

APS Midterm Upgrade Plan for Sector 3

“ μeV -resolution X-ray Spectroscopy”

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Summary

This upgrade plan is developed in consultation with the user groups that are active at the APS 3-ID beamline. The basis of science-driven ideas were presented at a comprehensive workshop held at the APS on July 20, 2006 and an update was reviewed by the newly formed User Advisory Committee for Sector 3 in light of the recent “Five Grand Challenges for the Basic Energy Sciences” presented by BESAC Panel on Dec 20, 2007. In particular, this proposal addresses at least three aspects of the challenges presented by the committee, namely, 1) “*How do we control material processes at the level of electrons?*” , 2) “*How do remarkable properties of matter emerge from complex correlations of the atomic or electronic constituents and how can we control these properties?*”, and finally 3) *How can we master energy and information on the nanoscale to create new technologies with capabilities rivaling those of living things?*

The two current scientific programs, namely nuclear resonant scattering and momentum resolved inelastic x-ray scattering would remain the same. New scientific opportunities are expected to arise with an increased brilliance and flux resulting from an upgrade of the Advanced Photon Source (APS). With a potential implementation of an APS storage ring and beamlines upgrade which will involve i) increased stored current, ii) extended straight sections, iii) superconducting and/or in-vacuum undulators, a gain of about a factor of ten in spectral flux in the 10 keV to 30 keV range can be realistically expected.

For nuclear resonant inelastic x-ray spectroscopy, this upgrade would enable a significant improvement of the energy resolution from the current value of 1 meV to 0.1 meV. We expect to complement the improved source with i) improved space for experiments by extending the station 3-ID-B, ii) improved cryogenically-cooled high-resolution monochromator, and iii) more efficient APD detectors.

For momentum-resolved inelastic scattering experiments, we propose to change the current horizontal scattering geometry to vertical geometry, thus increasing the momentum-transfer range from the current value of 34 nm^{-1} to over 100 nm^{-1} . Complemented with a multi-analyzer/multi-detector instrument comparable to a large multi-detector neutron time-of-flight spectrometer, e.g. ARCS at SNS, we expect an enhancement of data quality and collection efficiency by another order of magnitude. Furthermore, by changing the station layout, we propose to incorporate focusing optics to reduce the beam size to 10 micrometer level for high-pressure measurements.

In broad terms, we are proposing to

- 1) Change the undulator source at 3-ID,
- 2) Expand the experimental work space in 3-ID-B,
- 3) Re-build the IXS-spectrometer in the vertical geometry with increased solid angle coverage, and momentum-transfer range,
- 5) Provide unique sample environments, including high-pressure combined with high and low temperature, and high magnetic field, develop a UHV environment system for nano-scale magnetism experiments, and
- 6) Look for an opportunity to separate ^{149}Sm , ^{119}Sn , and ^{161}Dy experiments to another beamline, with the possibility of extending the nuclear resonance experiments to ^{121}Sb , and ^{145}Nd , ^{61}Ni .

The expected cost of this upgrade is in the range of 10 Million dollars over 5 years.

An alternate upgrade option proposes to convert the APS to an ERL. The calculated spectral flux for different operating modes is significantly lower even if compared to the present day APS. The bunch-to-bunch separation is too short to permit nuclear resonant scattering and ERL will seriously inhibit progress for momentum-resolved IXS and disable nuclear resonant scattering.

Scientific Aspects

In the last decade, inelastic x-ray scattering (IXS) spectrometers at highly brilliant synchrotron radiation facilities in the U.S., Europe, and Japan have provided exciting new opportunities for the study of vibrational and electronic properties of condensed matter. IXS experiments have attracted a variety of scientists to investigate cutting-edge problems in condensed matter physics, liquid dynamics, material science, biophysics, biochemistry, and geosciences. At present, the following IXS techniques are invaluable research tools for the scientific community.

