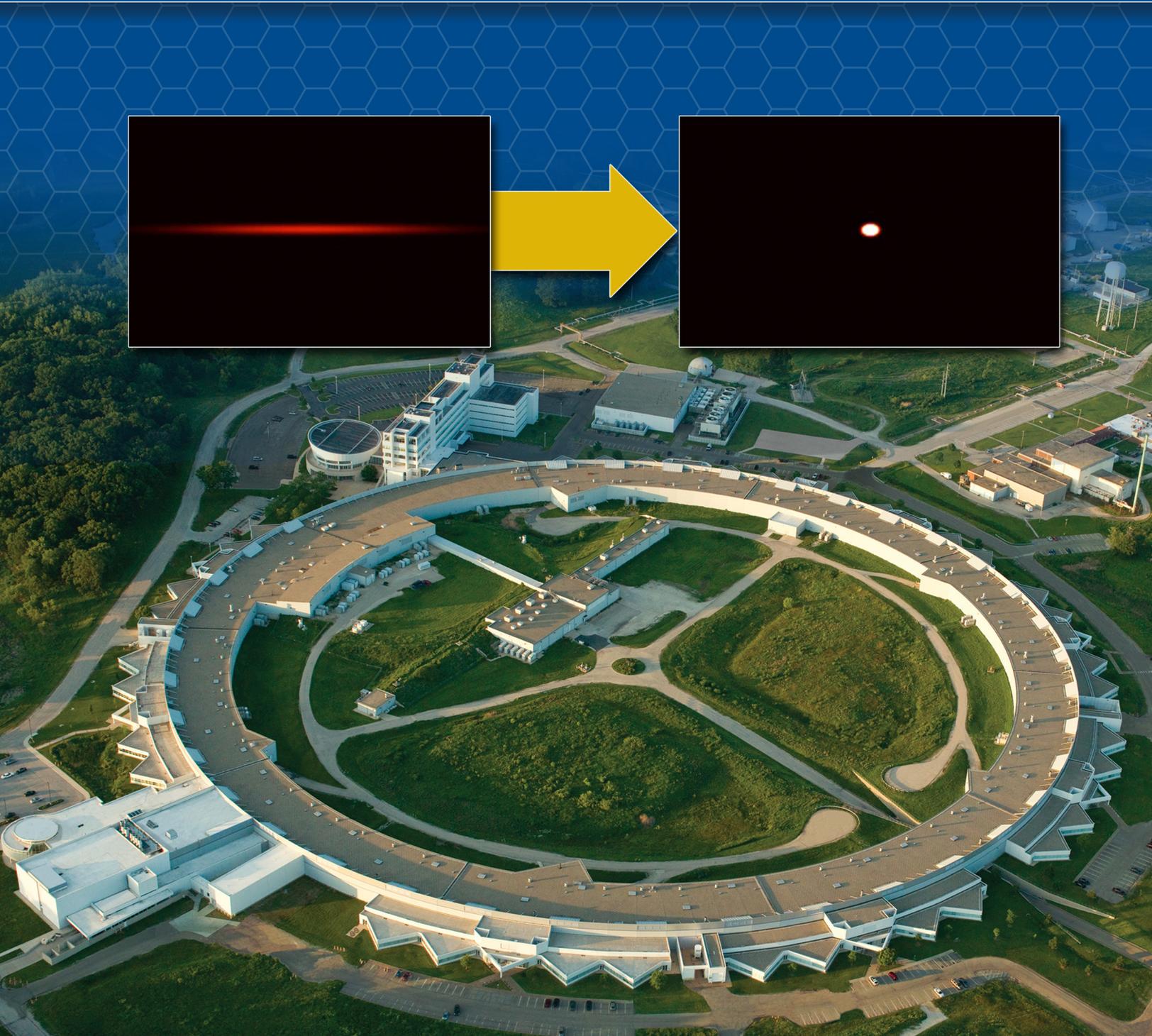
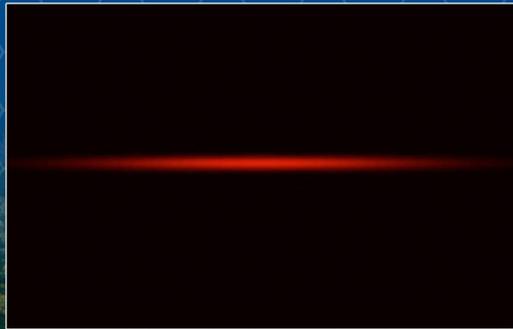


A MBA Lattice at the APS:

A New Generation

A preliminary report on the October 2013 workshop
on new science opportunities provided by a
multi-bend achromat lattice at the APS



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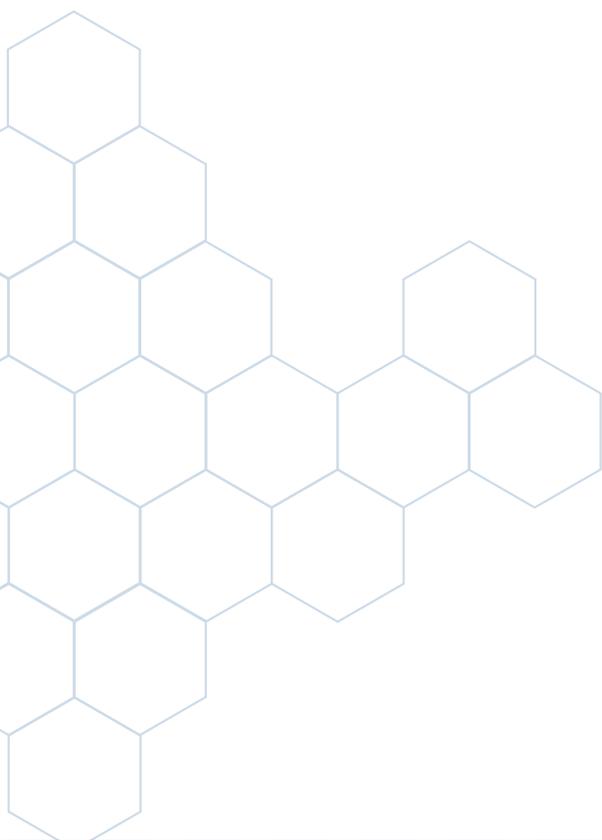


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1. EXECUTIVE SUMMARY

We are standing at the brink of a great opportunity – the possibility of building America’s first fourth-generation storage ring. At the Advanced Photon Source (APS), and throughout the global light source community, scientists are developing a new storage ring magnet lattice design – the multi-bend achromat (MBA). This new technology promises a revolutionary increase in brightness that could reach three full orders of magnitude beyond that of the current APS. The X-ray beams from this new, fourth-generation high-energy storage ring source will be nearly diffraction-limited, with smooth wavefronts that can focus the most flux into the smallest possible spot.

The new MBA lattice technology will provide three key improvements over the current APS design:

- ▶ The ability to focus all of the X-rays down to nanometer-size spots,
- ▶ 100 to 1,000 times increase in coherent flux, which will open up new experimental capabilities, such as coherent diffraction imaging and ptychography,
- ▶ 100 to 1,000 times increase in brightness per pulse for time-resolved experiments.

As we look ahead, it is clear that we are entering a new frontier of X-ray science – one that will give us unprecedented access to the inner workings of matter, and that will transform our ability to understand and manipulate matter at the nanoscale. The key improvements noted above will create an unparalleled X-ray microscope with the capability to access the full array of powerful X-ray contrast modes, from fluorescence and spectroscopy to diffraction and inelastic scattering. In a recent workshop held at the APS, representatives from a wide range of scientific disciplines discussed the potential impacts of these new capabilities, which will make it possible to find answers to fundamental scientific challenges that today remain beyond our grasp:

- ▶ The ability to observe and characterize individual structures as small as single atoms inside materials will be revolutionary, making it possible to solve vitally important problems in chemical catalysis, cell biology, environmental science, structural materials, and functional materials. For example, understanding and controlling the electron spin states of individual point defects in wide-bandgap semiconductors could provide the long-lived, controllable coherent quantum states necessary for quantum computing, allowing scientists to solve massive big-data problems that currently remain intractable.
- ▶ Probing all of the length scales of a battery *in operando*, from atoms to the full electrode, will enable researchers to measure transformation pathways, determine the local state of charge, and understand failure modes, all in a single experiment. This comprehensive approach will greatly enhance our understanding of the mechanisms that cause mechanical, surface, and chemical degradation, ultimately leading to technologies that will significantly extend battery life.

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- ▶ By understanding the molecular basis of function in increasingly complex biomolecular entities, from membrane protein assemblies to intracellular structures, we will answer fundamental questions of biology and potentially develop breakthrough treatments for disease. For example, recent research has focused on the critical role that metal ions play throughout biochemistry; a dramatic increase in X-ray brightness and stability will make it possible for researchers to observe the interactions between these metals and protein chemistry, yielding important insights into a wide range of biological processes, from metabolism to photosynthesis.
- ▶ The unprecedented coherent flux at high energies will facilitate exciting new research techniques, such as coherent diffraction imaging with resolution approaching the X-ray wavelength, and photon correlation spectroscopy for dynamic studies. This technology also will provide researchers with the highest possible spatial resolution over a broad temporal range, and with X-ray sensitivity to atomic structure and strain, elemental composition and chemical states, and electronic and magnetic structure. To take full advantage of this new source, we will invest in advanced X-ray beamline technologies and data infrastructure.

One of strengths of an MBA design at the APS is that it is very economical because large leaps in science output can be made using existing beamline infrastructure. Even larger benefits can be obtained with modest beamline investments. This provides a unique opportunity for phased improvements that will keep up with the future needs of the scientific community.

The MBA lattice is at the core of the APS Upgrade's goal – to deliver a powerful, versatile facility for science using high-brightness, high-energy X-rays. Incorporation of this game-changing technology into the APS will accelerate design of new high-performance materials, speed discovery of lifesaving pharmaceuticals, advance development of sustainable energy sources, and enable expansion of green manufacturing, giving the United States an enduring competitive edge across a wide array of industries and delivering profound impacts on the X-ray science community for decades to come.

2. INTRODUCTION

Each generation of X-ray sources has leapfrogged beyond its predecessor by incorporating revolutionary new designs and enabling transformational new science. The U.S. Department of Energy's current suite of facilities can be ranked as the most effective and prolific discovery machines ever built, across all fields of science and engineering. Although they have enabled many scientific discoveries, even more complex problems have arisen that require higher X-ray beam brightness to provide higher spatial resolution and improved sensitivity. We are now confident that developing a new storage ring magnet lattice design – the multi-bend achromat (MBA) – will deliver the fourth generation of storage-ring sources, with a thousand-fold increase in brightness and coherent flux, and performance approaching the ultimate diffraction limit.

When we first designed and built the APS, we were motivated by a vision of the transformative science that a new generation of storage-ring synchrotrons would make possible. The APS was the first third-generation hard X-ray synchrotron in the United States. Its undulators provided a huge leap in brightness over its predecessors, producing a corresponding leap in scientific capability and impact, and making it possible to meet – and exceed – our initial expectations. Today, the robust array of X-ray capabilities provided by the DOE's third-generation light sources are yielding important discoveries in physics, chemistry, biology, materials science, and many other disciplines.

Quantum spintronics

A

Nuclear spin

$B(t)$

$V(t)$

B

0 Height 7 nm

D

10 μm

Figure 2.1.

An ultimate challenge is to characterize individual structures at the scale of atoms, an ability that could revolutionize the field of quantum spintronics. The electron spin states of single point defects in wide-bandgap semiconductors (a) promise to provide the long-lived, controllable coherent quantum states needed for cryptography, sensing, and quantum computing to crack factoring and search problems inaccessible to the most powerful classical computers. Understanding how to create and manipulate interacting arrays of these “designer atoms” holds the key to developing this new technology. Optical studies show that each defect in an array can have different properties (b). But we can only guess at the defect structure and then use modeling to look for correspondence with its behavior. What we need is a probe sensitive to the defect's chemistry and its surrounding strain field, *in situ* during optical and electrical manipulation. A new generation of X-ray source with significantly higher brightness will open the way to these capabilities, through strain imaging using coherent X-ray diffraction and nanoprobe X-ray fluorescence studies approaching the ultimate sensitivity: individual atoms.

Images from D.D. Awschalom, *et al.*, Quantum Spintronics: Engineering and Manipulating Atom-Like Spins in Semiconductors. *Science*, 339:1174, 2013.

HIGHER BRIGHTNESS IS CRITICAL TO ACHIEVING KEY SCIENTIFIC GOALS

Increasingly, however, researchers require higher brightness X-ray beams than are currently available to answer complex experimental questions. We need higher brightness high-energy X-ray sources to observe systems as they function under real conditions and in extremes of pressure, temperature, and electric and magnetic fields. Increasingly, we also find that the systems with the most potential to meet global needs in health, energy, sustainability, and security are complex, heterogeneous systems that require probing across multiple length scales. Our scientific goals cannot be achieved without reaching higher resolutions in space, time, and energy and the ability to characterize individual structures at the atomic scale, combined with the full range of X-ray research techniques.

