resistance at 50 Gauss, and “colossal magnetoresistance materials” (CMR) that show 100000% increase in resistance at 6 T (at 77K). Recently, extraordinary magnetoresistance or EMR as large as 100% has been demonstrated in a nonmagnetic narrow-gap semiconductor ($\mu_e \sim 10^5$ cm²/Vs) with an embedded metallic inhomogeneity. The metal in a semiconductor acts as a short circuit, with most of the applied current passing through the metallic “inhomogeneity” in a zero magnetic field. However in large fields, $H > 1/m$ (where m is the carrier), the current is constrained to flow around the metallic inhomogeneity and the metallic inhomogeneity acts as an open circuit, and the total resistance becomes very high.

The magnetoresistance in a solid material depends on its intrinsic physical properties (carrier density and carrier mobility) and, in EMR materials, on its geometric properties (the shape of the solid and the shape metallic inhomogeneities, if any). Usually, the physical properties dominate the behavior, but metallic inclusions can add to the magnetoresistance through the geometric properties, which are dominant in EMR materials. The classic examples of EMR materials are InSb and Hg_xCd_{1-x}Te [50-52].

The electronic and dynamical behavior of the transition from metallic to non-metallic state in EMR materials are of primary interest with a view to understanding the interaction between physical and geometrical contributions. It is expected that the ¹²¹Sb and ¹²⁵Te nuclear resonances will provide characteristic information on the electronic properties and phonon properties, when the tools are well developed.

3.3.4 The biochemical case for ⁶¹Ni nuclear vibrational resonance spectroscopy

Nickel atoms are found at the active sites of many enzymes that are critical in biology and with respect to the environment. Among others, these reactions include:

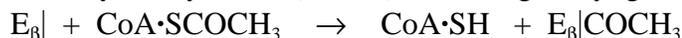
(1) H₂ uptake and evolution is accomplished by the enzyme hydrogenase (H₂ase) [53] :



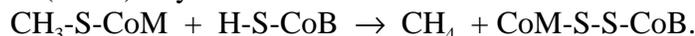
(2) CO oxidation and CO₂ reduction by carbon monoxide dehydrogenase (CODH) [54]:



(3) acetyl-CoA synthesis and cleavage by a multienzyme complex designated acetyl-CoA decarbonylase/synthase (ACDS), including acetyl group transfer [55]:



(4) the last step in methane production by methanogenic bacteria – the reduction of methyl-coenzyme M (CH₃-S-CoM) with coenzyme B (H-S-CoB) by methyl-coenzyme M reductase (MCR) to yield methane :



The first three enzyme active sites contain combinations of Fe and Ni (Figure 20). These are referred to as the “Ni-Fe cluster” of hydrogenase, the ‘C-cluster’ of CODH, and the ‘A-cluster’ of ACDS. The last reaction is catalyzed by an unusual mononuclear Ni in a reduced porphyrin ring. Although x-ray diffraction has provided crystal structures of all of these sites, questions remain about the catalytic mechanisms. The key intermediates often cannot be crystallized or only occur as modest fractions of the total sample.

If ^{61}Ni nuclear resonance vibrational spectroscopy (NRVS) were available, this technique could help solve important issues regarding these enzymes. Below we list just a few of the biochemical questions and how ^{61}Ni NRVS would help resolve them.

- (1) Does a hydride bridge occur between Ni and Fe in form C of the Ni-Fe cluster ?
 - observation of Ni-H and Ni-D bend frequencies
- (2) Does CO bind at Ni and/or Fe in reactive intermediate of the C-cluster ?
 - observation of Ni-C stretching frequency
- (3) Does a Ni-CH₃ bond form at the A-cluster ?
 - observation of Ni-C stretching frequency
- (4) Is reductive activation of MCR Ni-centered Ni(II) → Ni(I), ligand-centered, or both?
 - the Ni-centered vibrational spectrum would contribute to the answer

Apart from the NRVS spectrum, access to ^{61}Ni Mössbauer data on these samples would help in the electronic characterization of the Ni sites. Because the radioactive sources for ^{61}Ni Mössbauer are short half-life ^{61}CO (99 m) and ^{61}Cu (3.3 h) isotopes, time-domain Mössbauer using quantum beats might be an attractive alternative.

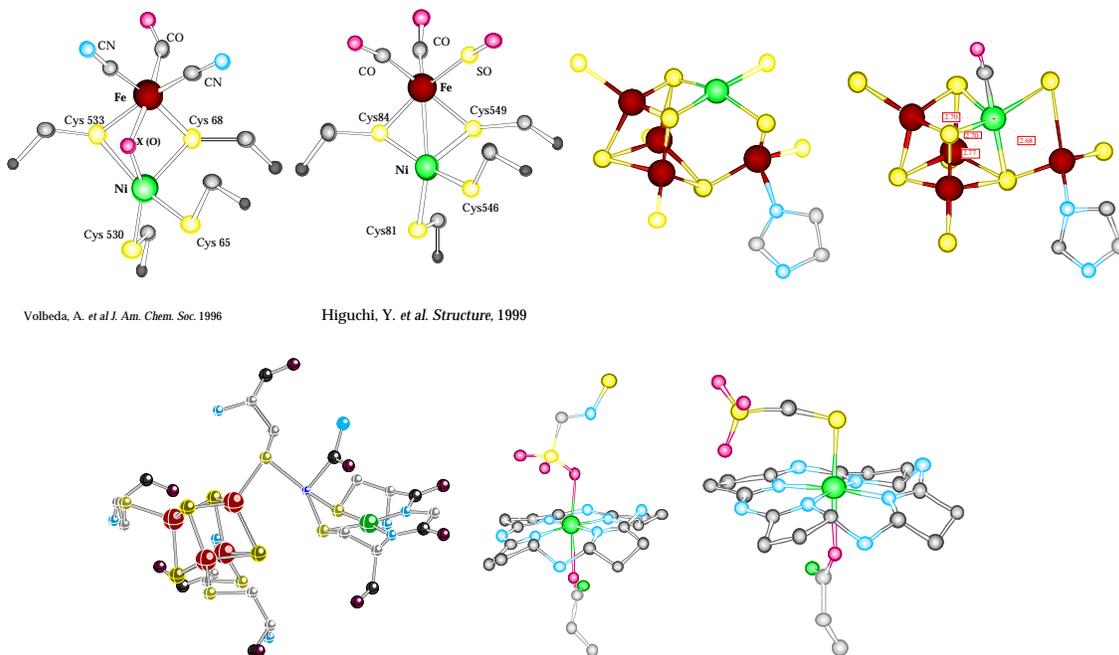


Figure 20. Top-left: Ball-and-stick figures of form A and reduced Ni-Fe cluster. Top-right: Bottom-left: A proposed structure for the A-cluster [56]. Bottom-right: MCR_{silent} and MCR_{ox1-silent} forms of the MCR enzyme.

3.4 X-ray metrology: Mass and Wavelength Standards, Isotopic Dependence of Lattice Constants

The path to x-ray wavelength standards in the metrology world has been through the use of visible wavelength standards. In 1973, Desaltes and Henins [57] published the definitive work on x-ray and visible wavelength ratios to establish the robust connection between these two disparate spectral regions. The use of combined x-ray and optical interferometry was the key to this approach. Recently, using nuclear resonant scattering (the Mössbauer effect) of ^{57}Fe , a new approach for x-ray wavelength standard was presented [58] from the APS. In this methodology the lattice constant of silicon is treated as a “constant of nature”, which is well accepted by the metrology community [59]. The accuracy in the measurement of the wavelength of this Mössbauer transition (86.02547×10^{-12} m) is true to a part in 10^7 . The technique has been recently applied to other radiation wavelengths based on nuclear resonant transitions using the EBB x-ray beam discussed in Section 3.2. [60]

Measurement of lattice constants with ultrahigh precision is fundamental to many properties of solid state. It focuses on defining the equation of state from such measurements as a function of temperature or pressure. The Bragg law simplifies to $\lambda=2d$ with the EBB condition, and, if the wavelength can be independently determined as discussed above (using nuclear resonant scattering), one can measure lattice constants with an unprecedented resolution of 1 part in 10^8 , only limited by the resolution of an analyzer. We have tested this concept by measuring the differing expansion coefficients of Ge single crystals made up of four different pure isotopes as a function of temperature [61] as shown Fig. 21. The data are taken at 14.4 keV using the NID station in backscattering geometry.

The measurement of differences in the lattice constants of different isotopes has implications both in the basic and applied sciences. The relative contribution of zero-point energy to interatomic distance can be evaluated, and the degree of anharmonicity in the interatomic forces can be measured. In addition, the role of strain in electronic band structure modification (also known as band-structure engineering) in device design relies heavily on the accurate knowledge of interatomic distance and its temperature dependence. Finally, the anomalous behavior of negative thermal expansion coefficient at low temperatures, which is related to negative phonon softening of transverse modes can be better understood if accurate information is available from pure isotopes. The interatomic potential like Stelling-Weber or *ab initio* methods like density functional theory can be tested only in presence of correct, precise and accurate data. Given the role of semiconductors in our modern technology, we believe that this is going to be an important application area for the EBB beamline. The potential for this type of work, both for metrology applications and in condensed matter physics investigations, is only limited by our imagination, and we expect to build a strong community around this unique capability of the EBB beam facility.