- ◆ IXS with meV resolution around 20-30 keV range for measurements of phonon dispersions in single crystals and collective excitations in liquids, biological molecules and solutions;
- ◆ X-ray Raman Spectroscopy around 8-15 keV to measure soft x-ray absorption edges in extreme environments, e.g., pressure, to provide bulk sensitivity and to distinguish dipole and quadrupole transitions by utilizing momentum transfer information;
- ◆ Resonant IXS with resolutions of typically 300 meV around the transition metal K-edges and momentum resolution that allows the study of electronic structure near the Fermi surface and addresses the issue of electron transport in manganites, nickelates, and cuprates, among others;
- ◆ X-ray Emission Spectroscopy with a resolution of typically 1 eV to study local electronic structure, e.g., valence and spin state, in extreme environments;
- ◆ Nuclear Resonant IXS with meV resolution to measure the phonon density of states and a dozen elastic and thermodynamic properties, e.g. velocity of sound, Grüneisen parameter, vibrational entropy, and specific heat, particularly in biomolecules and proteins, under extreme conditions, and in nano-structures;
- ◆ Nuclear resonant forward scattering with neV resolution as element and isotope selective magnetometer in nano-magnetism studies with a monolayer sensitivity as well as probe for valence and spin state under extreme pressure.

The next generation of IXS spectrometer with energy resolution significantly below 1 meV and improved collection efficiency would provide an invaluable tool to address many pressing scientific problems.

Geophysics

High-resolution inelastic x-ray scattering techniques provide the Earth and planetary science community with opportunities for new and exciting results on the properties of materials at high pressure and temperature conditions. These opportunities are possible due to the characteristics of third generation synchrotron sources such as the Advanced Photon Source. High-resolution IXS techniques fall into two broad areas. One is nuclear resonant scattering (NRS) which provides information on electronic, vibrational, and elastic properties, such as the density of states and sound velocities. It is also sensitive to solid-melt transitions. The other class of experiments is momentum-resolved IXS which directly gives the dispersion relation of low-energy collective excitations like phonons. Such measurements provide directional information on vibrational and elastic properties, such as the elastic tensor and sound velocities. Both methods are in many ways ideally or even uniquely suited for addressing a number of important geophysical questions. The following examples illustrate the potential use of high-resolution IXS in the Earth and planetary sciences.

Sound velocities and elasticity: A number of laboratories are attempting to measure sound

velocities at elevated pressure and temperature, using a variety of techniques. Such measurements allow one to interpret the seismic properties of the mantle and core. This is the primary motivation for IXS measurements of sound velocities. Note the method is suitable for metals and opaque minerals. The pressure range of 10-15 GPa and above is extremely challenging for velocity measurements, and inter-laboratory calibrations are necessary to assess absolute accuracy. Velocity measurements under P-T conditions of the lower mantle are mostly *terra incognita*. With nuclear resonant scattering one uses the ^{57}Fe isotope to obtain sound velocities from iron-containing compounds (Hu et al. 2003). The viability of this method has been demonstrated with materials under pressures up to 153 GPa and temperatures up to 1700 K (Mao et al. 2001, Lin et al. 2005, Mao et al. 2006). Momentum resolved IXS has been applied to determine sound velocities at pressures above 100 GPa and to obtain the elastic tensor (Fiquet et al. 2001, Antonangeli et al. 2004), and there is no obvious barrier to further application at simultaneous high temperatures. The improvement of energy resolution to values clearly below 1 meV will permit access to lower phonon energies thus providing a tremendous potential for sound-velocity determination.

Liquids: The physical properties of liquids such as viscosity, melting, and compressibility under high-pressure conditions are often poorly understood. However, current models of the Earth suggest that molten materials probably exist from Earth's surface down to the outer core. Therefore, measurements capable of extracting melt properties at pressures and temperatures reaching into the outer core P-T regime would be extremely valuable to substantiate, refine, and/or improve our understanding of Earth's interior dynamics. For example, the momentum resolved IXS technique was used to determine melt viscosities for $T > 3000$ K at ambient pressure (Sinn et al. 2003). The extension of such experiments into high-temperature and high-pressure regime would provide a wealth of new information that is not available today through other experimental methods. A multi-analyzer IXS instrument with significant improved flux would reduce the data collection time from hours to minutes, so that samples under extreme pressure and temperature, e.g. liquid iron or iron oxides, could be kept sufficiently stable. Sub-meV energy resolution is crucial to extract viscosity values in the range that is relevant to Earth sciences.