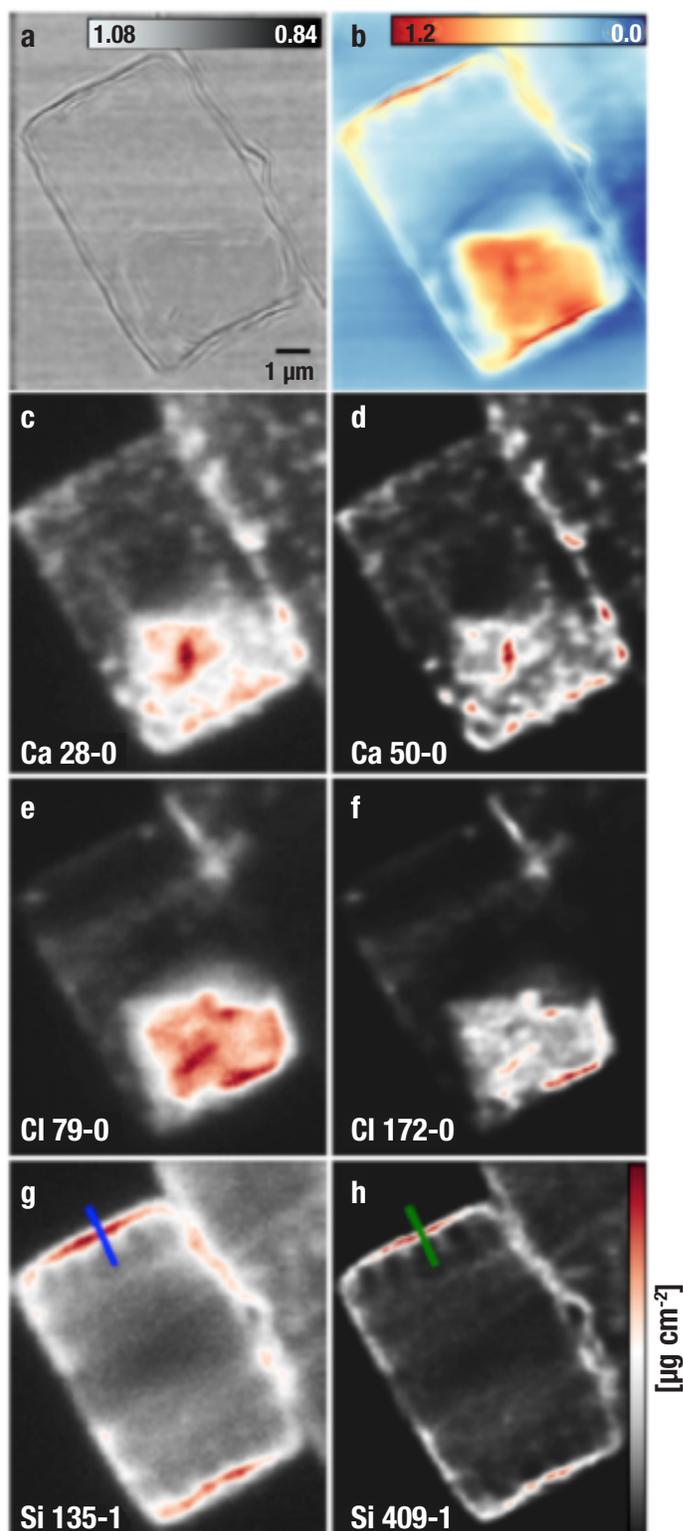
The increase in brightness of up to a thousand-fold delivered by an MBA lattice at APS will transform our capabilities for imaging and studies of dynamics. The unprecedented coherent flux, a two to three order of magnitude improvement, will enable widespread use of exciting new research techniques, such as coherent diffraction imaging with resolution approaching the X-ray wavelength, and photon correlation spectroscopy for dynamic studies reaching nanosecond time scale. The gain in brightness will allow the full array of powerful X-ray contrast modes, from fluorescence and spectroscopy to diffraction and inelastic scattering, to be used for scanning probe imaging with nanoscale resolution and improved time resolution, which enables measurements of dynamic processes. The high brightness at high energy provided by the MBA lattice at the APS will significantly enhance penetrating X-ray studies under extreme conditions and in real operating environments. This will transform our ability to observe nano- and meso-scale structures evolve *in situ* during synthesis and *operando*, enabling the highest possible spatial resolution over a broad temporal range. This also will provide X-ray sensitivity to atomic structure and strain, elemental composition and chemical states, and electronic and magnetic structure.

Over the past year, it has become clear that the MBA lattice will provide the orders-of-magnitude increase in X-ray brightness required to achieve these goals. Advances in accelerator simulation and engineering support our confidence in the feasibility of this technology.

The APS is the right place to deploy the MBA technology. It is the nation's largest X-ray synchrotron, and its large circumference ring takes full advantage of MBA technology. The APS is the nation's premier source for high-energy X-rays, which offer the greatest opportunity for increasing brightness, given that emittance can be reduced by orders of magnitude at high energies before reaching the diffraction limit.

So we now face a new opportunity to transform the field of X-ray science once more, giving our nation's scientists the tools that they need – and that they have requested – to overcome roadblocks to discovery.

Cellular imaging using ptychography and super-resolution nanoprobe



A key challenge in life sciences is to understand the molecular basis of function in increasingly complex entities, from membrane protein assemblies to intracellular structures. To gain this knowledge, we need not only to extend crystallographic structural determinations to smaller crystals with larger unit cells, but also to develop higher-resolution imaging capabilities into the nanometer range. A rapidly progressing imaging technique using diffraction of coherent X-rays known as “ptychography” promises breakthroughs in this area with the aid of the high coherent flux from MBA lattice technology. The spatial resolution of ptychography is not limited by the probe size and can approach the X-ray wavelength. It also provides a precise determination of the probe shape, which allows “super-resolution” analysis of scanning probe fluorescence images to sizes much smaller than the probe size. Here we see combined ptychographic and elemental fluorescence imaging of the freshwater diatom *C. meneghiniana*. Panels (a) and (b) show ptychographic phase and amplitude images. Resolution of original elemental images (c,e,g) is significantly improved (d,f,h) after deconvolution of probe shape.

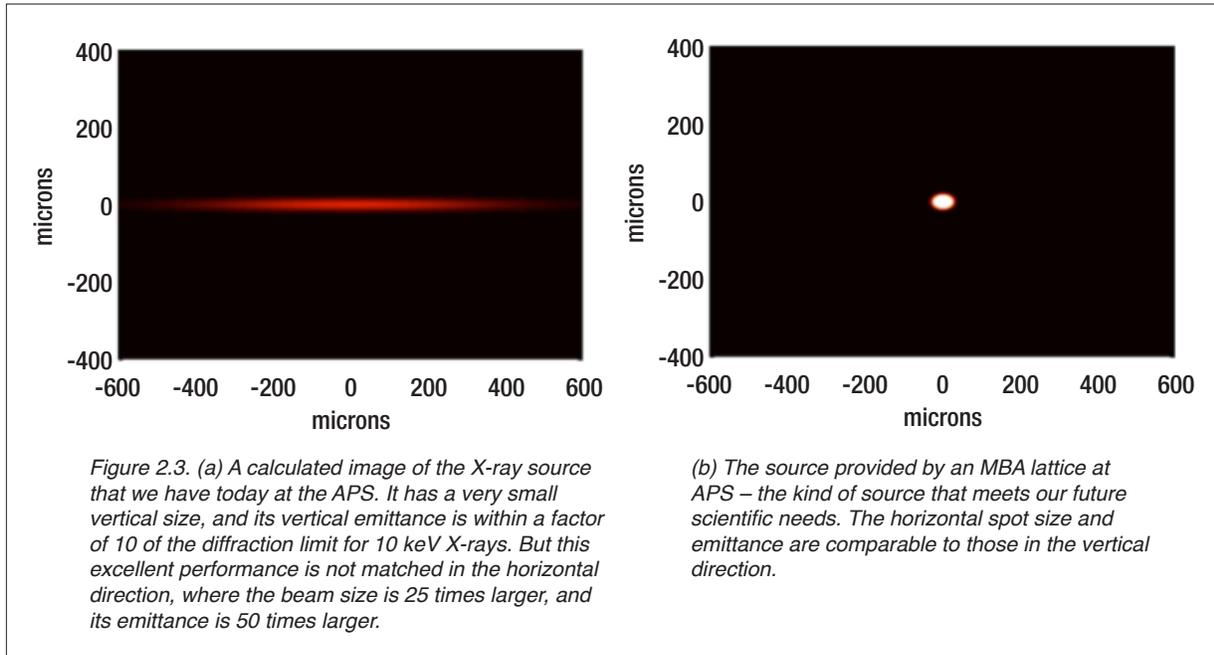
Images from D. J. Vine, *et al.*, Nanoscale fresnel coherent diffraction imaging tomography using ptychography. *Opt. Express*, 20:18287, 2012.

Figure 2.2

Highlights of Upgraded Techniques		
X-ray Technique	Key Benefit	New Capabilities and Improved Resolutions
Coherent Diffractive Imaging (CDI) & Ptychography	Lensless imaging technique that exploits coherence to reconstruct 2-D and 3-D structures. See page 60.	<ul style="list-style-type: none"> ▶ Signal increases of a factor of 100 to 1,000 ▶ Measurements of disordered structures ▶ Resolution approaching the atomic scale ▶ Time-resolved ptychography
X-ray Phase Contrast Imaging (PCI)	Technique that exploits variation in refractive index to increase contrast for penetrating high-energy X-rays. See page 57.	<ul style="list-style-type: none"> ▶ Projection microscope for full-field PCI with matched vertical and horizontal resolution ▶ Simultaneous optimization of image contrast and temporal resolution
X-ray Photon Correlation Spectroscopy (XPCS)	Method that uses temporal intensity variation of X-ray scattering to probe the dynamics of matter. See page 59.	<ul style="list-style-type: none"> ▶ Factor of 10,000 to 1,000,000 improvement in resolution ▶ Simultaneous nanosecond and nanometer temporal resolutions ▶ Large-angle XPCS approaches atomic length scale dynamics ▶ XPCS at higher energies and for diverse samples and environments
Scanning Probe Imaging	Raster scanning method that focuses the X-ray beam across a sample to produce an image.	<ul style="list-style-type: none"> ▶ Factor of 100 to 1,000 improvement in temporal resolution ▶ Microscopy of dynamic processes using the full array of powerful X-ray contrast modes ▶ Longer working distances ▶ <i>In situ</i>, real time nanoprobe experiments ▶ Ability to find rare events and characterize large populations using high throughput

THE MBA LATTICE FULFILLS THE RESEARCH MISSION OF THE APS UPGRADE

By incorporating MBA technology into the APS Upgrade, we can amplify its science mission and open up research opportunities that have previously been out of reach.



Plans for the APS Upgrade have been guided by two overarching themes developed in a series of science planning workshops with the community:

- ▶ Studying real materials under real conditions in real time, and
- ▶ Mastering structures across length scales from millimeters to nanometers through X-ray imaging.

The MBA technology offers a powerful new approach to achieving these Upgrade goals, providing orders-of-magnitude increases in source brightness and coherent flux to match advances in beamline instrumentation. This transformational increase in brightness provides three very big wins:

- ▶ The ability to focus all X-ray flux down to nanometer-size spots,
- ▶ Unprecedented brightness per pulse for time-resolved experiments, and
- ▶ A very high coherent flux that opens up new experimental capabilities, such as ptychography.

In Figure 2.3, the impact of the MBA lattice on the APS beam is immediately apparent. Figure 2.3 (a) shows a calculated image of the present electron beam at the APS. It has a very small vertical size (~25 microns full width at half maximum), and its vertical emittance is within a factor of 10 of the diffraction limit for 10 keV X-rays. But this excellent performance is not matched in the horizontal direction, where the beam size is 25 times larger (~650 microns full width at half maximum), and its

emittance is 50 times larger. Figure 2.3 (b) shows the source provided by an MBA lattice at APS. The spot size and emittance have been squeezed down to values nearly equal to those of the vertical, making the full beam much more useable.

MBA LATTICE ENABLES BREAKTHROUGH RESEARCH FOR APS USERS

In this report, we summarize a workshop held at the APS on October 21-22, 2013, in which we convened the user community to explore the scientific opportunities offered by an MBA design.

During the workshop, our partners in industry stressed the potential impacts of the brightness increase, which will create revolutionary capabilities to measure nanometer-sized buried structures in state-of-the-art electronic devices and photovoltaic cells. The increased brightness will result in increased sensitivity to detect individual atoms where we now must look at arrays of atoms and will enable study of dilute catalysts *in situ* and *operando*. Pharmaceutical researchers will be able to characterize difficult-to-crystallize macromolecules and to carry out studies at room temperature, accelerating drug discovery. APS users at the workshop noted that the increased brightness and coherence will make it possible to measure structural and electronic properties of matter with unprecedented sensitivity, with impacts in all areas of science. The MBA lattice will enable studies of materials synthesis and deformation, cell biology, and geophysics, with simultaneously applied combinations of sample environments, such as chemical, high pressure, temperature, and magnetic field. The workshop participants concluded that the increased brightness and coherence at high energies will be transformational, and will position APS to remain a world-leading scientific facility for many decades to come.

3. TRANSFORMING SYNCHROTRON SCIENCE WITH THE MBA LATTICE

A new storage ring technology, known as a multi-bend achromat (MBA) lattice, has been under study for several years, both globally and at Argonne National Laboratory, as a possible mechanism for developing a next-generation low-emittance X-ray light source. Until recently, the implementation of such a source was believed to be more than a decade in the future. Several developments, however, have led to this technology maturing much faster than expected. In particular, advances in accelerator simulation codes employing large-scale supercomputers and novel high-field gradient magnet designs have provided confidence that such an MBA lattice could be realized much sooner. In fact, an MBA-type lattice is already being incorporated into the design of two lower-energy synchrotron rings under construction in Sweden and Brazil, and is being considered by a large number of other facilities around the world. The great potential of such a high-brightness X-ray source to provide powerful new capabilities for scientific research using hard X-rays was presented by representatives of the scientific community, including some from the APS, to the Basic Energy Sciences Advisory Committee (BESAC) [1] at its meeting in July of 2013. The committee report endorsed consideration of incorporating this new technology into current plans for upgrading the APS.