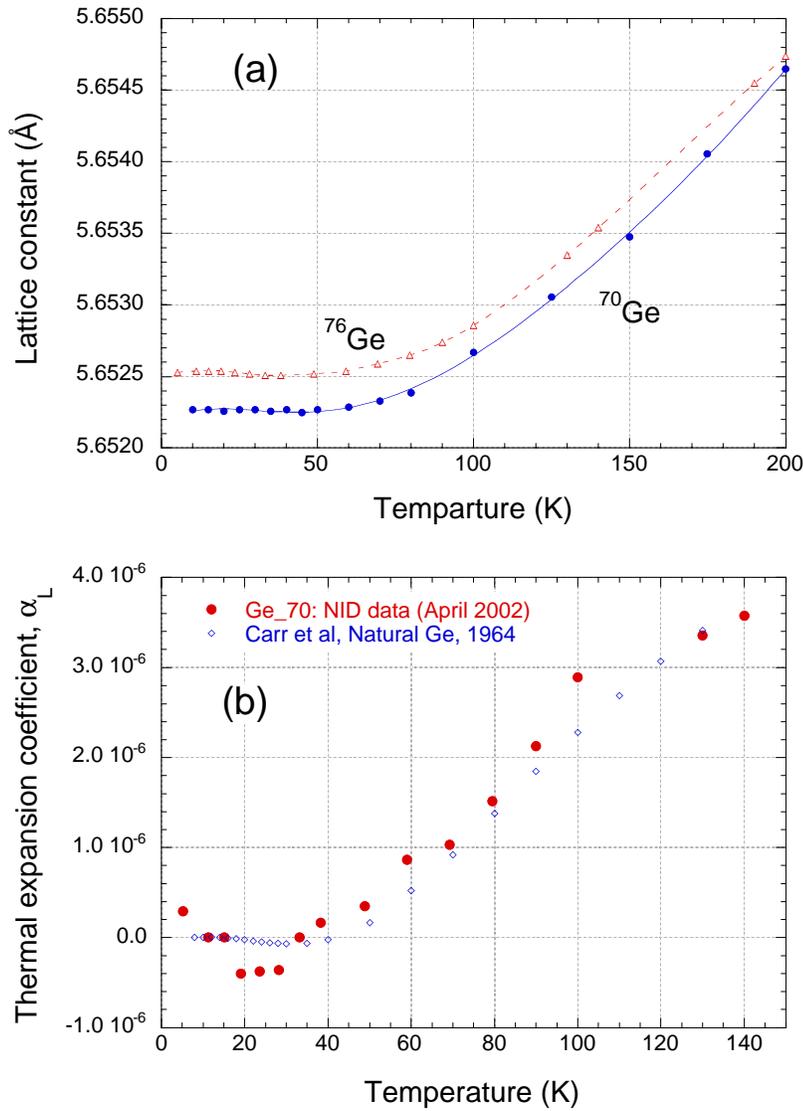


Figure 21. (a) The lattice constants of two different Ge isotopes as a function of temperature measured in the NID-X station with exact Bragg backscattering conditions measured using Ge (12 4 4) reflection at 14.536 keV with 5 meV resolution. Note that thermal expansion coefficient becomes negative below 40 K. (b) Comparison of thermal expansion coefficients obtained from isotopically pure ^{70}Ge and natural Ge. The data on natural Germanium (a mixture of Ge 70, 72, 73, 74 and 76) using the capacitance bridge technique is due to Carr et al. [62]. The latter data, however, was susceptible to experimental difficulties associated with pinholes forming on the silver coatings, and it would be difficult to perform on isotopically pure crystals with dimensions of a few millimeters, since it may require crystals as long as 10 cm.

In addition, an active group in the metrology community aims to replace the artifact kilogram standard with an absolute standard based on Avogadro constant, N_A , given by $(M \times n)/(\rho \times a_0^3)$. (The numerator involves molar mass M and atoms per unit cell, n . The denominator consists of density and cell volume. Great expertise exists at various metrology institutes in precisely measuring all the quantities other than the lattice constant. The direct approach to the determination of Avogadro constant could use ultraprecision lattice constant measurement with an EBB x-ray beam to obtain the macroscopic crystal density for isotopically enriched crystals. The kilogram standard we use today is almost 120 years old and it is based on a Pt-Ir alloy from a single charge. The mass standard is the only unit in SI system still defined in terms of a material artifact [63]. The project to establish a very precise value for N_A , the conversion factor between microscopic and macroscopic amounts of matter, is expected to set improved limits on the stability of the present standard of mass and to redefine the kilogram. An international Avogadro Group with membership from various metrology institutes has been formed under the auspices of the *Comite Consultif pour la Masse et le grandeurs apparentees (CCM)*. We expect to attract the experts from this metrology groups who would benefit from the capabilities of the EBB beam facility, while using their competence in key areas to improve our facilities for metrology work. The plan is to explore the new area of x-ray metrology at the EBB beam facility in which metrology specialists (e.g., from NIST, PTB, CSIRO, NRLM) could potentially form a new user community. We have an indirect collaboration with Peter Becker of PTB in Germany, and we have already initiated contacts with the Metrology Group at NIST.

3.5 X-ray Pulse Accumulation

Third generation synchrotron radiation facilities in the hard x-ray range are fully meeting expectations by supporting a broad spectrum of scientific research requiring high brilliance beams. The limitations of these storage-ring-based sources have recently become apparent in the forefront research area of temporal science experiments. Most of these experiments require either x-ray pulses of very high intensity and/or those with subpicosecond duration. Delivering such pulses has limitations that are intrinsic to the physics of storage rings.

In all pump-probe experiments, the pump laser has a repeat frequency of 100 Hz to 1 kHz, which is many orders of magnitude smaller than bunch frequency in a storage ring. For example, with 25 bunches filled at the APS, a sample “sees” x-rays from about five million bunches, all of which cannot be used in a time-resolved experiment. On the other hand, the pump process has to be repeated many thousands of times to collect adequate statistics, since each x-ray pulse is not sufficiently intense. This makes very inefficient use of the storage ring source. In addition, there is a class of experiments in which the chemical or spin dynamics is much faster than the width of the x-ray pulse from the storage ring to be useful.

The ideas presented to overcome these limitations are strategic to this section of the proposal and will provide new directions in performing a unique set of time domain experiments in the hard x-ray range, which otherwise would not be possible. The essence of this proposal includes development of a x-ray optical cavity [10, 64], which would perform x-ray pulse accumulation. As a result, the program will generate unique tools for performing a new class of x-ray pulse experiments in various areas of science.

While we focus here on the development of advanced x-ray pulse physics, it also addresses many exciting problems, such as the seeding physics for the conceptualization of the x-ray free-electron laser storage and distribution of x-ray pulses from an FEL to different beamlines, dynamical x-ray diffraction at normal incidence, and Fabry-Perot interferometer in the hard x-ray range. In fact, recent experiments involving two of our proposal members (Shvydko and Alp) to realize a Fabry-Perot interferometer in the x-ray regime has produced positive results, as shown in Figure 22 [65].

The electron bunch pattern at the APS with a limitation of 15 mA/pulse generates 10^7 photons/sec/eV/pulse. One can increase this number by an order of magnitude using an x-ray accumulation cavity as proposed here. We plan to demonstrate the principle of x-ray pulse accumulation and photons/pulse enhancement using an x-ray cavity made up of two sapphire crystals. The idea is to adjust the distance between the two reflecting crystals such that the time it takes to travel from one to the other is equal to the distance between the electron bunches in the storage ring. The length of the NID beamline along with the flexibility of locating the reflecting optics allows one to test these ideas. Maintaining temperatures of the reflectors to within a few millidegrees and optical alignment to within a few microradians would be some of the major challenges in the studies planned here. Also, the accumulated pulse has to be extracted from the x-ray

cavity using a synchronized optical scheme. The instrumentation meeting these stringent requirements has been conceived, and preliminary studies have been performed.

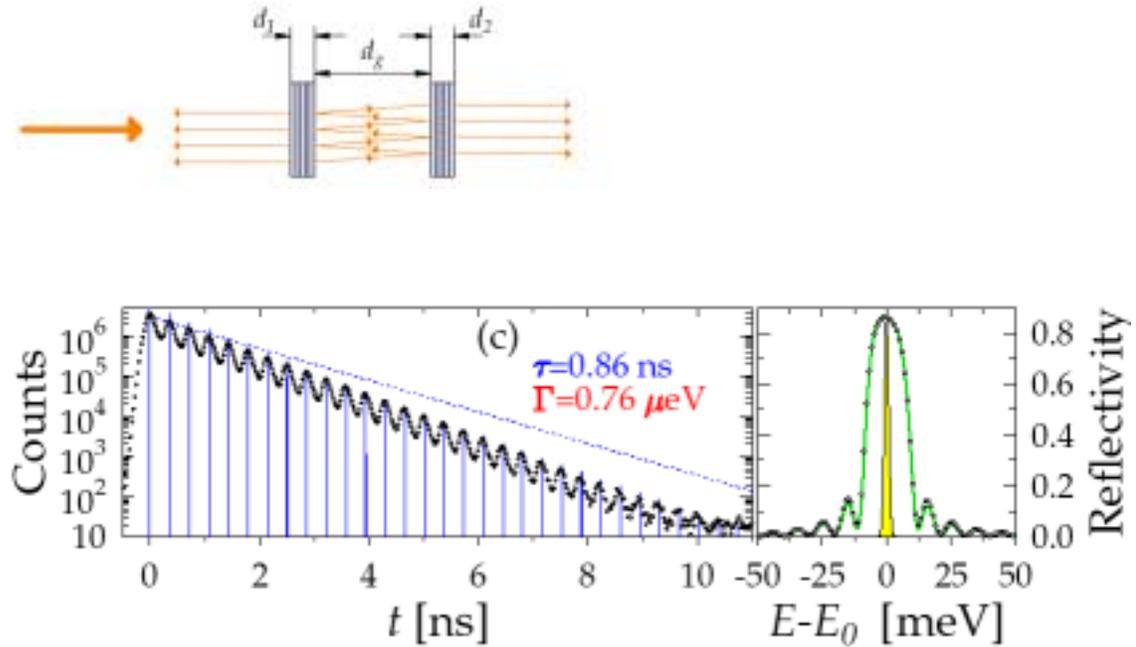


Figure 22. First successful demonstration of an x-ray Fabry-Perot interferometer using two sapphire backscattering crystals 5 cm apart. Data taken at the APS [65]. Top figure shows the geometry of the experiment. The time decay data indicate near-perfect reflectivity for Al_2O_3 (0 0 30) reflection at 14 keV.