High-spin to low-spin crossover: Recent synchrotron experiments indicated a high-spin to low-spin crossover (HS-LS) of the Fe in magnesiowüstite at lower-mantle pressures (Badro et al. 2003, Lin et al. 2005a). This crossover probably has an important influence on the partitioning of Fe and other elements, sound velocities, viscosity, and density of the lowermost mantle. The temperature dependence of this change of spin state, even though theoretically predicted (Sturhahn et al. 2005), has yet to be explored experimentally. NRS techniques are ideal to study such phenomena, e.g., a HS-LS crossover collapses the electric field gradient at the Fe nucleus and thereby the nuclear level splitting (Lin et al. 2006). NRS in the laser heated diamond anvil cell would therefore offer an independent means of studying HS-LS transitions at lower mantle pressures and temperatures.

Melting in Fe: Nuclear resonant forward scattering allows one to observe transitions from the solid to the liquid state. In the liquid state, the nuclear resonant forward scattering signal disappears. Therefore, the NRS technique is an alternative means of detecting melting that is complementary to more commonly employed x-ray diffraction techniques (Shen 1998, Boehler 2000, Shen 2001). The intensity of an x-ray diffraction signal is sensitive to grain growth and preferred orientation of grains, while NRS is not. Moreover, NRS can distinguish between an amorphous high pressure solid (Hemley 1988) and a true liquid. NRS should therefore allow one to investigate the melting of Fe and Fe alloys, which are the main constituents of the core. This could resolve controversies on the temperature of the Earth's core.

Recent publications in Geophysics and related areas:

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Badro, J et al. (2003) *Science* **300**, 789
Boehler, R (2000) *Rev. Geophysics* **38**, 221
Fiquet, G et al. (2001) *Science* **291**, 468
Giefers, H et al, (2007) *Phys. Rev. Lett*, **98**, 245502
Hemley, R J et al. (1988) *Nature* **334**, 52
Hu, M Y et al. (2003) *Phys. Rev. B* **67**, 094304
Lin, J-F et al. (2005) *Science* **308**, 1892
Lin, J-F et al. (2005a) *Nature* **436**, 377
Lin, J-F et al. (2006) *Phys. Rev. B* **73**, 113107
Mao, H-K et al. (2001) *Science* **292**, 914
Mao, W L et al. (2006) *Science* **312**, 564
Shen, G and Heinz, D L (1998) in Hemley, RJ (ed), *Ultra High Pressure Mineralogy - Physics and Chemistry of Earth's Deep Interior*, (Mineralogical Soc. Am., Washington DC) p 369
Shen, G et al. (2001) *Appl. Phys. Lett.* **78**, 3208
Sinn, H et al. (2003) *Science* **299**, 2047
Sturhahn, W et al. (2005) *Geophys. Res. Lett.* **32**, L12307
Sturhahn, W et al, *Geophys. Soc. Of America*, (2007) **421**, 157

Biophysics

The dynamical structure of biological compounds such as proteins are typically characterized by infrared or resonant Raman spectroscopy. However, these techniques require coupling to electric dipoles, and thus pose selection rules, eliminating the possibility of observing all modes, and the very limited range of momentum transfers by the scattered light does not permit the study of dynamic spatial correlations on the nanometer scale. Furthermore, the amplitudes of observed spectra do not correspond to real vibrational modes. Inelastic x-ray scattering techniques, with the proposed improvements in energy resolution, can address some of the fundamental issues related to functional dynamics of biological catalytic reactions.