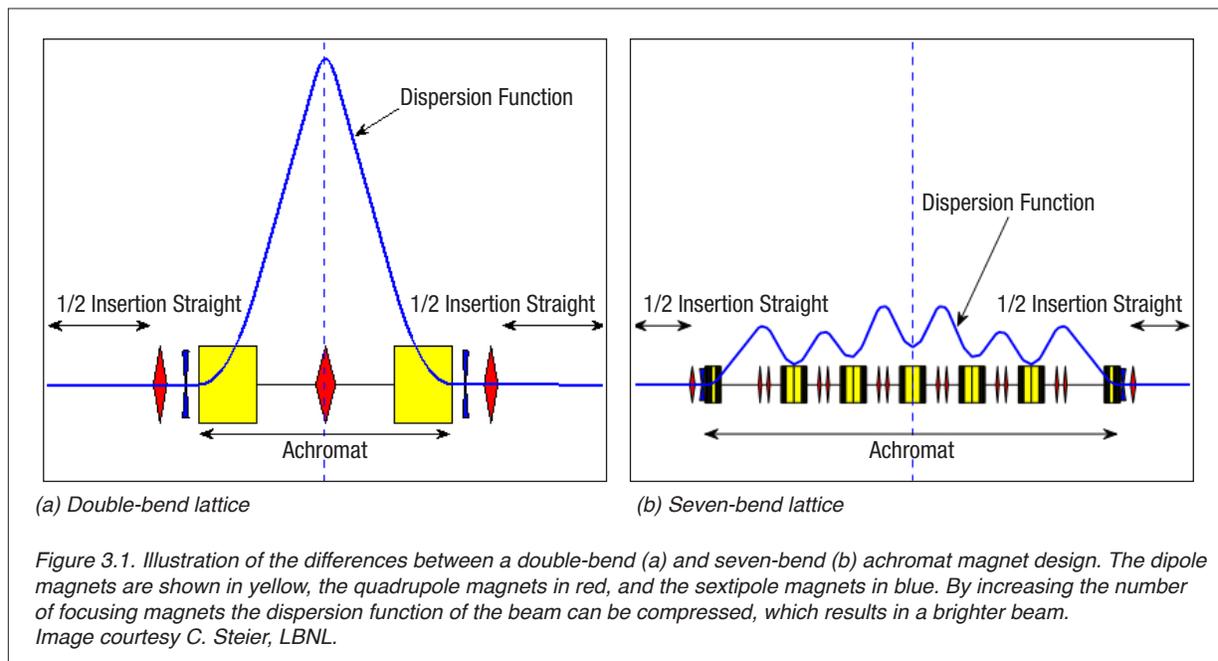
In evaluating possible MBA lattice designs for the APS storage ring, the following design goals were considered:

- ▶ Reducing the electron beam emittance by a factor of 30 to 50 from the present value of 3,100 picometers to under 100 picometers.
- ▶ Reusing the existing storage ring tunnel and maintaining the current X-ray source points for both the insertion devices and bending magnet beamlines.
- ▶ Increasing the beam current from 100 milliamps to 200 milliamps in order to increase the X-ray flux.
- ▶ Deploying on each beamline insertion devices optimized for high brightness in particular spectral ranges and for desired polarization characteristics.
- ▶ Minimizing the downtime for installation and commissioning of the new lattice.

PARAMETERS AND EXPECTED BRIGHTNESS

The key benefit of implementing an MBA lattice at the APS is that it significantly increases the X-ray brightness, which ultimately determines the amount of flux that can be put into a small focal spot and the coherence of the beam. Quantitatively, the brightness is simply the X-ray flux normalized by its size and its angular divergence, which can be no smaller than that of the electron beam producing the synchrotron radiation. The emittance of a storage ring is the product of the size and divergence of the electron beam. Thus, a lower emittance results in a higher brightness X-ray source.

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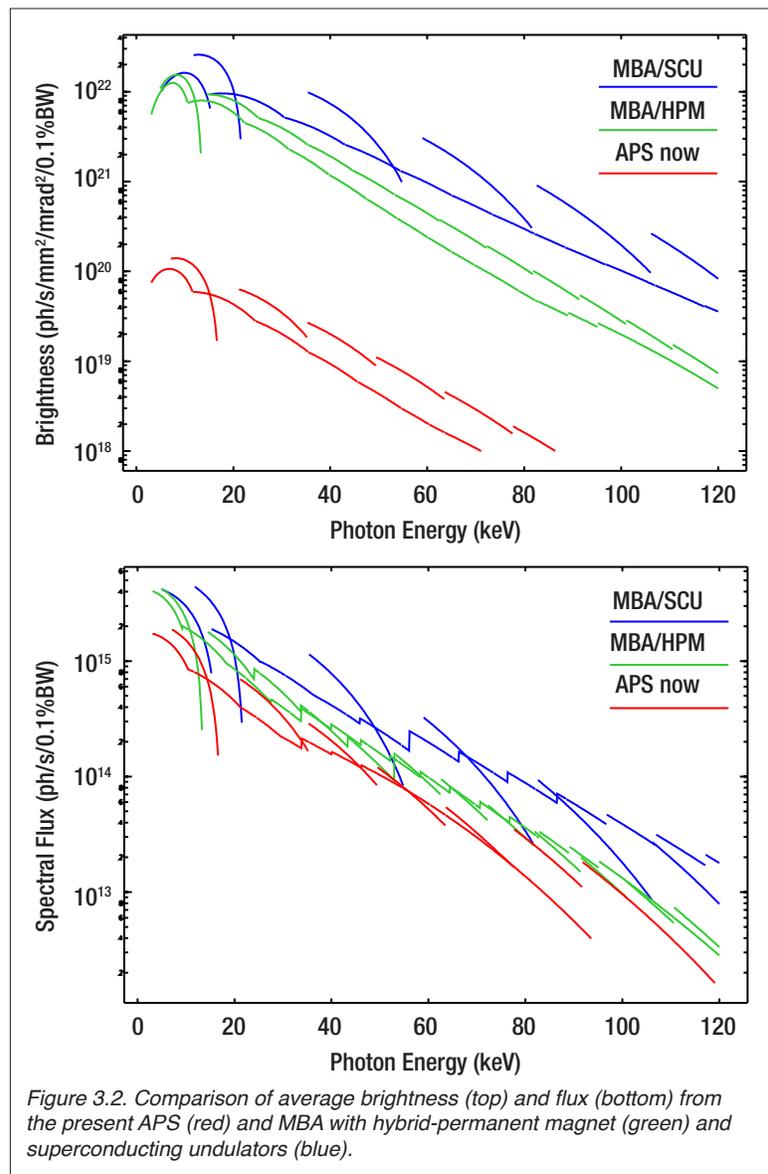
The current APS design has two bending magnets in each of the 40 sectors that make up the ring. This is referred to as a double-bend achromat (DBA) design. An MBA design takes advantage of the fact that the horizontal emittance scales with the inverse cube of the number of these bends, thus large reductions in the emittance can be realized by simply increasing the number of bends and placing additional horizontal focusing magnets between them. For example, increasing the number of bends from two to seven in the current APS storage ring could result in an emittance drop of $2^3/7^3 \sim 1/43$ of its present value. The emittance is also proportional to the square of the electron energy, so reducing the operating energy from 7 GeV to 6 GeV further reduces the emittance. These two changes would result in an electron beam with a horizontal emittance roughly equivalent to that of the vertical emittance of today's APS.

A preliminary MBA lattice design that retains the same circumference, number of sectors, and beamline positions as the current APS storage ring has been developed. Reusing the existing facility infrastructure greatly reduces both overall costs and time for implementing an MBA source, when compared to the construction of a completely new facility. The MBA design being considered is based on the seven-bend achromat (7BA) cell shown in Figure 3.1. This is similar to what is currently under construction at the MAX-IV synchrotron in Sweden and being studied for the upgrade of the ESRF synchrotron in France. The parameters of the current APS and expected performance for two possible MBA operating modes (with differing number of electron bunches in the ring optimized for timing and maximum brightness) are listed in Table 1 [2]. The table points to the key improvements in horizontal beam size that the MBA lattice will provide, which will not only result in smaller focal spots, but also greatly improve the efficiency of most optics.

Quantity	Symbol	Units	APS Now	APS MBA Timing Mode	APS MBA Bright. Mode
Beam Energy	E	GeV	7	6	6
Beam current	I	mA	100	200	200
Number of bunches	N_b		24	48	324
Bunch duration	σ_t	ps	34	70	68
Bunch spacing	T_b	ns	153	77	11
Bunch rep. rate	f_b	MHz	6.5	13	88
Emittance ratio	$\kappa = \epsilon_y/\epsilon_x$		0.016	1.0	0.1
Horizontal emittance	ϵ_x	pm	3100	42	60
Horizontal beam size	σ_x	μm	275	7.4	8.8
Horizontal beam divergence	$\sigma_{x'}$	μrad	11	5.7	6.8
Vertical emittance	ϵ_y	pm	40	42	6
Vertical beam size	σ_y	μm	10	10.9	4.1
Vertical beam divergence	$\sigma_{y'}$	μrad	3.5	3.8	1.4

Table 1: Preliminary MBA lattice parameters for insertion devices source points compared to current APS.

Unlike the present-day APS ring, the MBA lattice would be operated in on-axis injection mode (“swap-out” instead of “top-up”) [3,4]. Because of this, the new ring will not be restricted to traditional insertion devices with small vertical gaps and relatively large horizontal gaps. Instead, novel devices such as superconducting helical devices producing circular polarization could be implemented for the first time in a storage ring light source. Figure 3.2 shows calculations of the expected 100 to 1,000-fold improvement in X-ray brightness anticipated from this MBA lattice design, compared with those for the present-day APS. These calculations assume that all insertion devices would occupy the maximum possible length of 4.8 meters for permanent-magnet devices and 3.7 meters for superconducting undulators (SCUs). The lower emittance directly translates into a much higher coherence of the X-ray beam, approaching the so-called ultimate diffraction limit for lower X-ray energies (<5 keV). Such beams will truly revolutionize imaging and dynamic X-ray studies of materials.



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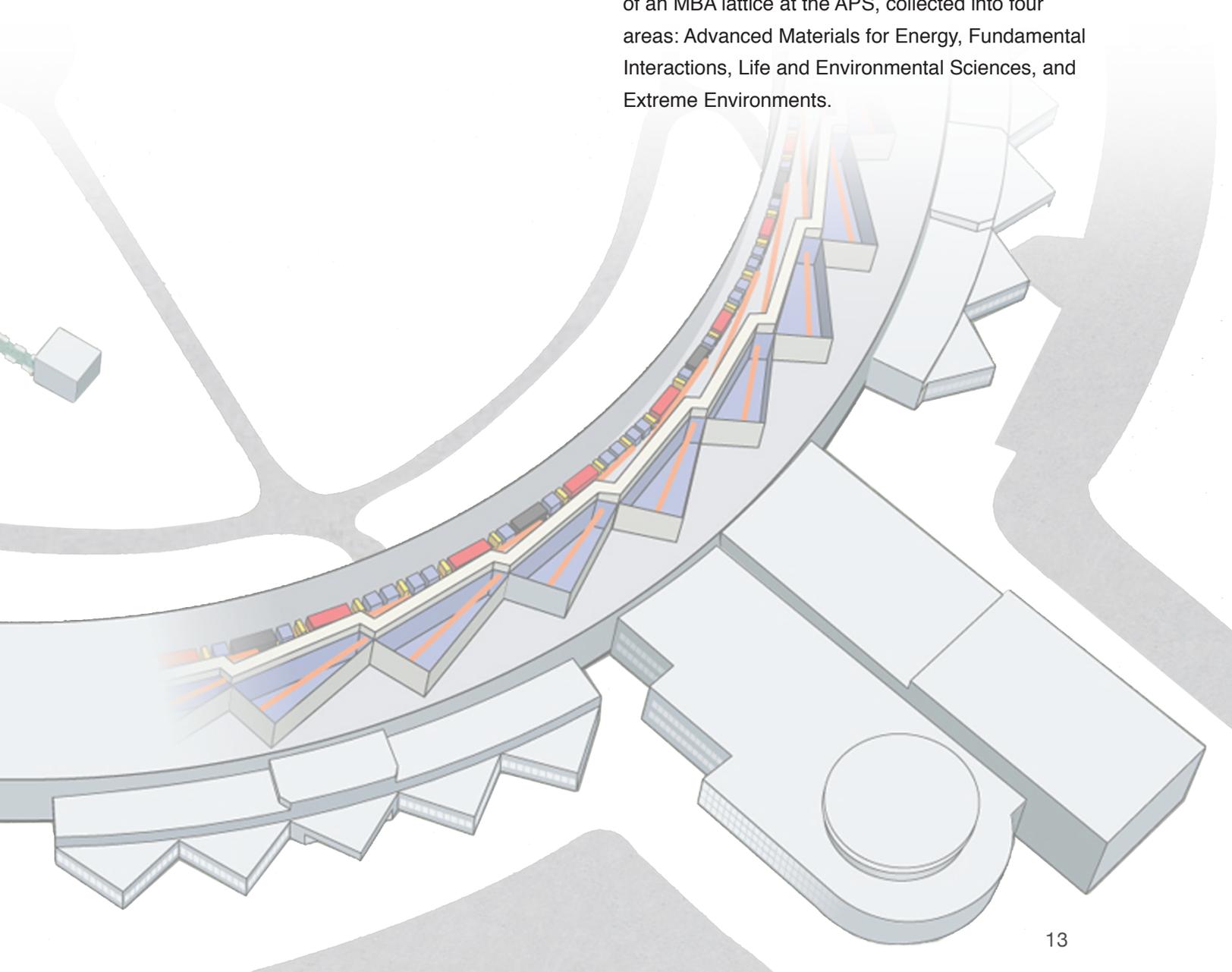
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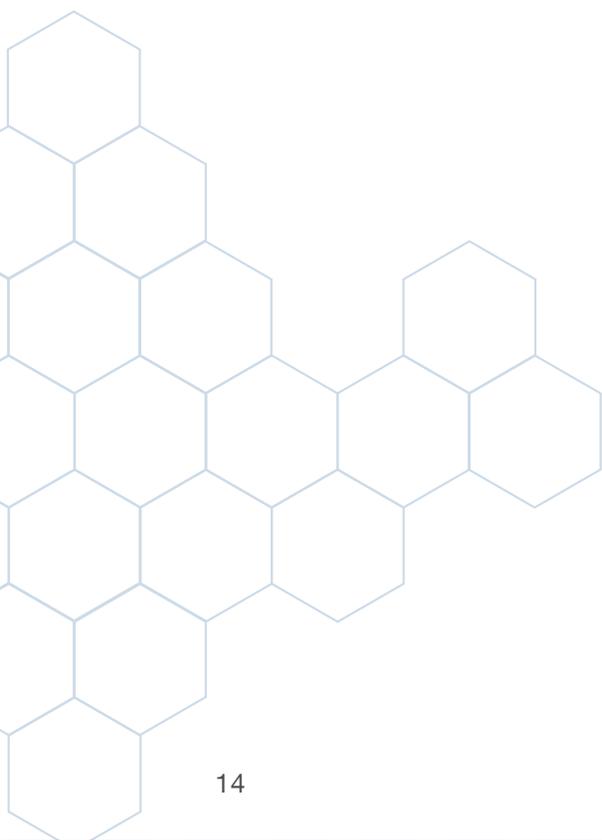
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4. SCIENTIFIC OPPORTUNITIES CREATED BY THE MBA LATTICE