The success of this capability will allow us not only to perform time-resolved experiments requiring intense pulses at lower repeat frequency but also to time slice the pulse to produce intense sub-picosecond pulses using the x-ray "switch" technique developed by researchers at MHATT CAT. The concepts developed in this proposal can be extended to design an x-ray storage ring with four crystal reflectors that will allow us to increase the energy bandpass, and eliminate the need for a specialized beamline [66, 67]

4. Beamline Technical Details

The layout of the facility along with the NID beamline is shown in Figures 1 and 2. A general description has been provided in Section 2. The new additions to build the EBB beamline facility include experiment stations (which will replace the temporary structure NID-X station) equipped with various instruments and a support laboratory adjacent to the station. The layout is shown in Figure 23.

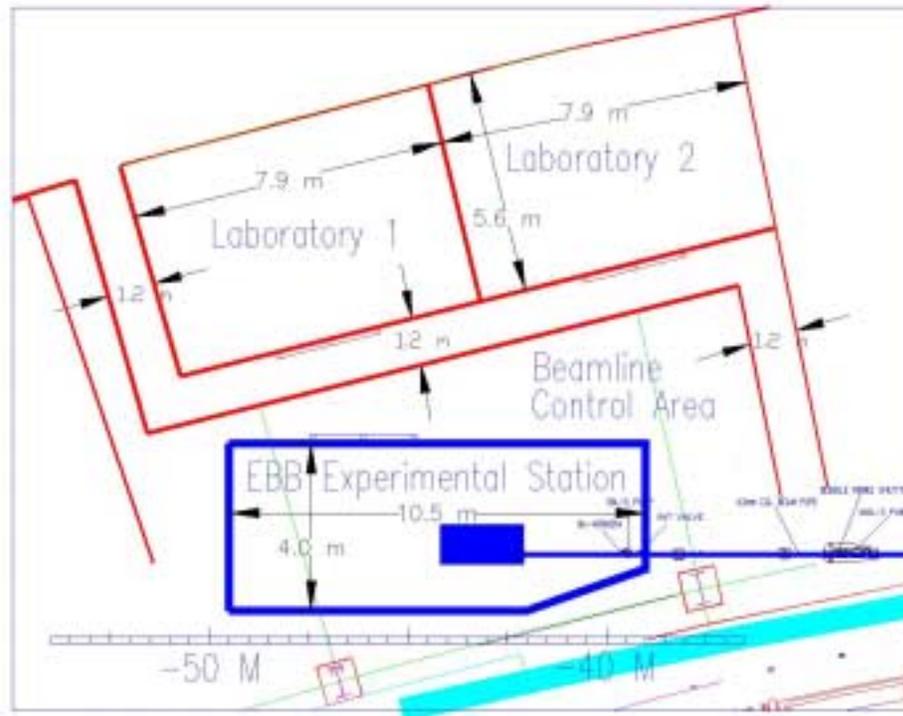


Figure 23. The proposed EBB station on the APS experimental floor and two laboratories. Since the location of this facility is in the area known as the “Early Assembly Area”, it is not possible to make use of a Laboratory Office Module, a standard support facility for other APS beamlines. Therefore, we propose to build two laboratories adjacent to the beamline station. The electrons on this picture are traveling from left to right, while the x-ray beam is in the opposite direction, being diffracted by a backscattering crystal about 80 meters downstream.

Since most of the needs of the NID beamline are already in place, the additional needs reflect the scientific program described above. The major capital and materials costs are for (a) a new undulator to meet the needs of both the SRI-CAT Sector 1 program, and the EBB facility program described here, (b) experiment stations along with all personnel-safety and equipment-safety systems, (c) support laboratory adjacent to the experiment station, (d) goniometers and nanomotion stages (e) monochromator crystals and mirrors, (e) ovens with capability of temperature control of better than a few millidegree, (f) beamline control electronics, (g) data acquisition electronics, (h) detectors, and (i) cryogenic capabilities.

The x-ray beam observed in the NID-X station is at the same height as the electron beam, and the station has a direct line of sight to the ring itself. This generates some background radiation that originates from the Compton scattering of the white beam from white beam slits, masks, and the first optic. We used a time-resolved detector in the NID-X station to measure the origin of the background and identified the location of these components, consistent with their distance from the observation point. A double-crystal monochromator or a pair of focusing mirrors will be used to eliminate this background.

The reflecting atomic planes of the sapphire crystals should be adjusted to be parallel with sub- μ rad or even nanoradian accuracy. The higher the finesse of the crystal surface, the more stringent is the requirement. The required range angular adjustment is defined for the proposed experiments by the angular mismatch between the reflecting atomic planes and the surface of the sapphire crystals. The requirement will be to build a two-dimensional rotation stage with about 10 nrad resolution and about 1 mrad range (a dynamic range of 10^5). Such devices are not available commercially. We have manufactured such stages and tested to our satisfaction their suitability for the NID-X station [68]. The Bragg energy changes with temperature are typically about a tenth of a meV/mK for high-order reflections like the (0 0 0 30) in sapphire. The energy width of the reflection is about 13 meV. Therefore, the temperature of all EBB crystals should be equal and stable within 10 mK so as to maintain the reflectivity peaks to within 1 meV. We have tested a combination of passive and active temperature controls. Based on our experience, the instrument would include a nanoradian stage with the sapphire crystal that will be thermally isolated from the environment. The sapphire crystals can be mounted to the flat surfaces of the nanoradian stage with the help of copper holders, which also incorporated wire heaters. The PT100 sensors are mounted on each copper holder and stabilized to an accuracy of 10 mK by using the heaters and computer control [69].

Competency of Personnel

All the personnel currently developing the EBB x-ray beam facility have extensive experience at most of the synchrotrons around the world including the Advanced Photon Source. All have experience in exact Bragg backscattering techniques and the various scientific programs proposed. We have already tested the basic concepts for an EBB beamline facility, and the applications of an EBB beam in demonstration experiments, pioneering many new areas of research. The personnel have extensive experience in the development of innovative instrumentation for various applications. The group also has a proven record in project planning, management and budget control. We plan to hire a senior member with a broad experience in the field to lead the effort and to train younger scientists and users.

In building a user program, the PIs plan to organize workshops with potential users on a regular basis, so that, during the facility development period, the new users can begin to perform early research in the available temporary station.

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Current involvement in other synchrotron-based projects

Inelastic scattering / photoemission beam line at SOLIEL, the planned French synchrotron VUV Raman project at the SASE Free Electron Laser test facility, DESY, Hamburg, Germany
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Selected activities or achievements

NSF International Research Fellowship, 2000-2001
Member of American Physical Society Committee on Applications of Physics, 1997 - 1999
Member of American Physical Society Task Force on Careers and Professional Development, 1996
Featured correspondent in *Science* magazine's *Next Wave* project, 1995 - 1997
Founder and operator of the *Open Forum on Alternative Careers for Physicists* at UIUC, 1994
Co-producer of *Science Left Out: A radio series on science and society*; aired on WEFT, 90.1 FM, Champaign, IL, 1994
University of Illinois Fellowship, 1993
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Selected Publications

1. "A Structural Probe of the Doped Holes in Cuprate Superconductors", P. Abbamonte, L. Venema, A. Rusydi, I. Bozovic, and G. A. Sawatzky, *Science*, **297**, 581 (2002)
Featured in the news item "Stripes Theory Beset by Quantum Waves", *ibid.*, p. 499
2. "Plasmons in Lithium Ammonia", C. A. Burns, P. Abbamonte, E. D. Isaacs, and P. M. Platzman, *Phys. Rev. Lett.*, **83**, 2390 (1999)
3. "Resonant Inelastic X-Ray Scattering from Valence Excitations in Insulating Copper-Oxides", P. Abbamonte, C. A. Burns, E. D. Isaacs, P. M. Platzman, L. L. Miller, S. W. Cheong, and M. V. Klein, *Phys. Rev. Lett.*, **83**, 860 (1999)
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Advisory Committees

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Honors and Awards

- University of Chicago, Distinguished Scientific Performance Award (1999)
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Recipient of International Atomic Energy Agency Fellowship Award (1980-1981).
Recipient of International Association for Exchange of Technical Students (IAESTE) award (1974).