Metalloproteins: Biologically active proteins and enzymes often contain transition elements like Fe near their active sites. The understanding of the relations between structure, dynamics, and functionality in enzymes like nitrogenase or hydrogenase can address problems of wide interest, e.g. the N₂-fixation problem in the production of fertilizers. Nuclear resonant IXS has been demonstrated to produce unique results in studies of nitrogenase (*Xiao et al. 2006*) and electron transfer proteins like rubredoxin (*Xiao et al. 2005*), myoglobin (*Sage et al. 2001*), hemoglobin (*Zeng et al. 2005, Adams et al. 2006*) and cytochrome-f (*Adams et al. 2006*). Furthermore, these studies have been extended to model compounds like porphyrins (*B. K. Rai et al, 2002*) and Fe-S clusters like cubanes (*Smith et al. 2005*). It has been experimentally observed that in the presence of counter-ions and off-center metallic cations, the vibrational spectra broaden, requiring better resolution than 1 meV to characterize low energy modes (*Jayasooriya et al. 2006, unpublished*). Recent advances in applying density functional theory to simulate bonding in model compounds and to calculate vibrational properties provide a real opportunity for further improvements in understanding the dynamics of large molecules at the atomistic scale (*Leu et al. 2004*). An energy resolution significantly below 1 meV would enable access to longer time scales and potentially open a new window to study collective protein dynamics. Also the proper analysis of line broadening and the observation of small shifts related isotopic substitution. An increase in

spectral flux would enable the detection of hydrogen atoms (protons) near the metal ion in an enzyme and promises great opportunities not available today.

Bio-membranes: Biological membranes which are mixtures of several lipids and amphiphilic proteins play a significant role in processes like ion-transport and signal transduction. They have been studied by a variety of methods including differential scanning calorimetry, NMR, ESR, x-ray and neutron diffraction, Brillouin scattering, and inelastic neutron scattering. However, studies of the in-plane collective excitations of lipid chains that are essential for the understanding of several aspects of the membrane's biological functions are scarce so far. Momentum transfers between 1 nm^{-1} and 5 nm^{-1} are particularly important but inaccessible by the aforementioned experimental techniques. A good energy resolution is particularly important to distinguish low-energy collective modes from often strong elastic scattering. Currently, inelastic x-ray scattering techniques have already shown the connection between in-plane phonon dispersion relations of certain bilayer phases and the order of the lipid molecules in the membrane (*Chen et al. 2003, Angelini et al. 2006*). However, excitations in these systems are often weak and barely distinguished from elastic scattering. An increase in spectral flux combined with sub-meV energy resolution would enable inelastic x-ray scattering techniques to provide sufficient constraints for various models proposed to explain the change in the elasticity of membranes upon phase change or intercalation of large molecules like cholesterol.

Recent publications in biophysics and related areas:

- Adams, K et al. (2006) *J. Phys. Chem. B* **110**, 530
- Angelini T et al. (2006) *Proc. Nat. Acad. Sci.* **103**, 7962
- Chen S et al. (2003) *Biophys. Chem.* **105**, 721
- Leu B M et al. (2004) *J. Am. Chem. Soc.* **126**, 4211
- Leu, B. et al, *Biophysics Journal* (2007) **92**, 3764
- Petrenko, T et al, (2007) *JACS* **129**, 11053
- Rai B K et al. (2002) *Biophys. Journ.* **82**, 2951
- Sage J T et al. (2001) *Phys. Rev. Lett.* **86**, 4966
- Silvernail, N., (2007) *JACS* **129**, 2200
- Smith M C et al. (2005) *Inorg. Chem.* **44**, 5562
- Xiao Y et al. (2005) *J. Am. Chem. Soc.* **127**, 14596
- Xiao Y et al. (2006) *J. Am. Chem. Soc.* **128**, 7608
- Zeng W et al. (2005) *J. Am. Chem. Soc.* **127**, 11200

Condensed matter physics

Collective excitations at low energy reflect a fundamental property of condensed matter. In the past century, a variety of experimental techniques were developed to study related phenomena like sound, phonons, and magnons. Inelastic x-ray scattering offer unique capabilities in this area, e.g. large momentum transfer, very good energy resolution, very small samples. The nuclear resonant scattering methods also provide perfect isotope selectivity albeit at the expense of momentum resolution. The proposed improvements in spectral flux and energy resolution would lead to unprecedented possibilities for fundamental and applied studies of condensed matter. Several examples are:

Localized phonon modes: In the field of phonon spectroscopy in crystals, recent studies show more and more the importance of localized phonon modes on material properties e.g. in ferro-electrics (*Egami and Billinge 2003*) or even in pure uranium (*Manley et al. 2006*). These

localized modes are often only visible in a narrow part of the momentum transfer range off the main symmetry axis. A multi-analyzer IXS-spectrometer would collect simultaneously spectra distributed all over the reciprocal space. One could then easily Fourier-transform the inelastic data from reciprocal into real space and obtain a so-called 'dynamic pair distribution function', which provides novel ways for data interpretation. The concept of recording the dynamic pair distribution function was recently implemented in the design of neutron time-of-flight spectrometers that are currently under construction, like MERLIN at ISIS and ARCS and SNS. A similarly capable inelastic x-ray spectrometer would enable new opportunities not available with neutron scattering studies, e.g. only small amounts of sample are available or in case of unfavorable neutron cross sections.

Energy conversion materials: Recent advances in thermoelectric materials with a large figure of merit, defined as $ZT = a^2s/\kappa$, where a is the Seebeck coefficient ($a \sim dV/dT$), s is the electrical conductivity, and κ is the total thermal conductivity, merits further systematic scientific studies. A good material would be $ZT > 2$, and achieve this at low temperatures, preferably lower than the superconducting transition temperatures of cuprates. Advances in this field will have significant consequences for computers, infrared devices, and small-scale power generation (*Tritt et al. 1999*). While an increase in carrier concentration through doping can optimize the electronic component or power factor, a^2s , an increase in phonon scattering can reduce the thermal conductivity, as it is suspected to happen in caged compounds like clathrates or skutterudites. The anharmonic nature of vibrations of a cluster of atoms in constrained cage-like environments stems from low-energy translational, librational or rotational motions. The energy of these excitations are typically less than a few millielectronvolt ($1 \text{ meV} = 4.14 \text{ THz} = 8 \text{ cm}^{-1}$), thus, limiting the utility of established techniques such as infrared spectroscopy. X-ray diffraction has been employed to estimate the amplitude of the motion of these cluster of atoms, but the information is indirect. Also, the size of the holes may be too big for an effective use of the positron annihilation technique. Thus, inelastic x-ray scattering emerges as a tool of choice. Currently, best energy resolution, achieved with crystal monochromators, is around 1 meV. A recent study carried out on Kr-doped clathrate hydrate indicates that there are strong phonon modes centered at 1 meV (*Tse et al. 2005*). Similarly, another recent work on a skutterudite of $\text{EuFe}_4\text{Sb}_{12}$ indicates that the low-energy excitations of rare-earth atoms are decoupled from iron vibrational modes at low energies limited to 5 meV (*Long et al. 2005*). A complicating aspect of energy conversion materials is that they are all comprised of multi-elements, and thus it is difficult to assess the impact of elemental doping, without having a technique that is element-selective. Resonant x-ray scattering techniques solve this problem, and thus enable an in-depth and systematic study. Recently, nano-engineered systems such as $\text{Bi}_2\text{Te}_3/\text{Sb}_2\text{Te}_3$ superlattices with a ZT value higher than 2 have been synthesized (*Venkatasubramanian et al. 2001*). One additional advantage of x-rays is their ability to work in grazing-incidence geometry, thus increasing the sensitivity down to monolayer levels. Thus, we propose to combine the most attractive aspects of inelastic x-ray scattering in terms of energy resolution, element-selectivity, and applicability to bulk as well as to quantum systems.

Metallic glasses: Glasses, compared to close-packed crystalline materials, have larger internal volume, or free space. Their vibrational characteristics are strongly dependent of this free volume. The most pronounced characteristic of the vibrational density of states is the presence of a strong "boson peak", a non-Debye energy dependence of low-energy phonon modes (*Keune et al. 2003*). It has been recently demonstrated that there is a strong correlation between the composition of binary glasses and the mode occupancy of the low energy vibrations around 3 meV. As the resolution of the inelastic scattering x-ray technique improves, the relation between "boson-peak" energy and occupation factor dependence becomes clearer. In addition, with

element selective inelastic x-ray spectroscopy, it is possible to differentiate any preferential surface segregation in the internal cavities and to better assess the potential of metallic or metal-oxide glasses as hydrogen or lithium storage devices in (*Idota et al. 1997*). Thus, we propose to extend the observable energy range for element selective resonant inelastic x-ray scattering technique.