This section provides examples of the scientific impact of an MBA lattice at the APS, collected into four areas: Advanced Materials for Energy, Fundamental Interactions, Life and Environmental Sciences, and Extreme Environments.





BETTER CAPABILITIES TO TACKLE GRAND CHALLENGES

Today the nation and the world face a multitude of roadblocks to progress, sustainability, safety, health, and economic prosperity. During the last decade, scientific advisory committees working with the U.S Department of Energy have distilled these roadblocks into five interrelated grand challenges and identified opportunities for overcoming them to obtain a truly transformational understanding of matter.

The upgraded APS will provide the needed research capabilities to help the nation speed discovery in each of these areas. Below are examples of how the APS Upgrade offers new capabilities to help the nation build a better future.

Grand Challenge #1. How do we control materials processes at the level of electrons?

- ▶ X-rays 1,000 times brighter than currently available will enable the single-atom/single-dislocation sensitivity studies needed to understand how to directly manipulate the charge, spin, and dynamics of electrons to control and imitate the behavior of physical, chemical, and biological systems, such as digital memory and logic. This could put quantum computing, cryptography, and long-lived controllable sensing within our grasp. (See pages 3 and 24.)
- ▶ An ability to offer a wider range of multimodal characterization at higher resolutions and in more-extreme environments will provide the data needed to synthesize conversion of the Sun's energy into fuel through artificial photosynthesis. This will require unprecedented real time 3-D structure profiling of *operando* chemical reactions. (See page 21.)

Grand Challenge #2. How do we design and perfect atom- and energy-efficient synthesis of revolutionary new forms of matter with tailored properties?

- ▶ Characterization of nano catalysts as small as 10 atoms under high temperatures and pressures will enable the design of selective catalysts that produce no unwanted byproducts. (See page 20.)
- ▶ *In situ* studies with spatial resolution of about 50 nanometers and dynamics in the 10-millisecond time scale will provide unparalleled opportunities to study materials that operate at the theoretical limits of strength and fracture resistance. Also, this will open up the ability to initiate small-fatigue cracks and observe them as they grow, even in the absence of strong-absorption contrast. (See pages 23 and 25.)

Challenge #3. How do remarkable properties of matter emerge from complex correlations of the atomic or electronic constituents and how can we control these properties?

- ▶ Very intense, tens of nanometer spot size X-ray beams combined with multimodal characterization will provide a path towards understanding the collective behavior of billions of electrons and atoms manifesting new phenomena, such as new states of matter or new functionality combining contradictory properties. (See pages 1, 20, 23, 30, 33, and 50.)

Grand Challenge #4. How can we master energy and information on the nanoscale to create new technologies with capabilities rivaling those of living things?

- ▶ A dedicated X-ray interfacial science facility for nondestructive *in situ* real-time monitoring of buried interfaces at atomic resolution providing the ability to synthesize fundamental new structures with atomic-scale precision. (See pages 21 and 31.)
- ▶ The MBA lattice will enable a new method to evaluate alternative barrier layer fabrication strategies to develop defect-tolerant electronic circuits by pinpointing *in situ* the location, quantities, structure, and chemical state of impurities. (See page 24.)

Grand Challenge #5. How do we characterize and control matter away - especially very far away - from equilibrium?

- ▶ The most extreme environments generally can only be realized across small volumes. The intense sub-micron X-ray beams generated by the MBA lattice will provide unprecedented opportunities for probing the structure, correlations, and dynamics of matter at extremes, including pressures beyond 1 megabar, magnetic and electric fields beyond 20 Tesla, and high temperatures. These capabilities will shed light on general principles of materials far away from equilibrium, and provide a path towards controlling these behaviors for new functionalities. (See pages 50, 51, and 53.)
- ▶ The MBA lattice will provide a small beam with high X-ray flux to study individual nanoparticle growth and changes at complex interfaces to achieve adaptive earth chemistry, environmental sustainability, and control of toxins and pollutants. (See pages 44 and 46.)

4.1 DEVELOPING NEW ADVANCED MATERIALS FOR ENERGY

INTRODUCTION

Many of the major global challenges facing society in the 21st century have at their core the inadequate production and inefficient use of energy resources. A critical step in meeting these needs lies in developing high-performance sustainable materials. The APS MBA Upgrade will provide a unique experimental tool for tackling a wide range of scientific and engineering hurdles that slow the discovery and deployment of these advanced materials.

For example, efficient catalysts are a key component in energy production, but in most cases, we lack a fundamental understanding of the synthesis and operation of catalysts. Similarly, understanding and improving the operation of photovoltaic solar cells requires acquiring detailed knowledge of the exciton generation, charge separation, and charge transport processes within the device itself. We can only harness photosynthesis in both natural and artificial materials through improved structural and chemical characterization of each component. But to do that, we need better tools to characterize at the nanoscale level heterogeneity common to many next-generation energy technologies.

The nanometer-scale X-ray beams that the APS MBA upgrade will generate can provide the spatial resolution and photon intensities needed to move research beyond today's practice of observing average material structure and behavior to probing the characteristics of individual nanostructures. Such individual measurements are the crux to providing advanced materials systems with improved energy performance.

Tackling energy challenges requires more efficient use of the energy sources we have today. One of the strongest areas of interest for increased efficiency is the creation of high-performance materials that enable vehicles to use fuel more efficiently, reduce maintenance costs on energy systems, and require less energy.

However, we are using antiquated information to create these lighter automobile components, more heat-resistant turbine coatings, and stronger nuclear power plant alloys. The models used today to understand materials fatigue and fracture behavior to design these high-performance materials are often based on decades-old theories. This produces insufficient information that can lead to large safety margins in designs and require empirical testing of expensive prototypes. The advanced X-ray techniques enabled by the APS MBA Upgrade will allow the direct validation of deformation mechanics simulations on real materials in real conditions to provide a new paradigm of design by simulation that will greatly shorten the development cycle of advanced, energy-efficient systems.

UNDERSTANDING DYNAMIC BEHAVIOR OF BATTERIES *IN SITU*

Many renewable energy sources, such as wind and solar, do not provide a constant source of power, but rather vary with time of day and weather conditions. Therefore, the development of efficient and reliable battery systems is key to integrating these alternative energy sources into the national electrical grid system. New types of batteries will also help propel the next generation of hybrid vehicles, which will travel hundreds of miles farther on a single charge, reducing noxious emissions and empowering national energy independence. However, a limited understanding of the atomic and molecular processes that govern battery efficiency, performance, and safety properties has slowed design, modeling, and implementing of these future-generation batteries.

A battery is an ensemble of complex structures and dynamics on a length scale from nanometers to millimeters and a time scale from femtoseconds to hours and beyond [1]. This presents a great challenge for understanding the structure and function of each component. For example, in an operating battery, the diffusional dynamics of ions in solid electrode materials or electrolytes is a key feature in determining performance. Today X-ray photon correlation spectroscopy (XPCS) can be used to study the diffusion of ions in compounds and alloys that are promising candidates for electrode materials, but only at time scales of seconds. Yet, the diffusive characteristic time of ions can be well below a millisecond, impossible to capture with a temporal probe such as XPCS. Likewise, imaging of battery charging and discharging requires X-ray spectromicroscopy at the nanoscale, which is extremely slow at third-generation synchrotrons because it demands high brilliance. Because of that, imaging a battery is only possible by controlling discharge at speeds well below normal usage rates.

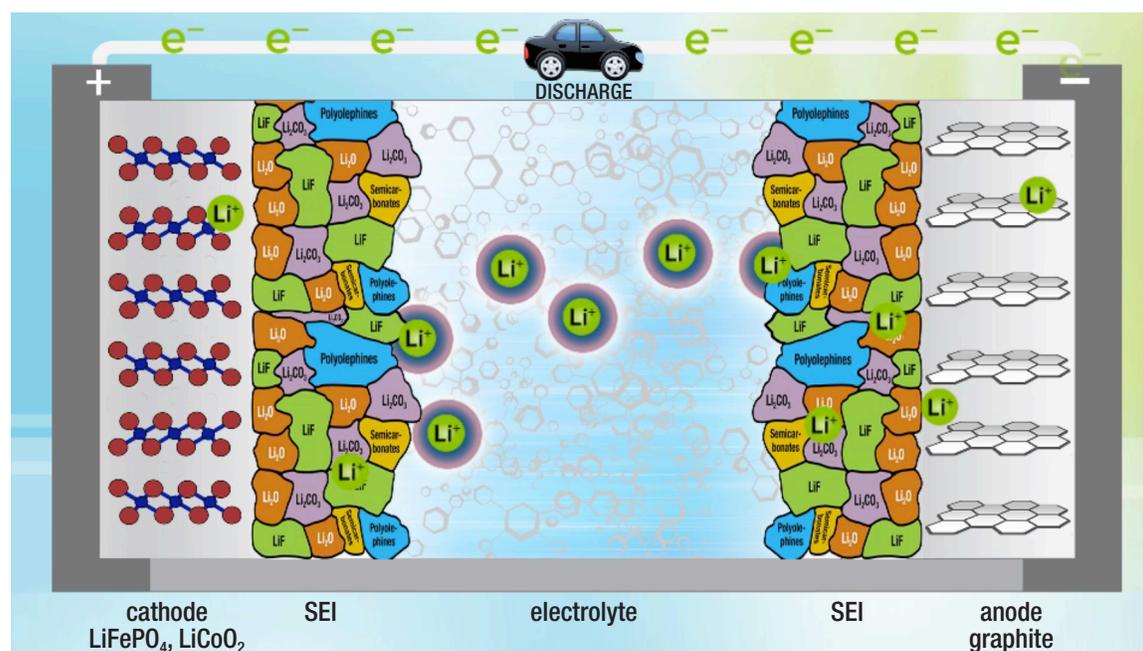


Figure 4.1.1. Schematic of a Li ion battery during a charging cycle. The diffusional dynamics of ions in battery structures is a key feature in determining performance, and needs to be studied below the seconds time scale of today's research. The MBA lattice will provide improved X-ray coherence, enabling studies of the ion diffusion on microsecond time scales. Image courtesy G. Crabtree, ANL.

APS MBA Strengths:

With the improvement of up to 1,000 in coherent photon flux provided by the MBA lattice at the APS, the time resolution for the XPCS will increase by 10^6 , well into the microsecond time scales needed to make feasible measurements of the diffusional dynamics of ions. The MBA source also will enable the use of XPCS for *in situ* and *operando* situations. Additionally, the dramatic increase in the coherent fraction at all energy ranges will enable the use of XPCS at photon energies much higher than possible today, greater than 20 keV. This will enable the penetration of the electrodes and electrolyte materials in a working condition and provide a much more complete view of how ion diffusion affects battery performance. For the study of battery charging and discharging, X-ray ptychography at an upgraded APS with an MBA lattice may allow not only spectromicroscopy at a much faster rate and with higher spatial resolution, but also provide an entirely new form of spectromicroscopy based on phase shift rather than absorption [1]. This “phase” spectromicroscopy is expected to be up to two orders of magnitude more sensitive in complex environments because the phase shift is much stronger than absorption for hard X-rays.