Patents:

- High Resolution X-Ray Monochromator (1997)
Redundantly Constrained Laminated Structures as Weak Link Mechanism (1999)

Some refereed recent publications in related fields:

1. Y. Shvyd'ko, M. Lerche, H.C. Wille, E. Gerdau, M. Lucht, H.D. Rüter, E. E. Alp, R. Khachatryan, X-Ray Interferometry with microelectronvolt resolution, *Phys. Rev. Lett.*, 90 (2003) 013904
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Education

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Recent Work Experience

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|-----------------------|-------------------------------|--|
| | May 2001-June 2002 | Visiting Scientist, ESRF |
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| Sept. 1999 – present | | Associate Professor, Western Michigan University |
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Some Recent Publications

- 1) Y. Tsui, N. Kalechofsky, **C. A. Burns**, P. Schiffer, “A Study of the Low Temperature Thermal Properties of the Geometrically Frustrated Magnet Gadolinium Gallium Garnet”, *J. App. Phys.* **85**, 4512 (1999).
- 2) Y. Tsui, **C. A. Burns**, J. Snyder, P. Schiffer, “Magnetic Field Induced Transitions from Spin Glass to Liquid to Long Range Order in a 3D Geometrically Frustrated Magnet”, *Phys. Rev. Lett.* **82**, 3532 (1999).
- 3) **C. A. Burns**, E. D. Isaacs, P. Abbamonte, and P. Platzman, “Electronic Excitations in Lithium Ammonia”, *J. Phys. Chem. Sol.* **61**, 411 (2000).
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- 11) Y.J. Kim, J. P. Hill, **C. A. Burns**, S. Wakimoto, R. J. Birgeneau, T. Gog, and C. T. Venkataraman, “Resonant Inelastic X-ray Scattering Study of Charge Excitations in La_2CuO_4 ”, *Phys. Rev. Lett.* **89**, 177003 (2002).

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Dr. R. Colella was born in Milan (Italy) in 1935. He received his academic education at the University of Milan, where he obtained his doctoral degree in 1958. In 1961, he joined the staff of Euratom Nuclear Research Center at Ispra (Italy) as a Research Scientist in the Solid State Division, with Dr. A. Merlini. In 1967 he came to the U.S. as a postdoctoral research associate at Cornell University, Department of Materials Science and Engineering, with Prof. B.W. Batterman, where he stayed until 1970. He joined the Physics Faculty of Purdue University on September 1, 1971, as an assistant professor. He was tenured and promoted to associate professor on July 1, 1975, and became a full professor on July 1, 1977.

During the academic year 1991-92 Dr. Colella was Visiting Professor at the University of Paris-Sud (Laboratoire de Physique des Solides-Orsay, France), and at the University of Paris VI and VII, Place Jussieu, (Faculté de Minéralogie et Cristallographie), Paris (France).

Honors:

- Fellow of the American Physical Society.
- North American Co-editor of *Acta Crystallographica*. (1980-1990).
- Honorable Mention from the Gravity Research Foundation (1980).
- Dr. Colella's work on neutron interferometry and gravity, in collaboration with Overhauser, Werner, Eagen and Staudenmann, has received ample coverage in the U.S. and international press. See, for example: *Physics Today* (August 1975, p. 17); *La Recherche* (France) **7**, n. 63, p. 66 and 60 (1976), and other journals. Popular descriptions of these experiments have been given in: *American Scientist*, **68**, 70 (1980) and *Scientific American* (May 1980). They are mentioned in standard textbooks on Quantum Mechanics and Optics, such as: "Quantique, Rudiments" by J.M. Lévy-Leblond and F. Balibar (Inter Editions, Paris 1984), "The Investigation of the Physical World," by G. Toraldo di Francia (Cambridge University Press, 1981), and: "Modern Quantum Mechanics," by J.J. Sakurai (Benjamin/Cummings, Menlo Park, CA, 1985).

Cited in the 1977 Yearbook of the MacGraw Hill Encyclopedia of Science and Technology, under the entry: Quantum Theory, Non Relativistic," (by R. Colella).

More recent work on the Phase Problem in diffraction has also attracted some attention. See, for example, the Editorial Comment published in *Nature*, (Vol. **329**, p. 201) and *Scientific American*, "The Science and the Citizen", (January 1988, p. 19).

- Chairman of the first Gordon Conference on "X-Ray Physics", New London, NH, August 7-11, 1989.
- JSPS Fellow (2/1/95-4/30/95); JSPS = Japan Society for the Promotion of Science).
- Member of the Organizing Committee of the "International School on X-ray and Neutron Dynamical Diffraction: Theory and Applications." (Erice, Italy, April 1996).
- Visiting Scientist at the European Synchrotron Radiation Facility (ESRF) and at CNRS (10/1/98-6/30/99), Grenoble, France.
- Member of the Editorial Board (2001) for the Encyclopedia of Condensed Matter Physics, to be published by Elsevier.
- Recipient of the McCoy Award, (April 2002), the most prestigious research award bestowed by Purdue University, for "significant contributions in the natural sciences".

Graduate Students over the past five years: R. Eisenhower, Y. Zhang, J. Sutter.

Total Number of Graduate Students Advised: 14.

Total Number of Postdoctoral Scholars Sponsored: 5.

Publication List (Only ten given):

[21.] “Observation of Gravitationally Induced Quantum Interference,” *Phys. Rev. Lett.* **34**, 1472 (1975). (w/A. Overhauser, and S. Werner).

[24.] “Observation of the Phase Shift of a Neutron Due to Precession in a Magnetic Field,” *Phys. Rev. Lett.* **35**, 1053 (1975). (w/A. Overhauser, S. Werner, and C. Eagen).

[31.] “Quantum Theory, Non Relativistic,” Title of an article published in the 1977 Yearbook of the McGraw-Hill Encyclopedia of Science and Technology. Article based on an experiment in which the phase of a neutron is shown to be affected by the presence of a gravitational field.

[45.] “Virtual Bragg Scattering: A Practical Solution to the Phase Problem in Diffraction,” *Phys. Rev. Lett.* **46**, 1578 (1981). (w/L.D. Chapman and D.R. Yoder).

[67.] “Solution of Phase Problem for Crystallography at a Wavelength of 3.5 Å,” *Nature*, **329**, 232 (1987). (w/Q. Shen. (See Editorial Comment on p. 201, *ibid.*).

[94.] “Multiple Bragg Scattering and the Phase Problem in X-Ray Diffraction. Perfect Crystals”. Text of lecture delivered at the International School on X-Ray and Neutron Dynamical Diffraction. Erice, Italy, April 9-21, 1996. Published in “X-Ray and Neutron Dynamical Diffraction. Theory and Applications”. Edited by A. Authier, S. Lagomarsino and B.K. Tanner. Plenum Press, New York, NY 1996.

[101.] “Dynamical Diffraction and X-ray Standing Waves from Atomic Planes Normal to a 2-fold Symmetry Axis of the Quasicrystal Al-Pd-Mn” (W/T. Jach, Y. Zhang, M. de Boissieu, M. Boudard, A.I. Goldman, T.A. Lograsso, D.W. Delaney and S.W. Kycia). *Phys. Rev. Lett.* **82**, 2904-07 (1999).

[106.] “Resonant Scattering in Germanium”. (T.L. Lee, R. Felici, K. Hirano, B. Cowie, J. Zegenhagen, and R. Colella). *Phys. Rev. B* **64**, 201316 (2001) (4 pages). Rapid Communication.

[108.] “X-ray Diffuse Scattering in the Icosahedral Quasicrystal Al-Pd-Mn”. (Y. Zhang, S.N. Ehrlich, R. Colella, M. Kopecky, and M. Widom). *Phys. Rev B* **66**, 104202, 1-7, (2002).

[109.] “The Effect of Isotopic Composition on the Lattice Parameter of Germanium Measured by X-ray Backscattering”. (M.Y. Hu, H. Sinn, A. Alatas, W. Sturhahn, E.E. Alp, H.-C. Wille, Yu.V. Shvyd’ko, J.P. Sutter, J. Bandaru, E.E. Haller, V.I. Ozhogin, S. Rodriguez, R. Colella, E. Kartheuser, M.A. Villeret. Accepted in *Phys. Rev. B*, (2003).

Takeshi Egami

Personal Data Born 15 July 1945 in Japan. Married, 3 children. U.S. Citizen

Education

1964-1968 University of Tokyo, B. Eng. in Applied Physics

1968-1971 University of Pennsylvania, Ph.D. in Materials Science

Professional Experience

2003- Distinguished Scientist, Oak Ridge National Laboratory/Distinguished Professor, University of Tennessee at Knoxville, Departments of Physics and Materials Science.

1980-2003 Professor, University of Pennsylvania, Department of Materials Science and Engineering, Department of Electrical Engineering, Graduate Group Chair (1988-93, 96-97), Chair of Materials Science Department (1997-2002).