Magnetic nanostructures: The magnetic properties of artificial structures like thin films, multilayers, and isolated nanoparticles are of great interest in condensed matter physics, material science, and applications of nanotechnology. Magnetic phenomena like spin rotation by interlayer coupling have been studied with nuclear resonant techniques that allow the investigation of specific regions of a complicated system by utilizing a unique isotope selectivity (*Röhlsberger et al. 2002, L'abbé et al. 2004*). So far monolayer sensitivity was demonstrated experimentally. However, for the effective study of isolated nanoparticles the signal-to-noise ratio needs to be increased. This is accomplished here by the significant reduction of the x-ray energy bandwidth which would provide us with the needed improvement for a novel and powerful tool to explore magnetism in the smallest structures.

Recent publications in condensed matter physics/materials science and related areas:

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Callens, R, J. Synchrotron Rad. (2007) **14**, 266
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Egami T and Billinge S (2003) Pergamon Press, Oxford, "Underneath the Bragg-Peak"
Idota Y et al. (1997) Science **276**, 1395
Keune W et al. (2004) J. Phys: Cond. Matt. **16**, S369
L'abbé C et al. (2004) Phys. Rev. Lett. **93**, 037201
Long G et al. (2005) Phys. Rev. B **71**, 140302
Manley M et al. (2006) Phys. Rev. Lett. **96**, 125501
Manley M et al, J. Alloys and Compounds, (2007) **444-445**, 129
Röhlsberger R et al. (2002) Phys. Rev. Lett. **89**, 237201
Tritt T M et al. (1999) Science **283**, 804
Tse J S et al. (2005) Nature Materials **4**, 917
Upton, M.H. et al, Phys. Rev. B (2007) **76**, 220501(R)
Venkatasubramanian R et al. (2001) Nature **411**, 597