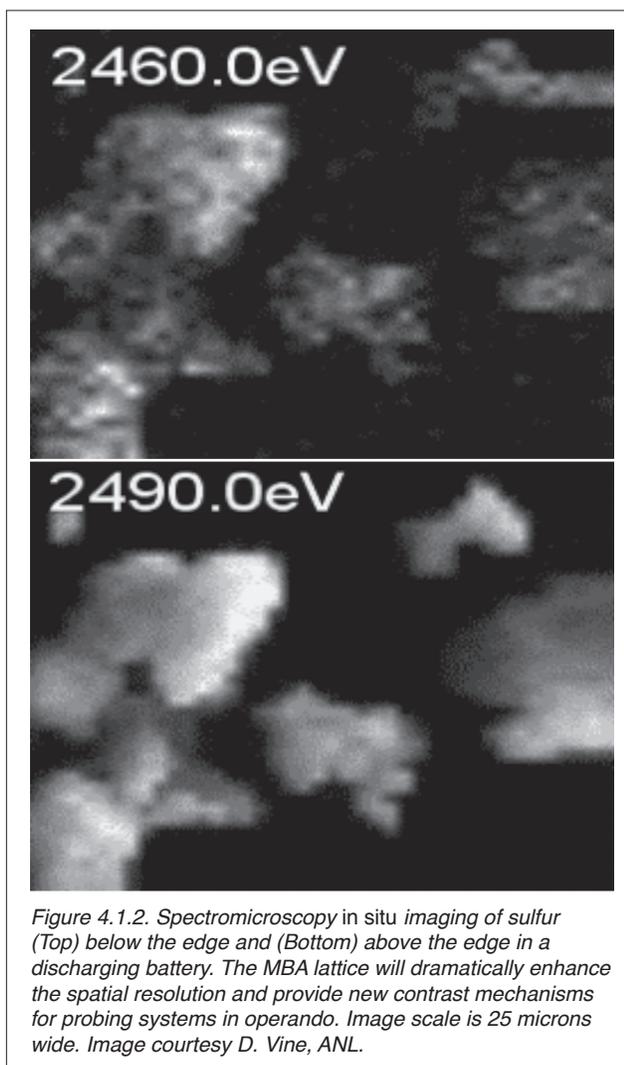


Figure 4.1.2. Spectromicroscopy in situ imaging of sulfur (Top) below the edge and (Bottom) above the edge in a discharging battery. The MBA lattice will dramatically enhance the spatial resolution and provide new contrast mechanisms for probing systems in operando. Image scale is 25 microns wide. Image courtesy D. Vine, ANL.

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Additional References

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MORE SELECTIVE AND EFFICIENT CATALYSTS FOR PRODUCTION OF BIOFUELS AND POLYMERS

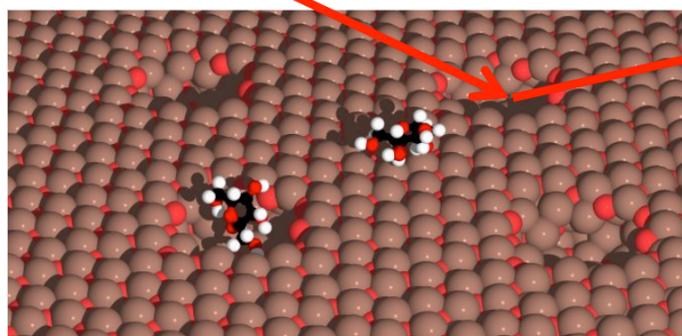
Nearly 90 percent of all chemical processes involve the use of catalysts. Improving the efficiency, lifespan, and effectiveness of these catalysts has become a key goal in chemistry and materials science. This is achievable by designing custom surfaces at the atomic level for better catalytic selectivity and for enhanced catalysis stability.

The creation of such designer catalysts hold promise for improved production of biofuels through the use of nano bowls with pitted pockets to hold individual catalysts in materials such as aluminum oxide and titanium oxide. Today single-angle X-ray scattering (SAXS) measurements must scan an array of nano bowls to draw inferences about the characteristics of individual nano bowls. Because many catalytic reactions are size dependent, it is critical to characterize very small catalytic sites.

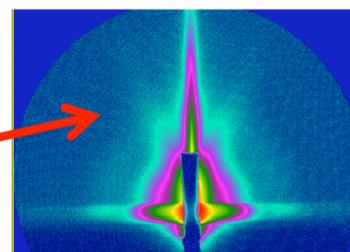
APS MBA Strengths:

The MBA lattice technology will provide a small beam with enough X-rays to see very dilute, small nano catalysts. Using a combination of X-ray techniques, including grazing incidence small-angle X-ray scattering (GISAXS), will enable the mapping of individual nano bowls on surfaces containing the small catalyst and allow the observation of changes with reactants and higher temperatures and pressures. This will make structures as small as 10 atoms measureable, down from 100 atoms, allowing for the design of smaller catalysts.

X-ray



Nano bowls containing catalysts



Grazing incidence scattering diffraction pattern from a nano-particle ensemble

Figure 4.1.3. Aluminum oxide surface with bowls that provide size selectivity for catalytic nano-particles (left). GISAXS using nano-scale beams can be used to map out nano particles on the surface and how they change with temperature and pressure. The MBA lattice will provide X-ray beams small enough to map individual nano bowls that are 10 atoms wide, compared to today's limit of 100-atom ensembles [1]. Image courtesy R. Winans, ANL.

This will benefit biofuel design in several ways. First, unprotected small catalysts quickly degrade during biofuel production. This is costly, and because many of the catalysts are made from noble metals, it uses up precious resources. The smaller catalysis enabled by the APS upgrade would potentially enable the production of hundreds of times more fuel per catalyst than is possible today.

Second, the smaller the design of the nano bowl, the more tailored it becomes for selecting small, pure products. This eliminates over-processing of molecules that can create harmful waste such as carbon dioxide. It also creates more efficient processing of biomass, which eliminates waste. It also allows for up-front separation of chemicals during large-batch processing, creating a purer, cleaner biofuel.

In general, the ability to observe smaller catalytic processes and to affordably create large batches of complex catalysts will open new avenues for the use of catalysis to create high-performance materials with new properties.

Reference

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DESIGNING TECHNOLOGIES THAT RIVAL THE CAPABILITIES OF LIVING THINGS

In many areas nature has designed highly selective systems, such as photosynthesis, that far exceed what mankind has been able to achieve. Yet, the ability to control matter on the nanoscale offers the opportunity to create new technologies with capabilities that rival those of living things and even enter areas untouched by nature. For example, natural photosynthesis is the model for capturing sunlight to drive energy-conserving catalytic chemistry. However, photosynthesis is not designed for optimized solar energy conversion, and photosynthetic systems that go beyond nature's design, such as an artificial leaf, could be developed for efficient, sustainable solar fuels production.

Progress in artificial leaf device design requires *in-situ* characterization of the catalysts and light-harvesting material layers, both spatially and time-resolved under functioning conditions. This will reveal the structures and fundamental physical-chemical reaction mechanisms that underpin artificial photosynthesis. Today a combination of synchrotron X-ray spectroscopy (XAFS and XANES) [1] and scattering (pair distribution function) [2] analyses have revealed some underlying chemistries between photosynthesis and amorphous oxides, which point toward unique design strategies. But, this is far from enough information to develop artificial leaf devices. The ability does not exist today to map the chemical and atomic structure in the detail needed.

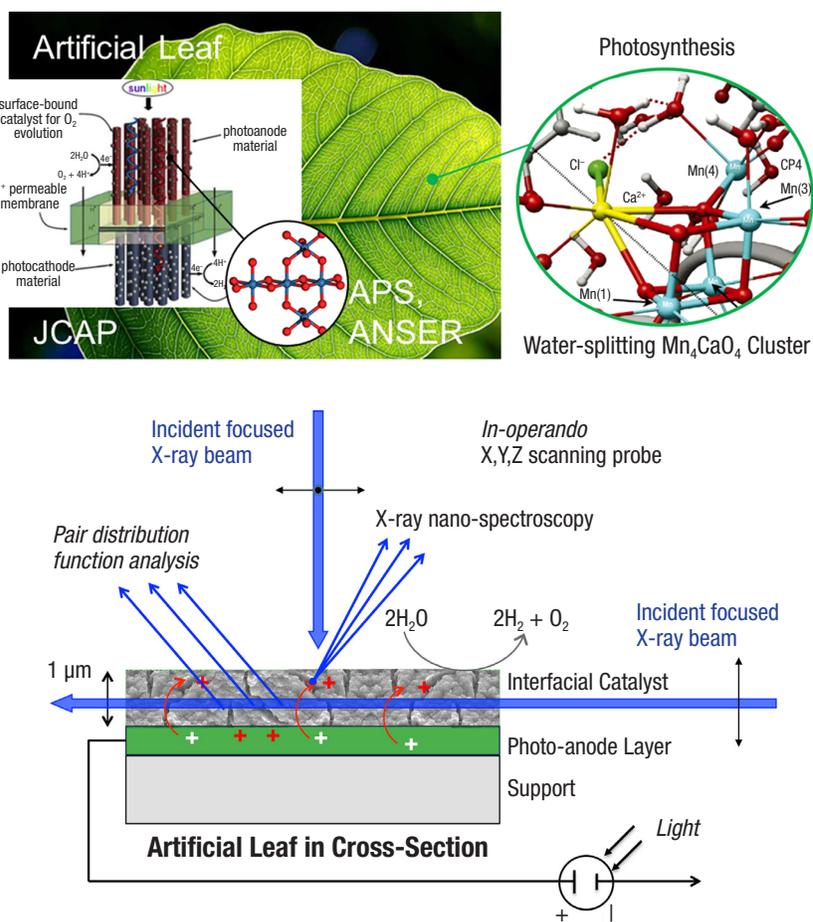


Figure 4.1.4. (Top) Nano-structured photocathode-photoanode artificial leaf architecture is a leading candidate for artificial photosynthesis design. (Bottom) The MBA upgrade will enable in-operando structure-function profiling within the catalyst layer in thin-film artificial leaf devices. Image courtesy D. Tiede, ANL.

APS MBA Strengths:

The MBA lattice technology will deliver the intense, collimated, nanoscale focused X-ray beams needed to provide unprecedented dynamically resolved three-dimensional direction structure profiling of light-harvesting and catalytic active layers under functional conditions in artificial leaf, thin film devices. Some of the key techniques making this possible will be XPCS to probe interfacial chemistry and kinetics within nanoscale domains, X-ray spectromicroscopy for mapping of chemical and atomic structure, and pair distribution function analysis to achieve directional profiling of atomic-scale solar catalyst structure.

References

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ENABLING MESOSCALE SCIENCE WITH HIGH-ENERGY X-RAYS

Polycrystalline materials are ubiquitous in society, from the ever-present concrete and steel to the most advanced state-of-the-art composites. Performance of polycrystalline materials is often dominated by how a material behaves at the level of where individual grains interact – the mesoscale. The ability to practice predictive mesoscale science is key to the development of advanced materials. Many models exist to predict materials behavior on these length scales, but little data is available to compare models to reality. Improved modeling will hasten the development of lighter, stronger materials for improving the energy efficiency of nearly all mechanical systems.

Nondestructive diagnostic tools to understand mesoscale behavior have been traditionally wanting, but recent innovations using X-ray diffraction microscopy have begun to change this. High-energy diffraction microscopy (HEDM) and sub-micron 3-D diffraction (S3DD) provide crucial information about individual grains and the interactions between grains. Among the mesoscale topics that have been studied are grain growth and reorientation, and stress distribution amongst grain ensembles and within grains. These measurements are very time consuming and often struggle to get past the demonstration phase. However, strong connections between these measurements and validated models are being made, promising predictive design of new materials and providing a strong motivation to improve the scope and fidelity of the measurements.

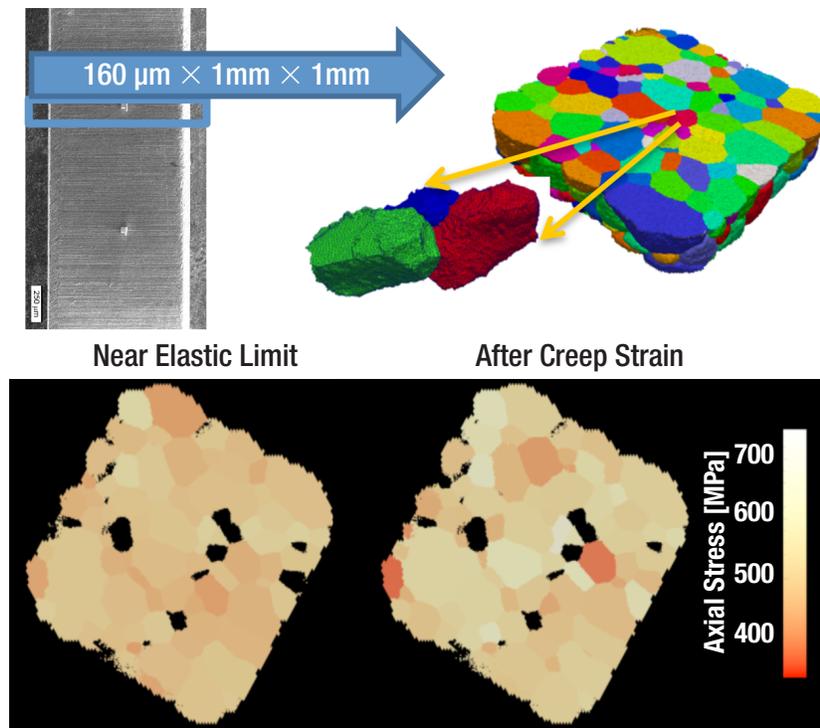


Figure 4.1.5. (Top) Distinct crystallographic grains in a turbine disk are shown in different colors. (Bottom) Near-field high-energy diffraction microscopy (HEDM) shows the local stresses before and after a Ti-7%Al sample deformed slowly under constant load. The inhomogeneous nature of the response is due to grain-to-grain interactions that are currently challenging for any model to reproduce. This was a first-of-its-kind in-situ measurement performed by a team led by the Air Force Research Laboratory. The MBA lattice promises to increase spatial resolution from the current level of about 5 microns to sub-micron, providing the insight about defects needed to design the next generation of high-performance materials. Image courtesy J. Schuren, Air Force Research Laboratory.