1976-80 Associate Professor, University of Pennsylvania

1973-76 Assistant Professor, University of Pennsylvania

2002 John Wheatley Scholar of LANSCE, Los Alamos NL; 1998 Guest Prof., KEK, Tsukuba, Japan; 1993 Guest Professor, Inst. for Mater. Res., Tohoku U., Sendai, Japan; 1988 Summer Faculty Visitor, IBM Lab, San Jose; 1987 Guest Prof., Dept. of Physics, U. of Tokyo, Tokyo, Japan; 1979-80, 1972-73 Visiting Scientist, Max-Planck-Inst. fur Metallforsch., Stuttgart; 1971-72 Postdoc. Fellow, U. of Sussex, Brighton

Honors

- ♦ B. E. Warren Diffraction Physics Award, Amer. Cryst. Assoc., 2003
- ♦ Metal Physics Achievement Award, Japan Institute of Metals, 1988
- ♦ Robert Lansing Hardy Gold Medal of TMS-AIME, 1974
- ♦ John Wheatley Scholar of LANSCE, Los Alamos National Laboratory, 2002
- ♦ Fellow, American Physical Society, 2000
- ♦ NSF Creativity Extension Award, 1999
- ♦ S. Reid Warren Distinguished Teaching Award of Tau Beta Pi, 1997

Current Research Interests

- ♦ Local atomic structure and lattice dynamics of electronic oxides including superconducting, ferroelectric, catalytic, and magnetic oxides, surface structure of oxides.
- ♦ Modeling of structure, molecular dynamics, theory of glass structure and glass transition.
- ♦ Theory of electron-lattice interaction, many-electron theories.
- ♦ Neutron scattering, synchrotron x-ray scattering, including atomic pair-distribution function analysis, energy-dispersive x-ray diffraction and differential anomalous x-ray diffraction.

Research Grants

NSF, NSF-MRL, ARO, ONR, EPRI, IBM, JRI, DOE

Selected Publications:

110. Magnetic Amorphous Materials : Physics and Technological Applications , T. Egami, *Rep. Prog. Phys.*, **47**, 1601 (1984).
169. "Observation of a Local Structural Change at T_c for $Tl_2Ba_2CaCu_2O_8$ by Pulsed Neutron Diffraction", B.H. Toby, T. Egami, J.D. Jorgensen and M.A. Subramanian, *Phys.Rev.Letters*, **64**, 2414 (1990).
211. "Lattice Effect of Strong Electron Correlation: Implication for Ferroelectricity and Superconductivity", T. Egami, S. Ishihara and M. Tachiki, *Science*, **261**, 1307 (1993).
244. Lattice Effect in High- T_C Superconductors , T. Egami and S. J. L. Billinge, in *Physical Properties of High Temperature Superconductors V*, ed. D. M. Ginsberg (World Scientific, 1996) p. 265-373.
256. Local Jahn-Teller Distortion in $La_{1-x}Sr_xMnO_3$ Observed by Pulsed Neutron Diffraction , Despina Louca, T. Egami, E. L. Brosha, H. R. der and A. R. Bishop, *Phys. Rev. B*, **56**, R8475 (1997).
282. Anomalous Dispersion of LO Phonons in $La_{1.85}Sr_{0.15}CuO_4$ at Low Temperatures , R. J. McQueeney, Y. Petrov, T. Egami, M. Yethiraj, G. Shirane, and Y. Endoh, *Phys. Rev. Lett.*, **82**, 628 (1999).
305. Local Atomic Structure of CMR Manganites and Related Oxides , T. Egami, in *Structure and Bonding*, vol. **98**, ed. J. B. Goodenough (Springer-Verlag, Berlin, 2001) p. 115.
310. Charge Localization in CMR Manganites: Renormalization of Polaron Energy by Stress-Field , T. Egami and Despina Louca, *Phys. Rev. B*, **65**, 094422 (2002).
325. *Underneath the Bragg Peaks: Structural Analysis of Complex Materials* , T. Egami and S. J. L. Billinge (Elsevier Science, Oxford, 2003), in press.

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Education

Princeton University, NJ: P.D. (2002) Department of Physics
Stanford University, Ca: Ph.D (2002) Dept. of App. Physics
Stanford University, Ca: M.S. (2001) Dept. of App. Physics
University of Texas at Austin, Tx: B.S. (1994) Dept. of Physics

Appointments and Affiliations

Princeton University, Princeton, NJ : Assistant Professor (2002-) Department of Physics.
Princeton University, Princeton, NJ : R.H. Dicke Fellow in Physics (2001-02) Dept. of Physics.
Bell Laboratories, Lucent Tech., NJ : Visiting Scientist/Affiliate (2002-) Semicond. Physics Div.
Princeton Materials Institute : Affiliate Faculty (2002-) PCCM/Princeton Materials Institute
Argonne National Lab, IL : Member (2001-) IXS-CAT Advanced Photon Source
Executive Board Member (2002-) CMC CAT Adv. Photon Source
European Synchrotron Rad. Facility, Grenoble, France : Guest Researcher (2000, 2002).
Brookhaven National Lab, NY : User Scientist (since 1998) Nat'l Sync. Light Source.
Lawrence Berkeley National Lab, Ca : User Scientist(since 1998) Advanced Light Source.
Stanford Synchr. Rad. Lab, SLAC, Stanford, Ca : User Scientist (p/o 1996-01).

Research Interests

O Complex Quantum Systems, Strongly Correlated Electrons & Biophysics Novel Spectroscopies Using High-Energy Synchrotron Facilities (both soft & hard X-rays) (Stanford/Bell-labs Press Rel. : <http://www.stanford.edu/dept/news/report/news/june14/electron-614.html> (2000)) (Syn.Rad.News Article :16-1, p15: "Future Sci. Opportunities with Ultra-High-Resolution. Soft X-rays"(2003))

Selected Publications (since 2000)

- o "Electronic Structure of Mott Insulators Studied by Inelastic X-ray Scattering", **M.Z. Hasan**, E.D. Isaacs, Z.X. Shen, L.L. Miller, K. Tsutsui, T. Tohyama and S. Maekawa *Science* 288, 1811 (2000).
- o "Particle-hole excitations in an antiferromagnetic parent cuprate"
M.Z. Hasan, E.D. Isaacs, Z.X. Shen and L.L. Miller *Physica C* 341-348, 781 (2000). *Physica C* 364-365, 618 (2001).
- o "Inelastic X-ray Scattering as a Novel Tool to Study Electronic Excitations in Complex Insulators"
M.Z. Hasan, E.D. Isaacs, Z.X. Shen and L.L. Miller *J. Elect. Spect. & Rel. Phen.* 114-116, 705 (2001) and NLSL/BNL AR-Research Highlight, 2-78 (2001)
 - o "X-ray Standing-Wave Investigations of Valence-Electronic Structure"
J. Woicik, E. Nelson, D. Heskett, L. Berman, **M.Z. Hasan**, I.Vartanyants, Z. Shen and P. Pianetta *Phys. Rev. B* 64, 125115 (2001)
 - o "Momentum-resolved Charge Excitations in a Prototype One Dimensional Mott Insulator".
M.Z. Hasan, P.A. Montano, E.D. Isaacs, Z.X. Shen, S.K. Sinha, H. Eisaki and S. Uchida *Phys. Rev. Lett.* 88, 177403 (2002)

Honors, Awards and Synergetics

Principal Organizer & Chair : Intern'l Workshop on "Future Scientific Opportunities with the Ultra-High Resolution Soft X-Rays", Oct-11 & 12, LBNL, Berkeley, California, 2002.
<http://www-als.lbl.gov/als/usermtg/mevworkshop.html>, and *SRN 16-1-15* (2003)
R. H. Dicke Research Award in Physics, Department of Physics, Princeton University, NJ, 2001
Young Scientist Award - IUCr (CMP), IXS-2001 (Helsinki/Haikko, Finland), 2001.
Hamilton (Research) Scholarship, Chemistry Department, Brookhaven National Laboratory, 1997.
Junior Fellow (Department of Philosophy) College of Liberal Arts, University of Texas, 1993-94.
Presidential Scholar (in Physics), Department of Physics, University of Texas at Austin

JOHN P. HILL, Physicist
Department of Physics, Building 510B
Brookhaven National Laboratory
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hill@bnl.gov

Education:

Massachusetts Institute of Technology, MA
Ph.D in Physics, 1992

Imperial College of Science and Technology
B.Sc. in Physics
1st class Honors, 1986

Professional Experience:

Brookhaven National Laboratory

Group Leader, X-ray Scattering 2001-present
Executive Director, IXS-CAT 2000-present
Physicist 1998-present (with tenure, March 1999)
Associate Physicist 1995-1998
Assistant Physicist 1993-1995
Postdoctoral Researcher 1992-1993

Research Interests:

The study of cooperative electronic and magnetic phenomena in condensed matter systems, including especially magnetic ground states and electronic excitations in metals and strongly correlated systems. Development and use of x-ray magnetic and inelastic scattering techniques.