Appendix 1. Layout of 3-ID beamline

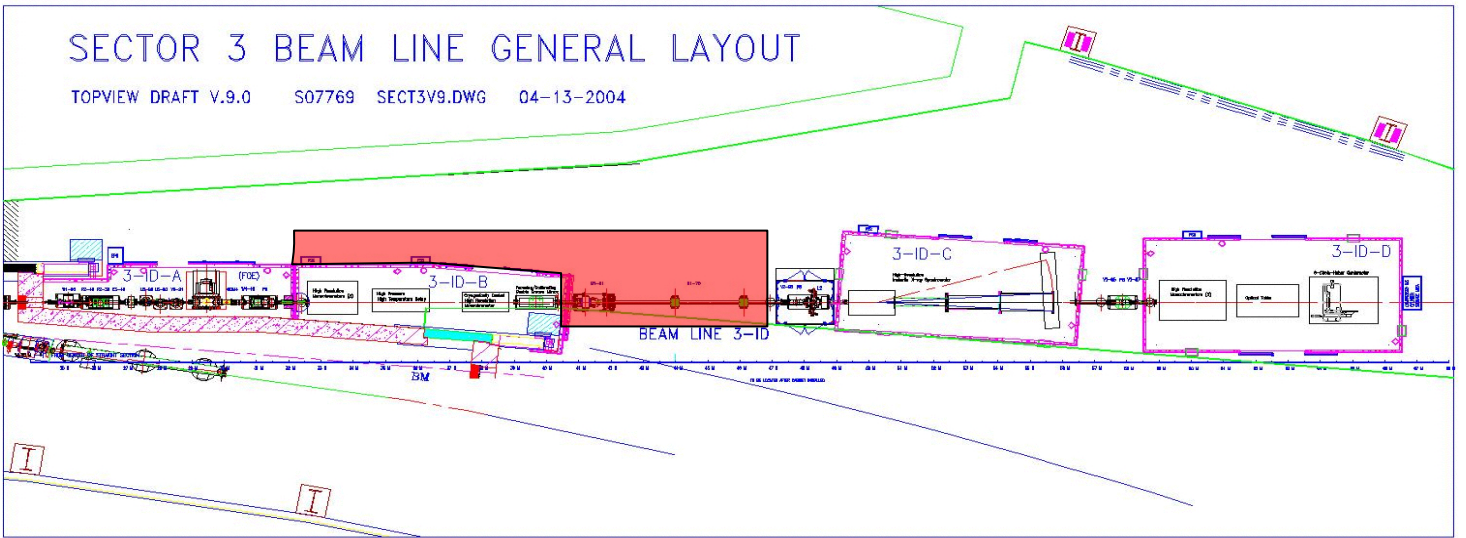
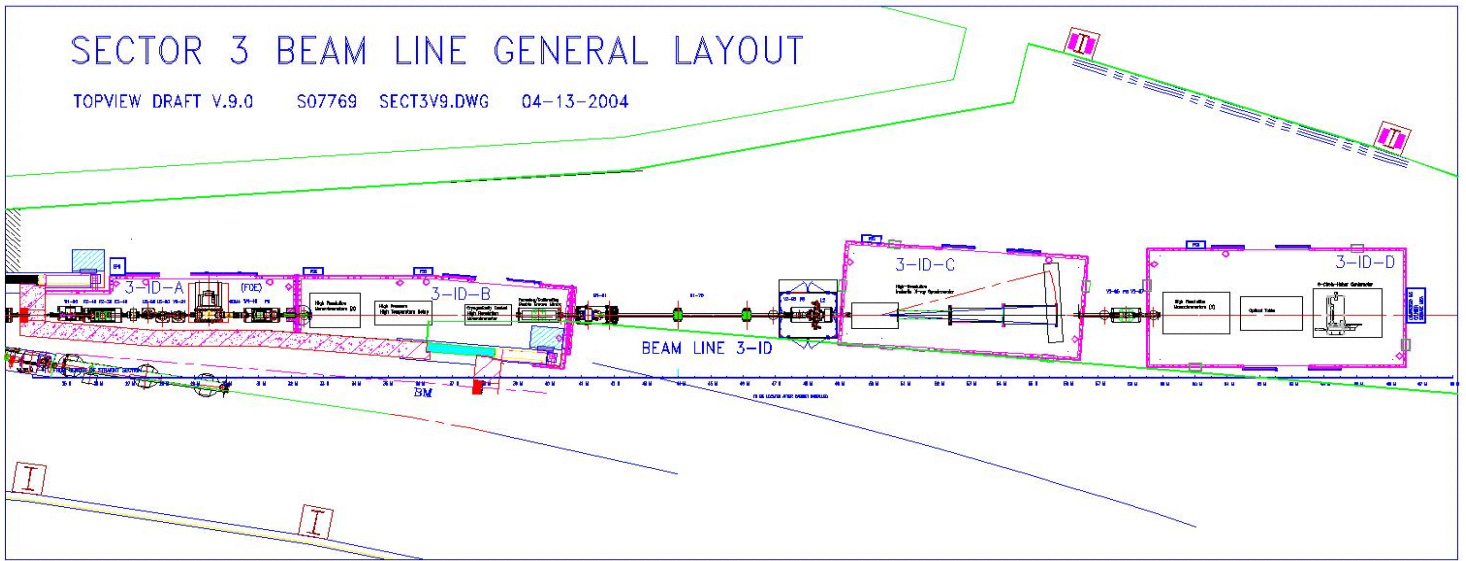


Figure 1. The current (above) and proposed (below) layout of Sector 3-beamline

Appendix 2. Undulator selection for 3-ID beamline

Sector 3 beamline has been at the forefront of undulator development since the beginning of the APS. The first short period device (2.7 cm period) was installed at 3-ID, as well as first full length device (i.e. Two 2.4m length devices) and the first short gap insertion device vacuum chamber (8.5 mm magnetic gap) were all used at this beamline. Now we would like to propose to have also an extended straight section (12.5 m long) and either cryogenically cooled in-vacuum device or better a superconducting device. For the purpose of discussion the following assumptions are made:

1. The straight section is extended to 12.5 m, and at least 10 m is available for the insertion device.

2. The minimum allowed gap is 7 mm.

3. Cryogenically cooled and hybrid type in-vacuum device is assumed, such that a magnetic field enhancement of 30 % is assumed over the room temperature. This, we believe is conservative, based on what is already achieved.