APS MBA Strengths:

The increased brightness from an MBA lattice directly translates into smaller beams and increased flux for higher spatial resolution and faster measurements. Rapid data collection will allow new experiments on materials undergoing dynamic changes (e.g., fatigue, annealing). Enhanced spatial resolution will reveal constituent responses of increasingly complex heterogeneous materials, including radiation-resistant steels and biomechanical systems (e.g., metal implants in bone). Furthermore, improved resolution will extend the reach of experiments to sub-micron grain sizes, enabling studies of additional energy-relevant materials including batteries. The capabilities of the MBA lattice will transform these mesoscale techniques from physics demonstrations to engineering tools.

PROBING SEMICONDUCTOR DEVICE DEFECT BEHAVIOR *IN SITU*

During the past 40 years, the information technology revolution has driven scaling of electronic devices down to nanometer dimensions. Recently the drive to enhance the performance of these devices under more energy-efficient operating conditions has required the incorporation of novel materials into these technologies. These new materials have different diffusion and failure characteristics than previous generations. These differences need to be understood on the nanometer level in order to push further the fundamental limits of performance and reliability.

The presence of impurities within electronic devices and the contact metallization plays a major role in controlling both carrier density and mobility. The median lifetime of the metallization elements that provide power to the underlying semiconductor devices, however, has been shown to decrease by 50 percent with each new technology node due to the effects of electro migration, particularly along key interfaces such as grain boundaries [1]. Further, the interface between contact materials that link the devices to the overlying metallization layers is designed with specific dopant concentrations to minimize the associated contact resistance. Assessing not only the locations and quantities of these impurities but also their structural and chemical state *in situ* within intact devices will provide essential feedback towards reducing carrier scattering at key interfaces in nanoelectronics.

One of the pressing concerns in future interconnect geometries is the scaling of barrier layer dimensions (Ta/TaN in Figure 4.1.6) below two nanometers commensurate with the current copper line widths. As new barrier layer materials are introduced, such as self-forming manganese silicate layers or Ru-based layers, there will be two dominating issues. First, whether they are effective at preventing copper diffusion into the dielectric and oxygen diffusion from the dielectric into the copper layer thereby impacting on its resistivity. Second, preserving the adhesion strength between the copper and the barrier covered side walls of the interconnect trench. It is the reduced adhesion strength between the copper and the barrier layer that may initiate void generation resulting from enhanced electromigration effects.

APS MBA Strengths:

The investigation of these processes will be possible with the next-generation nano-beam X-ray spectroscopic measurement capabilities made possible by the MBA upgrade with commensurate spatial resolution. This will enable for the first time such measurement in actual device geometries at elevated temperatures and in real time and will provide a powerful method to evaluate alternative barrier layer fabrication strategies for future interconnect generations. Additionally, crack propagation is an intrinsically intermittent and stochastic process, which requires a large field of view as well as fine temporal and spatial resolution.

Reference

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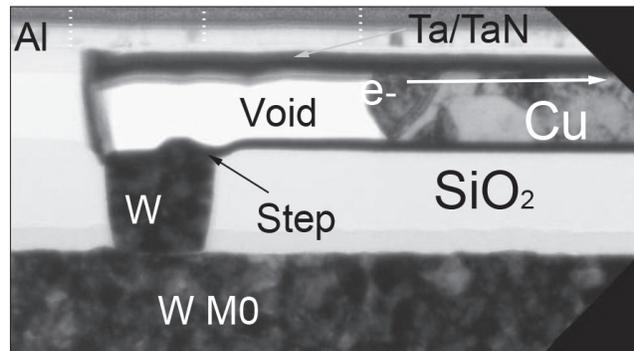


Figure 4.1.6. Interfacial defects at metal semiconductor contacts dictate the performance of nanoelectronics. For example, the reduced adhesion strength between copper and the barrier layer of tantalum may initiate void generation resulting from enhanced electromigration effects. Studying such interconnect geometries at smaller length scales will become increasingly important and will be a strength of the MBA lattice. The size of nano wires in transistors is expected to decrease from about 22 nm today to about 5 nm by 2020. The MBA lattice will allow enable these studies in actual device geometries at elevated temperatures and in real time. Image scale is about 1,400 nm wide. [C.K. Hy et al., *IEEE 42nd IRPS*, 222 (2004)]. Image courtesy C .Murray, IBM.

CONDUCTING DYNAMIC STUDIES OF FATIGUE CRACKS

Understanding the growth of fatigue cracks under cyclic loading remains the key challenge in fault-tolerant design in a variety of applications including aerospace vehicles and pressure tubes for power plants. *In-situ* studies of the growth of small-fatigue cracks under cyclic loading are a critical need in this area. While the behavior of long cracks is relatively well understood and therefore predictable, the growth of small cracks is much more variable; in some cases the growth rate of small cracks vastly exceeds that of long cracks and is highly microstructure-dependent. This is a critical and potentially dangerous situation because the useful life of engineering structures is usually estimated from fatigue-life calculations based on growth rates of long cracks [1]. As another example, a recent trend in airframe construction is fabrication of monolithic

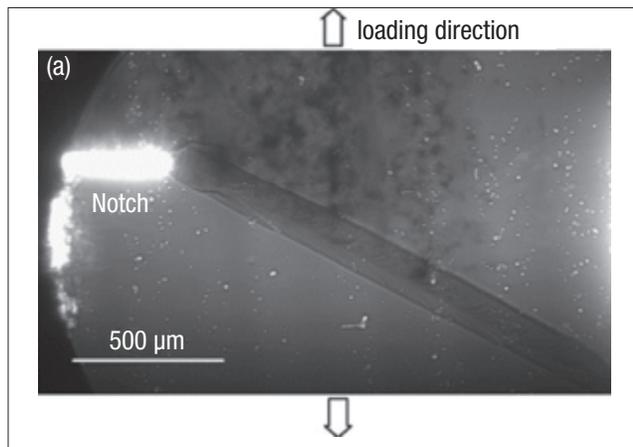


Figure 4.1.7. Static X-ray phase contrast image of a fatigue crack initiated at a notch in a nickel-based super alloy. The MBA lattice will allow higher resolution studies of such phenomena. Image courtesy L. Liu et al. *Modeling grain size dependent optimal twin spacing for achieving ultimate high strength and related high ductility in nanotwined metals. Acta Mater.* 59:5103-5115, 2011.

components through high-speed machining of thick aluminum alloy plate. The interplay between the loading state and local variations in material anisotropy leads to turning of fatigue cracks in components where inspection is difficult and, as in the case of the growth of small cracks, requires analysis outside the usual engineering practice for fatigue-life estimation.

APS MBA Strengths:

Today we can view crack propagation at its mid and end points, which typically occurs in the 1,000-nanometer size range and 100-millisecond time scale. An MBA lattice at the APS will enable characterization of the initial formation of cracks and their early propagation, which occurs in the 50-nanometer range and 10-millisecond time scale. The combination of high coherent flux from the MBA lattice with high X-ray energies (>60 keV) creates unparalleled opportunities for studying fatigue behavior in bulk materials. Because the image formed with a coherent beam is sensitive to gradients in electron contrast, internal interfaces and surfaces are readily observable even in the absence of strong-absorption contrast. With a coherent high-energy X-ray beam, it will become possible to perform studies in which small-fatigue cracks are deliberately initiated, and then observed while they grow (Figure 4.1.7). For example, high-speed imaging could be performed at a frame rate >20 kHz while the crack is subjected to cyclic loading at about 1 kHz, allowing a complete evaluation of the crack opening and closing process. Alternatively, or in conjunction with high-speed imaging, slower tomographic reconstructions of the 3-D crack-tip morphology will permit a complete description of the crack as it advances through the microstructure of the material. Complementary diffraction measurements of lattice strain and orientation of individual grains (Figure 4.1.8) will be pursued to provide the driving forces associated with crack growth. The capability to conduct these experiments would revolutionize our understanding of fatigue crack behavior, ultimately providing predictive capability and mitigation strategies.

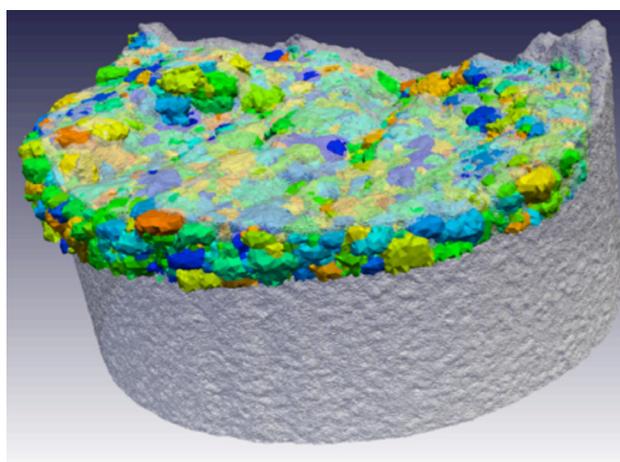


Figure 4.1.8. Fatigue fracture surface region of a 1.1-mm diameter nickel superalloy, measured post-mortem with high-energy X-rays ($E=65$ keV). The gray-scale is a tomographic image of the sample illustrating a rough top fracture surface. The colors are the superimposed grain structure measured with high-energy X-ray diffraction microscopy (HEDM). The MBA upgrade would reduce the time for HEDM collection from tens of minutes to seconds, enabling in-situ, real-time measurements as the fracture process proceeds. Image courtesy R.M. Suter, Carnegie Mellon University.

Reference

1. R.O. Ritchie and J. Lankford. *Mater. Sci. Eng.*, 84, 11-16, 1986.

NEW POSSIBILITIES FOR THE *OPERANDO* STUDY OF ELECTRODES ACROSS ALL LENGTH SCALES

Inhomogeneity across various length scales underpins critical performance parameters in many materials. Yet it also makes it impossible to create accurate predictive models of how matter behaves from spatially averaged information. For example, studies of batteries demonstrate that capacity is lost by diffusion and reaction process across the entire scale of the electrode but a lack of research tools prevents scientists from determining how this inhomogeneity dictates performance.

Finding a way to bridge the gap between existing technologies to recover accurate spatial measurements of inhomogeneity across individual particles would enable a new understanding of electrochemical systems and enable better control of such systems. The MBA lattice will let us do just that. In the case of batteries, this could speed the discovery of the next-generation of materials for smart phones, laptops, grid storage and electric vehicles that can hold charges longer, charge and discharge faster and extend the lifetime of batteries. This will be particularly beneficial for studies of lithium-ion and magnesium-ion batteries where untapped capacity is thought to exist in the inhomogeneous mesoscale. Today these batteries have a capacity of about 180 milliamps but theory predicts that the current material should be able to reach about 240 milliamps. An improvement on that order could lead to smart phones and laptops holding charges nearly twice as long as they currently do.

APS MBA Strengths:

The MBA lattice will shrink the X-ray beam size and improve brightness by two orders of magnitude, making the upgraded APS the only facility in the U.S. with the capability to create an entirely new X-ray tool to characterize meso-scale complexity in batteries. The high-energy X-rays provided by the APS also will reduce the changes induced in the sample, producing the purest representation of battery function.

The possibility of 50-nanometer high-energy beams with energies above 50 keV will enable the development of a singular measurement technique that combines pair distribution function and small-angle scattering and tomography that will probe length scales from the atomic bond continuously through to the dimensions of a full electrode in a battery system. Today PDF and SAXS studies average reactions over many thousands of nanoparticles but with the MBA lattice at the APS, measurements of 100 nanoparticles contained in an ensemble of 20 to 100 nanometers are feasible. Likewise, PDF measurements that today produce 3-D spatial resolution across an area of about a 100-microns cubed, will be able to capture data from a 50-nanometer cubed section. The power of a low-emittance source is that these measurements could be cross-correlated with tomographic reconstructions with similar resolutions, providing a full picture of the workings of the electrodes under real operating conditions. The theoretical basis for this approach has been recently established and the required next-generation fast-frame rate detectors are set to come online in the next few years.

4.2 UNDERSTANDING FUNDAMENTAL INTERACTIONS AT THE NANOSCALE

INTRODUCTION

X-rays have long been used to study fundamental behavior of materials. The incorporation of an MBA lattice into the APS Upgrade will allow a leap forward in several areas of fundamental science. It will push high-energy X-ray materials science to research levels that are faster, smaller, more precise. This will strongly benefit the characterization of the dynamics of condensed matter, a goal of many scientific experiments because of its crucial nexus between data and theory. Many scientific applications benefit from the large increase in coherency associated with the low-emittance lattice, but there is in particular a huge boost in the capability of X-ray correlation spectroscopic techniques (XPCS). Structural, chemical, or magnetic fluctuations in the sample produce intensity fluctuations in the speckle pattern, and these can be measured to probe the underlying dynamics with relevant statistics. It may be possible with the upgrade of the APS to push the use of this key technology down to the sub-nanosecond time domain.

Knowledge across a wide variety of length scales is also required for any robust understanding of a material. Improved focusing capabilities will provide spatial resolution comparable to the length scales of phase segregation in functional materials, electronic textures of complex condensed matter systems, and individual devices in advanced microelectronics. An orders of magnitude increase in source brightness will translate into significantly improved analytical sensitivity at the highest spatial resolution. For example, spatial resolution for inelastic scattering studies will improve by a factor of 1,000. The improved brightness will also dramatically increase analytical speed, allowing the extension of nanoscale imaging capabilities to much larger specimen domains, including looking at linear and non-linear bulk rheology.