Honors and Awards:

Fellow of the American Physical Society, 2002
Presidential Early Career Award, 1996.
D.O.E. Young Independent Scientist Award, 1996.
Wolfe Fellowship, 1991-1992.
S.E.R.C. Overseas Scholarship, 1986-1989

Five Key Publications:

1. *Resonant inelastic x-ray scattering study of charge excitations in La_2CuO_4 .* Y.-J. Kim, J.P. Hill, C.A. Burns, S. Wakimoto, R.J. Birgeneau, D. Casa, T. Gog, and C.T. Venkataraman. Phys. Rev. Lett. **89**, 177003 (2002).
2. *Interplay between charge, orbital and magnetic order in $Pr_{1-x}Ca_xMnO_3$.* M. v. Zimmermann, J.P. Hill, D. Gibbs, M. Blume, D. Casa, B. Keimer, Y. Murakami, Y. Tomioka and Y. Tokura. Phys. Rev. Lett. **83**, 4872 (1999).
3. *Resonant inelastic x-ray scattering in Nd_2CuO_4 .* J.P. Hill, C.-C. Kao, W.A.C. Caliebe, M. Matsubara, A. Kotani, J.L. Peng and R.L. Greene. Phys. Rev. Lett. **80**, 4967-4970 (1998).
4. *Inelastic X-ray Scattering Study of solid and liquid Li and Na.* J.P. Hill, C.C. Kao, W.A.C. Caliebe, D. Gibbs and J.B. Hastings. Phys. Rev. Lett. **77**, 3665-3668 (1996).
5. *An x-ray-induced insulator-metal transition in a magnetoresistive manganite.* V. Kiryukhin, D. Casa, J.P. Hill, B. Keimer, A. Vigliante, Y. Tomioka and Y. Tokura, Nature **386**, 813-815 (1997).

Young-June Kim
Department of Physics
Brookhaven National Laboratory
Upton, NY 11973-5000

Education:

Harvard University, Ph. D. in Applied Physics, 1999
Seoul National University, B. S. in Physics, 1993

Professional Experience:

Brookhaven National Laboratory, Goldhaber Fellow, August 2001 – present
Brookhaven National Laboratory, Postdoctoral Associate, September 2000 – July 2001
Massachusetts Institute of Technology, Postdoctoral Associate, June 1999 – August 2000

Research Interests:

Resonant and non-resonant inelastic x-ray scattering, x-ray diffraction, neutron scattering, strongly correlated electron systems, quantum magnetism, and superconductivity

Honors and Awards:

Goldhaber Distinguished Fellowship, Brookhaven National Laboratory, 2001

Publications:

1. Y. J. Kim, J. P. Hill, C. A. Burns, S. Wakimoto, R. J. Birgeneau, T. Gog, and C. T. Venkataraman, *Resonant inelastic x-ray scattering study of charge excitations in La₂CuO₄*, Phys. Rev. Lett. **89**, 177003 (2002).
2. V. Kiryukhin, T. Y. Koo, Y. J. Kim, C. S. Nelson, J.P. Hill, D. Gibbs, and S.-W. Cheong, *Common features of charge-ordered nanoclusters in magnetoresistive manganites with ferromagnetic low-temperature state*, Phys. Rev. B **65**, 094421 (2002).
3. Y. J. Kim, R. J. Birgeneau, F. C. Chou, R. W. Erwin, and M. A. Kastner, *Critical spin dynamics of the 2D quantum Heisenberg antiferromagnets: Sr₂CuO₂Cl₂ and Sr₂Cu₃O₄Cl₂*, Phys. Rev. Lett. **86**, 3144 (2001).
4. Y. J. Kim, A. Aharony, R. J. Birgeneau, F. C. Chou, O. Entin-Wohlman, R. W. Erwin, M. Greven, A. B. Harris, M. A. Kastner, I. Ya. Korenblit, Y. S. Lee, and G. Shirane, *Ordering due to quantum fluctuations in the 2D Heisenberg Antiferromagnet Sr₂Cu₃O₄Cl₂*, Phys. Rev. Lett. **83**, 852 (1999).
6. K. Yamada, C. H. Lee, K. Kurahashi, J. Wada, S. Wakimoto, S. Ueki, H. Kimura, Y. Endoh, S. Hosoya, G. Shirane, R. J. Birgeneau, M. Greven, M. A. Kastner, and Y. J. Kim, "Doping Dependence of the Spatially Modulated Dynamical Spin Correlations and the Superconducting La_{2-x}Sr_xCuO₄", Phys. Rev. B **57**, 6165 (1998).

Stephen P. Cramer, Ph.D
Professor, University of California, Davis

| | | | |
|--|-----------|-----------|-----------|
| Williams College, Williamstown, MA | B. A | 1969-1973 | Chemistry |
| Stanford University, Stanford, CA | Ph.D. | 1973-1977 | Chemistry |
| California Institute of Technology, Pasadena, CA | (postdoc) | 1977-1978 | Chemistry |

Selected peer-reviewed publications – 2000-present (in chronological order).
(Publications selected from 146 peer-reviewed publications)

- [1.] "X-ray Raman Spectroscopy of Carbon in Asphaltene: Light Element Characterization with Bulk Sensitivity", Bergmann, U.; Mullins, O. C.; Cramer, S. P. *Anal. Chem.*, **2000**, *72*, 2609-2612.
- [2.] "Ni L-Edge Soft X-Ray Spectroscopy of Ni-Fe Hydrogenases and Model Compounds -- Evidence for High-Spin Ni(II) in the Active Enzyme", Wang, H.; Ralston, C. Y.; Patil, D. S.; Jones, R. M.; Gu, W.; Verhagen, M.; Adams, M. W. W.; Ge, P.; Riordan, C.; Marganian, C. A.; Mascharak, P.; Kovacs, J.; Miller, C. G.; Collins, T. J.; Brooker, S.; Croucher, P. D.; Wang, K.; Stiefel, E. I.; Cramer, S. P. *J. Am. Chem. Soc.*, **2000**, *122*, 10544-10552.
- [3.] "Characterization of Heterogeneous Nickel Sites in CO Dehydrogenases from *Clostridium thermoaceticum* and *Rhodospirillum rubrum* by Nickel L-Edge X-Ray Spectroscopy", Ralston, C. Y.; Wang, H.; Ragsdale, S. W.; Kumar, M.; Spangler, N. J.; Ludden, P. W.; Gu, W.; Jones, R. M.; Patil, D. S.; Cramer, S. P. *J. Am. Chem. Soc.*, **2000**, *122*, 10553-10560.
- [4.] "Structural investigations of $\text{Li}_{1.5+x}\text{Na}_{0.5}\text{MnO}_{2.85}\text{I}_{0.12}$ electrodes by Mn X-ray absorption near edge spectroscopy", Horne, C. R.; Bergmann, U.; Kim, J. K.; Striebel, K. A.; Manthiram, A.; Cramer, S. P.; Cairns, E. J. *J. Electrochem. Soc.*, **2000**, *147*, 395-398.
- [5.] "Conversion of some substituted phenols to the corresponding masked thiophenols, synthesis of a dinickel(II) dithiolate macrocyclic complex and isolation of some metal- and ligand-based oxidation products", Brooker, P.; Caygill, G. B.; Croucher, P. D.; Davidson, T. C.; Clive, D. L. J.; Magnuson, S. R.; Cramer, S. P.; Ralston, C. Y. *J. Chem. Soc. - Dalton*, **2000**, 3113-3121.
- [6.] "Fiske modes in superconducting tunnel junction detectors", Friedrich, S.; Cunningham, M. F.; Frank, M.; Labov, S. E.; Barfknecht, A. T.; Cramer, S. P. *Nucl. Inst. Meth. A*, **2000**, *444*, 151-155.
- [7.] "Correlating electronic structure with cycling performance of substituted LiMn_2O_4 electrode materials: A study using the techniques of soft X-ray absorption and emission", Grush, M. M.; Horne, C. R.; Perera, R. C. C.; Ederer, D. L.; Cramer, S. P.; Cairns, E. J.; Callcott, T. A. *Chem. Mat.*, **2000**, *12*, 659-664.
- [8.] "Electronic Structure of Chemically Prepared $\text{Li}_x\text{Mn}_2\text{O}_4$ Determined by Mn XANES", Horne, C. R.; Bergmann, U.; Grush, M. M.; Cairns, E. J.; Cramer, S. P. *J. Phys. Chem. B*, **2000**, *104*, 9587-9596.
- [9.] "⁷Li MAS-NMR, X-Ray Spectroscopy, and Electrochemical Studies of LiMn_2O_4 -Based Spinel for Lithium Rechargeable Batteries", Tucker, M. C.; Braun, A.; Bergmann, U.; Wang, H.; Glatzel, P.; Reimer, J. A.; Cramer, S. P.; Cairns, E. J. *Electrochem. Soc. Proc.*, **2000**, PV2000, 36.
- [10.] "High resolution x-ray spectroscopy of rare events: A different look at local structure and chemistry", Bergmann, U.; Glatzel, P.; Robblee, J. H.; Messinger, J.; Fernandez, C.; Cinco, R.; Visser, H.; McFarlane, K.; Bellacchio, E.; Pizarro, S. A.; Sauer, K.; Yachandra, V. K.; Klein, M. P.; Cox, B. L.; Nealson, K. H.; Cramer, S. P. *J. Syn. Rad.*, **2001**, *8*, 199-203.
- [11.] "A Quantitative Description of the Ground State Wavefunction of Cu_A by X-ray Absorption Spectroscopy: Comparison to Plastocyanin and Relevance to Electron Transfer Function", George, S. D.; Metz, M.; Szilagy, R. K.; Wang, H.; Cramer, S. P.; Lu, Y.; Tolman, W. B.; Hedman, B.; Hodgson, K. O.; Solomon, E. I. *J. Am. Chem. Soc.*, **2001**, *123*, 5757-5767.
- [12.] "L-edge X-ray Absorption Spectroscopy of Some Ni enzymes: Probe of Ni Electronic Structure", Wang, H.; Patil, D. S.; Gu, W.; Jacquamet, L.; Friedrich, S.; Funk, T.; Cramer, S. P. *J. Electron Spec.*, **2001**, *114*, 855-863.
- [13.] "L-edge X-ray Magnetic Circular Dichroism of Ni Enzymes: Direct Probe of Ni Spin States", Wang, H.; Patil, D. S.; Ralston, C. Y.; Bryant, C.; Cramer, S. P. *J. Electron Spec.*, **2001**, *114*, 865-871.
- [14.] "Nickel(II) in an almost regular tetrahedral thiolate environment: a first generation synthetic analogue of the active site of CO-dehydrogenase." Smith, M. C.; Longhurst, S.; Barclay, J. E.; Cramer, S. P.; Davies, S. C.; Hughes, D. L.; Gu, W.-W.; Evans, D. J. *J. Chem. Soc. Dalton*, **2001**, 1387-1388.