4. The period of the device (1.8 cm) is chosen such that at the shortest possible gap, the first harmonic energy is 14 keV.

(1) T. Hara, et al, *Physical Review Special Topics - Accelerators and Beams*, v. **7**, 050702 (2004)

(2) T. Tanaka, et al, *New Journal of Physics* 8 (2006) 287

5. The device for Sector 3 is tunable between 14 and 22 keV, given by the ^{57}Fe and ^{151}Eu nuclear resonance energy and Si (18 6 0) back-reflection of the IXS analyzer.

6. A second beamline should be used for ^{83}Kr , ^{149}Sm , ^{119}Sn , and ^{161}Dy , ^{121}Sb , and ^{145}Nd , ^{61}Ni isotopes, as well as development of high-resolution optics. An insertion device designed for 9-13 keV in the first harmonics can cover these isotopes. This will provide a realistic chance for these applications to get sufficient beamtime. Approximately, %30-60 % of beamtime at another beamline should be available during the timing modes at the APS.

Appendix 3. Detector development for nuclear resonant scattering

The main detector difficulty for nuclear resonant scattering is the ability to handle large incident flux (10^9 Hz or more), good time resolution, reasonable efficiency, and for inelastic scattering applications large area. Some of the desired parameters can be combined into an array detector like the one specified below. The detector is an Avalanche Photodiode Detector array. A desired set of specifications could be as follows:

Time resolution:	1 nsec
Area:	$10 \times 10 \text{ mm}^2$
pixel size:	$0.3 \times 0.3 \text{ mm}^2$
Thickness:	0.1-0.2 mm Si
Bump bonded ASIC,	
Integrated electronics (amplifier + threshold + time discriminator)	
Count rate:	10^7 Hz
Fast frame readout	< 10 ns

It turns out that such detectors are also needed for intensity fluctuation spectroscopy, thus we see a common ground with them. Similar detectors are being developed as European/Japanese collaboration, and either we take place in such development projects, or we end buying some version of the commercial detectors a few years later.

We prefer that our detector group at the APS spearheads an effort and obtain/participate/develop APD based detectors.

Appendix 4: New optics for inelastic x-ray scattering

Here we need to separate the need for high-resolution momentum-resolved inelastic x-ray scattering (IXS) and nuclear resonant scattering (NRS).

For momentum resolved IXS, we need to upgrade the current spectrometer to extend the momentum transfer range without paying a penalty to polarization. Employing a vertical scattering geometry, and using array detectors to avoid a scanning arm can best accomplish this feature. We have conceptual ideas, and we would like to develop these ideas into a feasible project if resources can be made available. This effort will also require to build ~100 new analyzers, with good reflectivity and reproducibility.

For NRS, we need to put renewed effort into better resolution tunable monochromators. We believe 0.1 meV is feasible at the APS as User instrument for $10 < E < 30$ keV. Furthermore, we need to develop new crystal optics for the 30-100 keV ranges, which will require a new approach.

Finally, we need to dedicate new focusing optics to accommodate each instrument separately to minimize the set-up time, optimize the beam size with no compromises. This would require a combination of new state-of-art bimorph K-B mirrors.

Appendix 5: Special Environments

Today, almost all beam lines at modern synchrotron sources have specialized equipment, including high pressure, high or low temperature, high magnetic field, powerful lasers, ultra high vacuum in-situ deposition systems, etc. We have some of these equipments, we would like to extend the range by acquiring more stable fiber laser sources, and in-situ deposition system for nano-magnetism and lattice dynamics of thin layers and interfaces, high magnetic fields exceeding 10 T for multi-ferroic systems under high pressure, membrane cells for remote-controlled high-pressure experiments, and in-situ pressure reading Raman systems. For each of these systems we have substantial user base so that we are in a position to articulate the need.

Appendix 6: Cost estimate

Layout modifications of 3-ID beamline	1,000,000
Undulators	2,000,000
Detectors	1,500,000
New optics for 3-ID beamline	3,000,000
Special environments	3,000,000
Total	10,000,000 US \$