MAPPING DEFORMATIONS IN MATERIALS TO IMPROVE PERFORMANCE

Deformation and flow are integral to the performance of many materials. The flow properties of coolant fluids and lubricants under extreme conditions directly affect the efficiency and reliability of many energy technologies. In addition, the ability of structural materials to deform elastically and plastically under high stress is critical to material toughness and failure resistance. While X-ray diffraction has long been used to map strains in crystalline alloys, microscopic characterization of flow in fluids and non-crystalline solids has been more elusive. Observing molecular flow distributions on the micron scale can provide key insight in a multitude of areas, such as boundary layer effects and heterogeneous dynamics in complex fluids and glasses. For example, mapping flow patterns in materials can explain

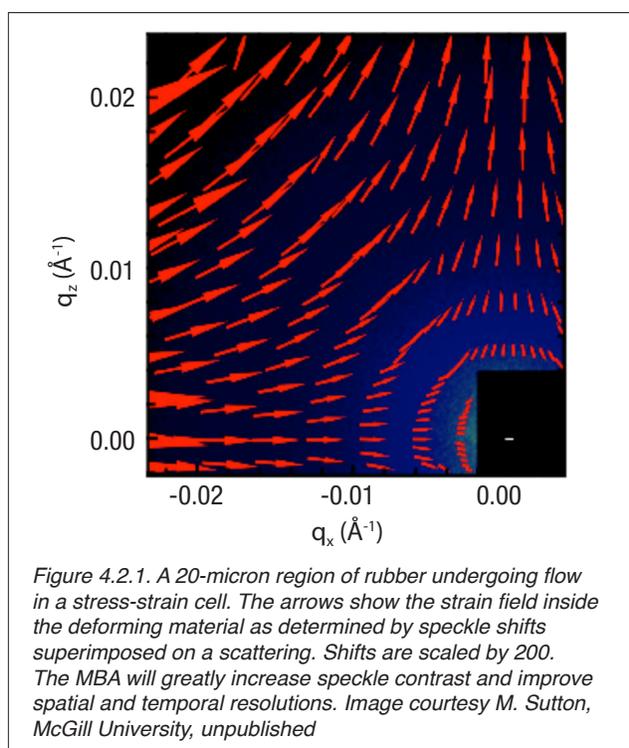
how melting permafrost in the tundra will affect the stability of structures such as drilling platforms, provide early indications of weaknesses in capillary walls, show how additives speed the extraction of oil from tar sands, and show individual molecules in complex polymers, such as rubber, react differently to the same strain to provide information about defects in tires.

Researchers have been increasingly using coherent X-rays to observe dynamics through X-ray photon correlation spectroscopy (XPCS). Fluctuations in the structural, chemical, and magnetic order in the material are revealed through time correlations in the evolving speckle patterns. Recently it has been shown that an extension of this analysis to include space-time cross-correlations reveals the local deformation occurring in a material (Figure 4.2.1). In principle this provides a powerful new way to map the strain fields in fluids and solids down to the molecular scale. However, due to the relatively low coherent X-ray flux of current sources, its applicability is limited to very slow deformations.

APS MBA Strengths:

The increased coherent flux provided by the MBA upgrade at the APS will revolutionize XPCS because its time resolution scales as the square of the source brightness. The 100 to 1,000 times increase in brightness will translate into a factor of a 10,000 to 1,000,000 increase in the accessible dynamic range. With the MBA upgrade, XPCS will reach nanosecond and nanometer time and space resolutions.

These new capabilities will create a new, powerful way to analyze the mechanisms of deformation in diverse samples in diverse environments. The high coherent flux at high energies will improve sample



penetration and give sufficient X-ray speckle signal to observe flow and strain fields inside materials and near boundaries and defects with sub-micron spatial resolution. This will have wide applicability to fundamental studies of complex fluids as well as to applied research, such as structural materials and nanofluidics.

Reference

F. Livet, F. Bley, F. Ehrburger-Dolle, I. Morfin, E. Geissler, and M. Sutton. X-ray intensity fluctuation spectroscopy by heterodyne detection. *J. Synchrotron Rad.*, 13:453, 2006.

NANOSCALE DYNAMICS AND MACROSCOPIC RHEOLOGY

Rheology is the study of flow and deformations in materials to an induced shear force. Understanding how this behavior occurs at the nanoscale presents an opportunity to create new high-performance materials.

For example, a novel application takes advantages of the phenomena of reversible shear thickening where material undergoes a colossal increase in the viscosity (liquid-to-solid-transition) at high-shear flows. Liquid body armor used by the military capitalizes on this phenomenon. The shockwave caused by a projectile impact results in shear thickening in the body armor, dissipating the impact. The underlying mechanism is related to the nanoscale lubrication forces between the nanoparticles in the fluid, which causes the formation of so-called hydro clusters deemed responsible for this phenomena. An understanding of this mechanism remains elusive because of an inability to peer at nanoscale dynamic behavior of such materials.

APS MBA Strengths:

X-ray photon correlation spectroscopy, XPCS, studies today only offer measurements in the 100-nanometer-scale range, with limited resolution of near-surface effects. The increased brightness, coherence, and higher energy provide by the MBA lattice upgrade at the APS will allow tens-of-nanometer sensitivity at microsecond time scales and a deeper penetration to better study real materials in operation.

The increased coherence provided by the MBA upgrade at the APS will revolutionize XPCS use for rheology

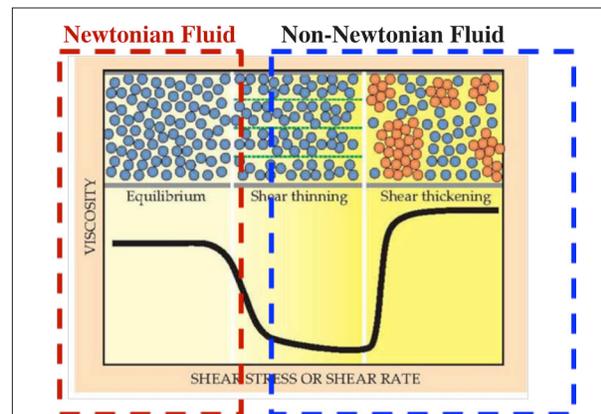


Figure 4.2.2. The relationship is complex between microstructure and viscosity for hard-sphere colloidal suspensions. In equilibrium, random collisions among particles make them resistant to flow. As shear increases, particles first become organized in flow, lowering viscosity, but at higher shears hydrodynamic interactions begin to dominate, creating ordered clusters (orange spheres) and increasing the viscosity. This phenomena of fluid dynamics under deformation induced by a shear force can be studied at a greater than 10,000 increase in accessible dynamic range with XPCS. The increased coherence provided by the MBA upgrade at the APS will revolutionize XPCS use for rheology because its applicability scales as the square of the source brightness. Image from N.J. Wagner, University of Delaware, and J.F. Brady, Shear thickening in colloidal dispersion, Physics Today, 27-32, October 2009.

because its applicability scales as the square of the source brightness. The 100-times increase in the brightness of X-rays will translate into a greater than 10,000 increase in the accessible dynamic range. We will be able to look at linear and nonlinear bulk rheology and its relationship to nanoscale dynamics in complex fluids.

Reference

W.R. Burghardt, M. Sikorski, A.R. Sandy, and S. Narayanan. X-ray photon correlation spectroscopy during homogeneous shear flow. *Phys. Rev. E*, 85:021402, 2012.

NANOSCALE CRYSTAL STUDIES OF NEW MATERIALS

Novel materials, developed by design or serendipity, are a key factor in much of the most interesting condensed matter and materials science research. Complex materials are often difficult to synthesize, and are rarely available as the large single crystals that are needed for many experimental methods. For example, it took more than a decade to grow high-T_c superconducting materials in single crystals large enough to use for standard X-ray and neutron diffraction and inelastic scattering experiments.

X-ray microbeam techniques can select small crystals out of polycrystalline aggregates, removing, in some cases, the need for large single crystals. However, the intensity of the focused beam often precludes flux-intensive experiments, such as inelastic X-ray scattering. This creates a significant hurdle to discovery because many important electronic materials, including high-T_c superconductors, metal-insulator transition metal oxides, CMR manganites, etc. are intrinsically inhomogeneous. They require inelastic scattering and other measurements with 10-nanometer beams to resolve these spatial inhomogeneities at relevant length scales.

APS MBA Strengths:

The high-brightness X-rays produced by the MBA lattice at the APS will greatly enhance the ability to study newly synthesized materials. Dramatically improved focusing will transform what are currently challenging microcrystal studies into routine experiments and open the door to studies of submicron crystals. This will make complex studies of defects and nanoclusters feasible. This also opens up the use of the full array of nanoprobe techniques to generate a rapid understanding of materials and speed the pace of materials exploitation. Today inelastic scattering studies can be performed on samples as small as 50 microns, but that will be enhanced to about 10 nanometers, a factor of 1,000 improvement.

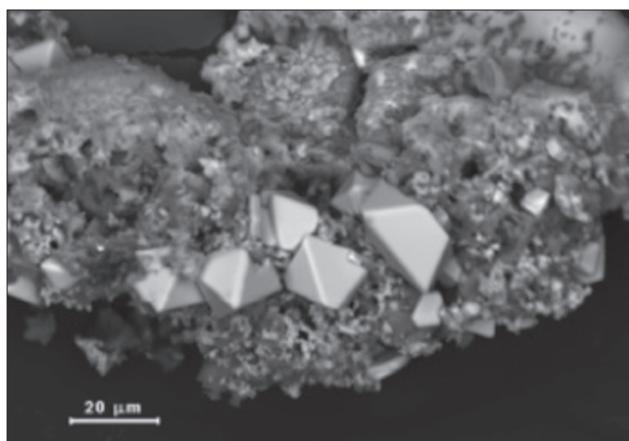


Figure 4.2.3. For $\text{La}_{2-x}\text{Ba}_x\text{CuO}_4$ at $x=1/8$, it took 15 years to optimize conditions for crystalline growth and to produce a single crystal large enough to use in X-ray experiments. The Upgraded APS will allow advanced X-ray analysis to occur immediately following discovery or synthesis of new materials, even when available only in small crystals as shown above.

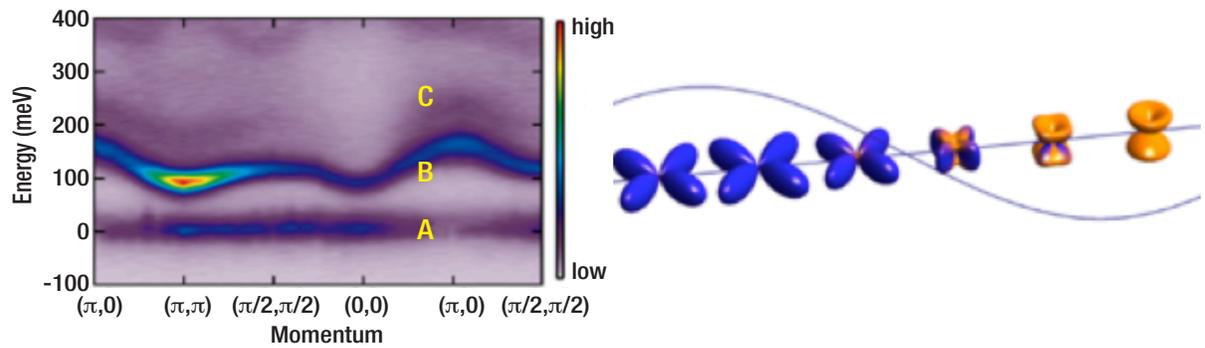


Figure 4.2.4. (Left) Resonant inelastic scattering (RIXS) spectra showing the dispersion of a single-magnon spin excitation (Feature B) in $\text{Sr}_2\text{Ir}_3\text{O}_7$, as a function of the momentum transfer Q along high symmetry lines in the Brillouin zone. Feature A is the elastic line, while the weak feature C is suggestive of a two-magnon state. (Right) A real-space schematic of a single-magnon spin excitation observed in a related material, Sr_2IrO_4 . The MBA lattice at the APS will enable such measurements from samples 1,000 times smaller than currently possible.

GROWTH AT THE ATOMIC SCALE

Many of our current technologies rely on the fabrication of materials with a level of precision almost unimaginable only a few decades ago. With modern synthesis and processing tools, along with the many remarkable advances in computational materials science, we now have the unique opportunity to design and create truly novel forms of matter with custom-tailored, and, potentially, transformable and adaptive properties. Such materials will have an enormous impact on how our society is able to manipulate, transport, and store both energy and information. For example, the computational speed of today's computers is limited by inefficient hardware that wastes vast amounts of energy through heat. To make faster, low-power electronics that are financially feasible, we need to design new materials that will enable computation with dramatically less heat loss.

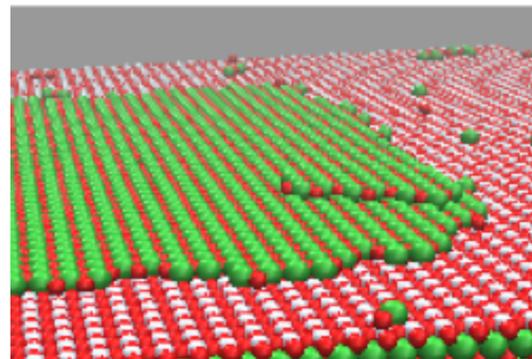
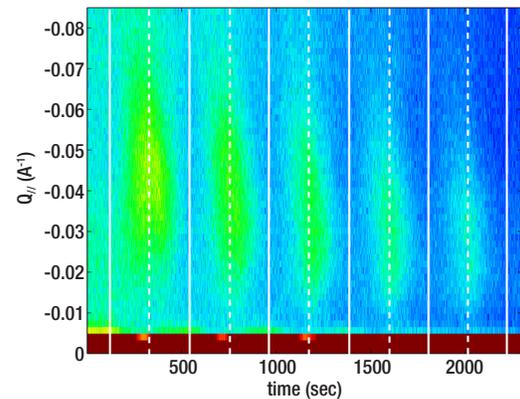


Figure 4.2.5. (Top) In situ X-ray scattering during complex oxide synthesis by oxide molecular beam epitaxy. Islands form and coalesce on the growing surface, giving rise to oscillations in the intensity of the diffuse scatter. (Bottom) Complementary computer simulations of the thin film growth process. While the scattering techniques employed in the current studies allow an understanding of the average island behavior, the dynamics of island formation and growth, as could be measured with XPCS, cannot be investigated with the current source. The increased coherent flux provided by the MBA will enable XPCS studies of the dynamics during growth. (D.D. Fong, ANL, J.W. Freeland, ANL, D. Morgan, University of Wisconsin-Madison, et al.)