- [15.] "Mn K-Edge XANES and K β XE Studies of Two Mn-Oxo Binuclear Complexes. Investigation of Three Different Oxidation States Relevance to the Oxygen-Evolving Center of PS II", Visser, H.; Anxolabehere-Mallart, E.; Bergmann, U.; Glatzel, P.; Robblee, J. H.; Cramer, S. P.; Girerd, J.-J.; Cinco, R. M.; Sauer, K.; Klein, M. P.; Yachandra, V. K. *J. Am. Chem. Soc.*, **2001**, *123*, 7031-7039.
- [16.] "Absence of Mn-Centered Oxidation in the S₂ \rightarrow S₃ Transition: Implications for the Mechanism of Photosynthetic Water Oxidation", Messinger, J.; Robblee, J. H.; Bergmann, U.; Fernandez, C.; Glatzel, P.; Visser, H.; Cinco, R. M.; Holman, K., M.; Bellacchio, E.; Pizarro, S. A.; Cramer, S. P.; Sauer, K.; Klein, M. P.; Yachandra, V. K. *J. Am. Chem. Soc.*, **2001**, *123*, 7804-7820.
- [17.] "Influence of the Core Hole on K β Emission following photoionization or orbital electron capture: A comparison using MnO and ⁵⁵Fe₂O₃", Glatzel, P.; Bergmann, U.; DeGroot, F. M. F.; Cramer, S. P. *Phys. Rev. B*, **2001**, *6404*, U111-U119.
- [18.] "Dioxygen Activation by a Nickel Thioether Complex: Characterization of a Ni^{III}₂(μ -O)₂ Core", Mandimutsira, B. S.; Yamarik, J. L.; Brunold, T. C.; Gu, W.; Cramer, S. P.; Riordan, C. G. *J. Am. Chem. Soc.*, **2001**, *123*, 9194-9195.
- [19.] "A superconducting detector endstation for high-resolution energy-dispersive SR-XRF", Friedrich, S.; Niedermayr, T.; Drury, O.; Cunningham, M. F.; van den Berg, M. L.; Ullom, J. N.; Loshak, A.; Funk, T.; Cramer, S. P.; Batteux, J. D.; See, E.; Frank, M.; Labov, S. E. *Nucl. Inst. Meth. A*, **2001**, *467*, 1117-1120.
- [20.] "The Fe-only Nitrogenase from *Rhodobacter capsulatus*: identification of the cofactor, an unusual high-nuclearity iron-sulfur cluster, by Fe K-edge EXAFS and ⁵⁷Fe Mössbauer Spectroscopy", Krahn, E.; Weiss, B. J. R.; Kröckel, M.; Grppe, J.; Hekel, G.; Cramer, S. P.; Trautwein, A. X.; Schneider, K.; Müller, A. *J. Biol. Inorg. Chem.*, **2002**, *7*, 37-45.
- [21.] "Anisotropic valence \rightarrow core x-ray fluorescence from a [Rh(en)₃][Mn(N)(CN)₅] · H₂O single crystal: Experimental results and density functional calculations", Bergmann, U.; Bendix, J.; Glatzel, P.; Gray, H. B.; Cramer, S. P. *J. Chem. Phys.*, **2002**, *116*, 2011-2015.
- [22.] "Bulk-sensitive XAS characterization of light elements: from X-ray Raman scattering to X-ray Raman spectroscopy", Bergmann, U.; Glatzel, P.; Cramer, S. P. *Microchem. J.*, **2002**, *71*, 221-230.
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- [26.] "Refinement of the Nickel Site Structure in *Desulfovibrio gigas* Hydrogenase Using Range-Extended EXAFS Spectroscopy", Gu, W.; Jacquemet, L.; Patil, D. S.; Wang, H.-X.; Evans, D. J.; Smith, M. C.; Millar, M.; Koch, S.; Eichhorn, D. M.; Latimer, M.; Cramer, S. P. *J. Inorg. Biochem.*, **2003**, *93*, 41-51.
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- [28.] "High-Resolution X-Ray Imaging Based on Curved Bragg Mirrors: First Results", Bergmann, U.; Ivanovic, M.; Glatzel, P.; Cramer, S. P. **2003**, *50*, in press.
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Employment:

- 1/2000-Present Staff Scientist, Stanford Synchrotron Radiation Laboratory,
Stanford Linear Accelerator Center, Stanford University
- 1994-1999 Research Assistant, the State University of New York, Stony Brook
- 1991-1994 Research Assistant, Chinese Academy of Sciences

Professional Activities:

- Proposal Review Panel, Advanced Photon Source, Argonne National Laboratory, 2002 – 2004.
- International Advisory Board for the 2nd International Workshop on Noncrystallographic Phase Retrieval, Australia, July, 2003.
- Chair, X-ray Imaging and Spectro-Microscopy Workshop, SLAC, Stanford, Oct. 8-9, 2002.
- Chair, Microsymposium on Holography and X-ray Microscopy, XIX Congress and General Assembly of the International Union of Crystallography, Geneva, Switzerland, Aug. 8-15, 2002.
- Co-chair, International Phasing Workshop: New Approaches to the Phase Problem, Berkeley, May 17-19, 2001.

Recent Publications:

1. J. Miao, K. O. Hodgson, T. Ishikawa, C. A. Larabell, M. A. LeGros and Y. Nishino, "Imaging Whole *Escherichia Coli* Bacteria by Using Single Particle X-ray Diffraction", *Proc. Natl. Acad. Sci. USA* **100**, 110-112 (2003).
2. J. Miao, T. Ohsuna, O. Terasaki, K. O. Hodgson and M. A. O'Keefe, "Atomic Resolution Three-Dimensional Electron Diffraction Microscopy", *Phys. Rev. Lett.*, **89**, 155502 (2002).
3. J. Miao, T. Ishikawa, B. Johnson, E. H. Anderson, B. Lai and K. O. Hodgson, "High Resolution 3D X-ray Diffraction Microscopy", *Phys. Rev. Lett.*, **89**, 088303 (2002). (Cover Story)
4. J. Miao, K. O. Hodgson and D. Sayre, "A New Approach to 3-D Structures of Biomolecules Utilizing Single Molecule Diffraction Images", *Proc. Natl. Acad. Sci. USA* **98**, 6641-6645 (2001).
5. J. C. H. Spence, M. Howells, L. D. Marks and J. Miao, "Lensless imaging: a workshop on new approaches to the phase problem for non-periodic objects", *Ultramicroscopy* **90**, 1-6 (2001).
6. B. Winn, H. Ade, C. Buckley, M. Feser, M. Howells, S. Hulbert, C. Jacobsen, K. Kaznacheyev, J. Kirz, A. Osanna, J. Maser, I. McNulty, J. Miao, T. Oversluiszen, S. Spector, B. Sullivan, Y. Wang, S. Wirick and H. Zhang, "Illumination for coherent soft X-ray applications: The new X1A beamline at the NSLS," *J. Synch. Rad.* **7**, 395-404 (2000).
7. J. Miao and D. Sayre, "On possible extensions of X-ray crystallography through diffraction pattern oversampling," *Acta Cryst. A* **56**, 596-605 (2000).
8. J. Miao, J. Kirz and D. Sayre, "The oversampling phasing method," *Acta Cryst. D* **56**, 1312-1315 (2000).
9. J. Miao, P. Charalambous, J. Kirz and D. Sayre, "Extending the methodology of X-ray crystallography to allow imaging of micrometre-sized non-crystalline specimens," *Nature* **400**, 342-344 (1999).
10. H. N. Chapman, S. Vogt, C. Jacobsen, J. Kirz, J. Miao, Y. Wang, B. Winn and T. Oversluiszen, "A Shutter-Photodiode combination for UV and soft X-ray beamline," *J. Synch. Rad.* **6**, 50 (1999).
11. J. Miao, D. Sayre and H. N. Chapman, "Phase Retrieval from the Magnitude of the Fourier transform of Non-periodic Objects," *J. Opt. Soc. Am. A* **15**, 1662-1669 (1998).
12. D. Sayre, H. N. Chapman and J. Miao, "On the Extendibility of X-ray Crystallography to Noncrystals," *Acta Cryst. A* **54**, 232-239 (1998).

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EDUCATION:

B.S. Engineering Physics, Cornell University, 1970
M.S. Physics, Massachusetts Institute of Technology, 1973
Ph.D. Physics, Massachusetts Institute of Technology, 1975

EMPLOYMENT:

9/01 to Present: Senior Scientist and Advisor to Laboratory Director, and MIT Visiting Professor
5/87 to 9/01: Associate Laboratory Director, Argonne National Laboratory
3/99 to 3/01: Executive Director, Spallation Neutron Source, Oak Ridge National Laboratory
4/85 to 12/90: Senior Research Associate and Group Head, Exxon Corporate Research
1/82 to 4/85: Physicist and Group Leader, Brookhaven National Laboratory
5/75 to 1/82: Member of Technical Staff, Bell Laboratories

PROFESSIONAL:

Fellow, American Physical Society
Member, American Association for the Advancement of Science
Consultant, Bell Laboratories (1982-84)
Consultant Exxon Corporate Research (1984-85, 1990-1993)
Member (1980-81) and Chairman (1982-83) of the Stanford Synchrotron Users Association
Committee Member, Planning Study for Advanced National Synchrotron Facilities (1983-84)
Member (1985-86) and Chairman (1987) of the Advanced Photon Source Steering Committee
Member of the Proposal Review Panel for the Cornell High-Energy Synchrotron Source (CHESS) (1987-1989)
Member of the Basic Energy Sciences Advisory Committee (1987-89)
Member, Materials Research Advisory Committee for the National Science Foundation (1990-1993)
Member, Policy and Advisory Board for the Cornell High-Energy Synchrotron Facility (CHESS) (1987-1996)
Niels Bohr Institute Advisory Committee, University of Copenhagen, Denmark (1996-2000)
MIT Materials Research Science and Engineering Center Advisory Board (1994-present)
Member, Solid State Sciences Committee, National Research Council (1997-2001)
External Member, Plenary Research Committee, Paul Scherrer Institut, Switzerland (1997-present)
Alumni/ae Representative, MIT Corporation Visiting Committee for the Dept. of Nuclear Engineering (1998-present)
Member, Scientific Advisory Committee for the Spallation Neutron Source (SNS) Project, Oak Ridge National Laboratory (1998-1999, 2001-present)
American Physical Society, Study Panel on National Missile Defense (2001-present)
American Physical Society, Physics Policy Committee (2002-)
Founder Member of the Science Advisory Committee to the Central Laboratory of Research Councils (United Kingdom) (2002 -)

AWARDS:

Outstanding Scientific Accomplishment in Solid State Physics, U.S. Dept. of Energy 1985 Materials Research competition. "Synchrotron X-ray Studies of the Magnetic Structure of Holmium."
Department of Energy's Ernest Orlando Lawrence Memorial Award, 1987, for development of high resolution synchrotron x-ray scattering techniques and their applications to diverse materials systems.
Award of Recognition by the Chicago Area Sigma Xi Chapters, 1995, for contributions to the advancement of research in materials science, and for the construction of the Advanced Photon Source.
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EXPERIENCE:

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| 2001-Present | Senior Scientific Advisor, Advanced Photon Source |
| 2002- Present | Member of International Scientific Advisory Committee for Australian Synchrotron Light Source |
| 2001 | Interim Associate Laboratory Director, Advanced Photon Source |
| 1999-2001 | Argonne National Laboratory, Senior Scientific Director, Advanced Photon Source. |
| 1999-Present | Member, Scientific Advisory Committee for the LCLS, Stanford |
| 1998 — Present | Member, Scientific Advisory Committee for the LANCE Spallation Source |
| 1989-1999 | Argonne National Laboratory, Division Director, Experimental Facilities Division, Advanced Photon Source. |
| 1988-1989 | Associate Division Director, Advanced Photon Source Project |
| 1984-1988 | Group Leader, Advanced Photon Source Project. |
| 1984-1988 | Group Leader, Materials Science Division, Argonne National Laboratory.. |
| 1981-Present | Senior Scientist- Argonne National Laboratory |
| 1976-1981 | Physicist, Materials Science Division, Argonne National Laboratory. |
| 1974-1976 | Visiting Scientist, Materials Science Division, Argonne National Laboratory |
| 1972-1974 | Research Associate, Centre de Recherches Nucleaires, C.N.R.S., Strasbourg, France. |
| 1971 | Visiting Scientist, Technical University of Helsinki, Otaniemi, Finland.. |
| 1970-1972 | Scientific Associate, Technical University of Munich, Garching, Germany. |
| 1967-1970 | Postdoctoral Appointee, Solid State Science Division, Argonne National Laboratory, Argonne, |
| 1966-1967 | Visiting Fellow, Tata Institute of Fundamental Research, Bombay, India |
| 1964-1966 | Senior Research Associate, The Institute of Science, University of Bombay |

PROFESSIONAL SOCIETIES:

American Association for the Advancement of Science
American Physical Society

HONORS AND AWARDS:

Fellow, American Association for the Advancement of Science
Fellow, American Physical Society
Distinguished Scientist Award by American Chapter of the Indian Physics Association, 1991
Argonne National Laboratory Pacesetter Awards, 1986 & 1988.
University of Chicago Award for Distinguished Performance, 1986.

PUBLICATIONS:

Over 300 publications, book chapters, books

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Yuri V. Shvyd'ko

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BORN: April 9, 1955, Krasnodar, Russia

EDUCATION:

1972-1978 BS. Moscow Engineering Physics Institute (State University).

1979-1984 PhD in physics at the Kurchatov Institute of Atomic Energy (KIAE), Moscow. Subject: "Time Dependence of Coherent Interaction of γ -Radiation With Nuclei in Crystals". Diploma FM-022401, 6 March 1985.

1998-2001 Habilitation (right to teach) in physics at the Hamburg University. (X-ray Resonators and other Applications of Bragg Backscattering).

EXPERIENCE:

1978 - 1985 Junior scienti_c employee, Kurchatov Institute of Atomic Energy (KIAE), Moscow

1985 - 1988 Scienti_c employee, KIAE

1988 - 1993 Senior Scientist, KIAE

1993 - 1995 Research Fellow of the Alexander von Humboldt Foundation, at the Hamburg University

1995 - 1998 Scienti_c employee, Hamburg University, II. Institut für Experimentalphysik.

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AWARDS:

1987 Young Scientist Prize of Moscow for "Experimental Studies of the Nuclear Excitations in Crystals"

MAIN FIELDS OF RESEARCH: X-ray optics, solid state physics, materials science, metrology, γ -optics.

SELECTED PUBLICATIONS in the last five years (1998-2003). Altogether about 60 papers were published in refereed physics journals since 1980.

1. Yu. V. Shvyd'ko, M. Lerche, H.-C. Wille, E. Gerdau, E. E. Alp, M. Lucht, H. D. Rüter, and R. Khachatryan "X-ray Interferometry with Microelectronvolt Resolution." Phys. Rev. Lett. 90 (2003) No.1.
2. H.-C. Wille, Yu.V. Shvyd'ko, E. Gerdau, M. Lerche, M. Lucht, H.D. Rüter, and J. Zegenhagen. "Anomalous Isotopic Effect on the Lattice Constant of Silicon". Phys. Rev. Lett. 89 (2002) 285901.
3. Yu.V. Shvyd'ko, M. Lucht, E. Gerdau, M. Lerche, E.E. Alp, W. Sturhahn, J. Sutter, T.S. Toellner. "Measuring wavelengths and lattice constants with the Mössbauer wavelength standard" J. Synchrotron Rad., 9 (2002) 17-23 .
4. Yu.V. Shvyd'ko, M. Gerken, H. Franz, M. Lucht, E. Gerdau. "Nuclear Resonant Scattering of Synchrotron Radiation from ^{161}Dy at 25.61 keV" Europhys. Letters 56 (2001) 39.
5. E.L. Saldin, E.A. Schneidmiller, Yu.V. Shvyd'ko, and M.V. Yurkov. "X-ray FEL with a meV bandwidth" Nucl. Instrum. and Methods A 475 (2001) 357-362.
6. Yu.V. Shvyd'ko, M. Lerche, J. Jäschke, M. Lucht, E. Gerdau, M. Gerken, H.D. Rüter, H.-C. Wille, P. Becker, E.E. Alp, W. Sturhahn, J. Sutter, and T.S. Toellner. " γ -ray wavelength standard for atomic scales" Phys. Rev. Lett 85 (2000) 495.
7. V.G. Kohn, Yu.V. Shvyd'ko, and E. Gerdau "On the theory of an x-ray Fabry-Perot interferometer" Phys. Stat. Sol. b 221 (2000) 597-615.
8. Shvyd'ko Yu.V. "Nuclear Resonant Forward Scattering of X Rays: Time and Space Picture." Phys. Rev. B 59 (1999) 9132
9. Shvyd'ko Yu.V, Gerdau E., Jäschke J., Leupold O., Lucht M., and Rüter H.D. "Exact Bragg Backscattering of X-rays " Phys. Rev. B 57 (1998) 4968
10. Shvyd'ko Yu.V, van Buerck U., Potzel W., Schindelmann P., Gerdau E., Leupold O., Metge J., H.D. Rüter, and Smirnov G.V. "Hybrid Beats in Nuclear Forward Scattering of Synchrotron Radiation" Phys. Rev. B 57 (1998) 3552