A MBA Lattice at the APS: A New Generation

The synthesis of these new, artificial materials will require control on the level of atoms and the design of assembly routes not found in nature. With detailed, time-dependent data describing the material surface with atomic-scale resolution, we will be able to create computer models that can process through the complex atomic structure and behavior to tell us the optimal recipe for constructing a pathway to new high-performance material. Progress in the realm of new materials requires high-precision synthesis techniques as well as direct monitoring of atomic behavior in the growth environment. With the use of *in-situ* synchrotron X-ray scattering and spectroscopy during materials synthesis, several research groups are gaining considerable insight into understanding how a material takes on its properties, even in the embryonic stage. Unfortunately, the present limitations of the synchrotron source are leaving large gaps in our understanding of surface behavior during growth. This leaves researchers unable to reconstruct the why and how of the different atomic mechanisms that are taking place.

APS MBA Strengths:

With the new MBA lattice technology, the dramatic increase in coherent flux will make it possible to fill in these gaps and allow true real-time studies of materials synthesis, with the spatial and temporal resolution necessary for true progress to be made in the development of novel materials. While we can spatially resolve nanometer-scale objects on the surface today, with the improved coherence from the MBA lattice we will be able to reach the desired atomic-scale resolution. Furthermore, the improved brightness will allow us to push down today's time resolution of X-ray photon correlation spectroscopy measurements. Experiments that today take about one second will take one microsecond, and other experiments that today take one microsecond will take one nanosecond, even at high temperature and in highly reactive growth environments. These new insights can then be used in computational models to facilitate the formulation of the growth strategies necessary for stabilizing designer materials.

4.3 ADVANCING LIFE AND ENVIRONMENTAL SCIENCES

INTRODUCTION

The life sciences are a major part of research activities at the APS. This field involves about 40 percent of the APS users and is a vibrant community with a large scientific impact. For example, 20 percent of all protein structures deposited in the Protein Data Bank are the result of research at the APS. Also, two recent Nobel prizes stem from work performed on APS macromolecular crystallography (MX) beamlines. APS users are leaders in understanding the roles of trace metals on health and disease, and in the structure-based design of novel drugs to improve health and cure disease. This approach to drug design relies on determining the three-dimensional structure of molecules at the atomic level. Four major categories of life sciences research are pursued at the APS. The first is macromolecular crystallography, which determines the structure of proteins and various macromolecular assemblies at atomic resolutions. This attracts by far the largest number of users. Second is direct imaging of biological structure across a wide range of length scales, from individual molecules to intact organisms. The third is real-space mapping of trace elemental content, chemical state, and, potentially, crystallographic makeup of samples. The fourth category is studies of non-crystalline, less-ordered systems by structural and spectroscopic approaches.

Grand challenges at the frontiers of structural biology address questions such as how complex molecular machines embedded in cell membranes work, exactly how drugs interact with their targets, how side effects arise, and how drugs can be improved. Macromolecular crystallography is a very powerful tool for determining structure at the atomic level, but it is limited by the necessity to prepare crystals of sufficient size and quality. For many grand-challenge questions, it is often only possible to grow tiny crystals. The present experimental capabilities generally require crystals with dimensions greater than 5 microns, but even these can be hard to prepare. The MBA lattice will extend these capabilities dramatically by creating an unprecedented opportunity to routinely study even smaller microcrystals of 0.5 microns, which are likely to be easier to obtain in well-ordered form. In addition, the brighter beam will enable routine room temperature analysis by allowing for data collection that outruns the secondary radiation damage. The use of room-temperature crystals will yield sharper diffraction spots and improved resolution. The X-ray beams available from the MBA lattice will allow users to effectively address the grand-challenge questions.

To fully exploit these new capabilities, new experimental approaches are under development. The APS's high X-ray energies and sub-micron beams will help mitigate radiation damage. Recent studies show that small beams produce less radiation damage per photon than larger beams because absorbed energy from photoelectrons is deposited outside the spot being illuminated.

To study biological systems and their hierarchical structure, X-ray microscopy and radiographic imaging permit direct visualization of specimen structure. The much reduced lateral source size of the MBA lattice will directly improve the achievable spatial resolution to below one micron, and permit visualization of *in vivo* specimens with unprecedented detail.

Structure must be complemented by exploration of local chemistry and functionality. About one-third of all proteins require a metal co-factor for proper, regulatory, or catalytic function. Understanding how these trace metals play their roles in fundamental questions of biology is therefore critically important. Scanning probe microscopic and spectroscopic approaches visualize, at the subcellular level, both the elemental content of trace metals and their local chemistry of metals. Today these approaches are limited to moderate spatial resolution of typically 100 nanometers, and to problems where a substantial signal is present. The enhanced brightness offered by the X-ray beams from the MBA lattice will dramatically change this by increasing the realistically achievable spatial resolution and sensitivity by one or more orders of magnitude. For example, novel nanocomposites are being developed to effectively combine diagnosis and therapy for diseases such as cancer. In order to assess their functionality and potential side-effects, we need to visualize how individual nanocomposites interact with tissues, cells, and organelles. The MBA lattice will make this possible for the first time by providing improved spatial resolution of better than 20 nanometers, across even the large field of view of tissue sections.

Additional Reference

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INTEGRAL MEMBRANE PROTEINS PROVIDE KEY DRUG TARGETS

Of the estimated 2 million human proteins, about one-third are integral membrane proteins, which are structurally and functionally diverse. Integral membrane proteins play key biological roles including trafficking, as seen in voltage-gated ion channels, biochemical pathway regulation, as seen in protein kinases, and physiological function, as seen in G-protein coupled receptors. These proteins have been implicated in many health problems including cystic fibrosis, epilepsy, infertility, diabetes, hypertension, cardiovascular disease, neurodegeneration, and Alzheimer's. They also play a role in various cancers such as leukemia, breast, prostate, lung, pancreatic, liver, and ovarian. They are also the targets of both "good molecules" such as hormones and "bad molecules" such as cocaine and neurotoxins. Because of their

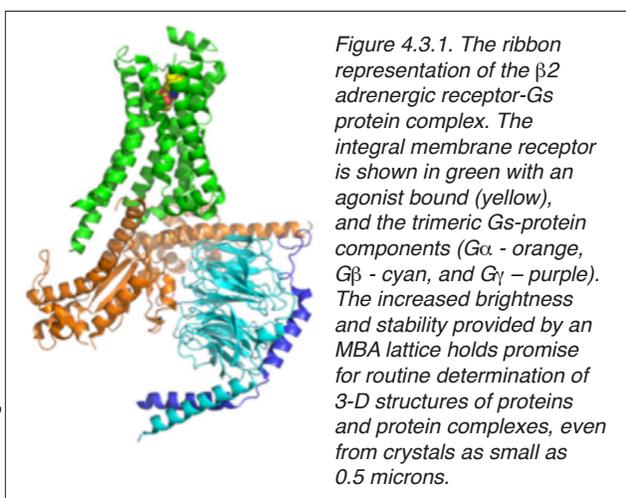


Figure 4.3.1. The ribbon representation of the β 2 adrenergic receptor-Gs protein complex. The integral membrane receptor is shown in green with an agonist bound (yellow), and the trimeric Gs-protein components ($G\alpha$ - orange, $G\beta$ - cyan, and $G\gamma$ - purple). The increased brightness and stability provided by an MBA lattice holds promise for routine determination of 3-D structures of proteins and protein complexes, even from crystals as small as 0.5 microns.

central role in so many biological processes, integrated membrane proteins are the target of more than 50 percent of all drugs. Understanding the 3-D atomic resolution structure of these proteins will enable the development of more effective drugs with fewer side effects to treat or prevent diseases. The biomedical importance of determining the 3-D structure of such molecules has been recognized by the awarding of three Nobel Prizes in Chemistry (1988, 1998, and 2012).

Integral membrane proteins and functional protein complexes are notoriously difficult to produce in sufficient quantity to crystallize. If they do crystallize, they tend to yield either small, micron, or larger heterogeneous crystals. In either case, they diffract poorly due to the small size or the poor internal order. Recent advances in microcrystallography techniques have enabled the structural determination of important integral membrane protein complexes such as the β 2-adrenergic receptor-Gs-protein complex [1] shown in Figure 4.3.1. However, the current brightness of the APS and the large unit-cell parameters of the crystals limit the minimum useful beam size, and therefore the crystal size, to about five microns or larger. This is a major bottleneck for structure determination of many systems, especially larger complexes. The low intensity of the five-micron beam also makes the experiments extremely challenging.

APS MBA Strengths:

The increased brightness and stability with an MBA lattice will provide a 100-fold increase in intensity and allow routine structure determination from crystals as small as 0.5 microns. The improved stability is necessary to keep a sub-micron X-ray beam aligned with a sub-micron crystal. The list of diseases that could be affected by this research is long, and their consequences for human health are great. The MBA lattice holds promise that the 3-D structure of these proteins and protein complexes can be determined routinely and become the next breakthrough area for the treatment of diseases.

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STUDYING KINETOCHORES TO TACKLE GENETIC DISEASES

Kinetochores hold particular interest for their role in regulating genetic material. These large, complicated macromolecular assemblies attach chromatin (chromosomes and their protective proteins) to microtubules of the mitotic spindle during mitosis (cell division) [1]. During mitosis, chromosomes are duplicated and must then be separated, equally and accurately, between the two daughter cells. Flaws in the microtubule function or structure lead to diseases such as albinism, peripheral neuropathy, cancer, and even cell death [2]. The kinetochore in humans is about 100 nanometers in size and is composed of multiple copies of about 38 distinct proteins that work in conjunction to bind the chromatids to the microtubules and ensure proper separation of the genetic material. Although the structures of some of the individual subcomponents are known, the structural details of the full

kinetochore remain elusive. Knowledge of the kinetochore at atomic resolution structure will provide a better understanding of how microtubules attach to chromatin, and will enable the development of drugs specifically targeted to related diseases.

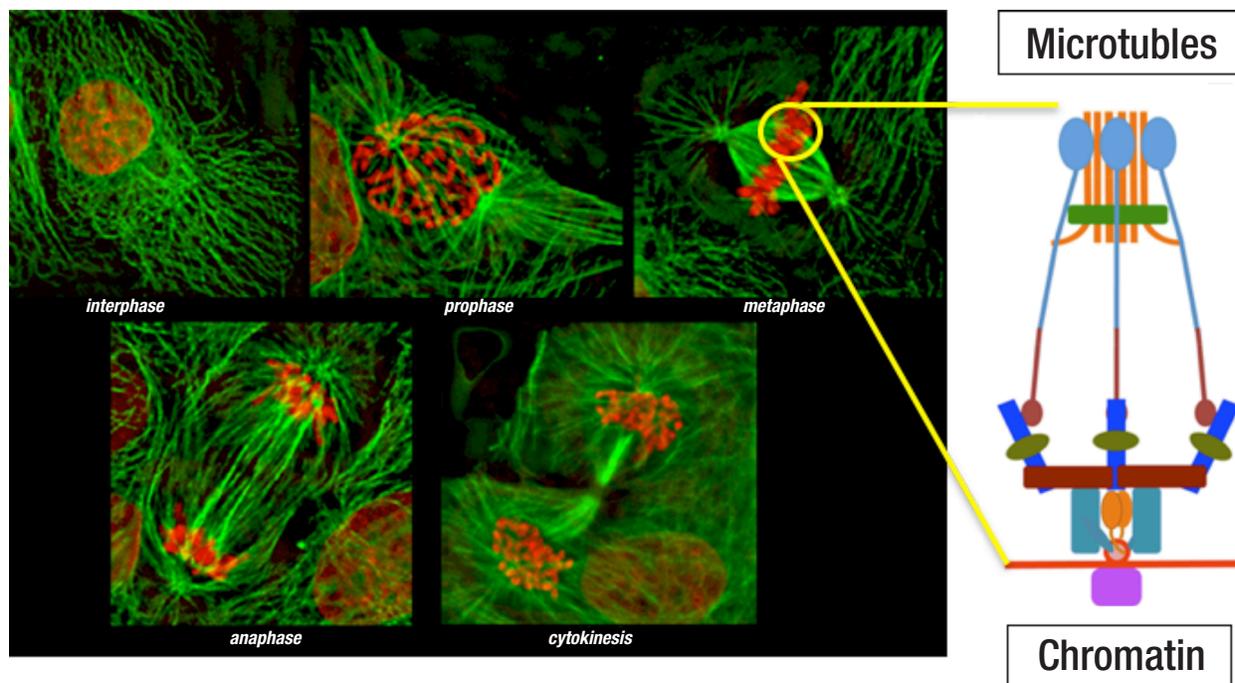


Figure 4.3.2. Left: Fluorescence images of cells during mitosis. The microtubules of the mitotic spindle are shown in green and chromatin is shown in red. Right: A cartoon of the kinetochore connecting chromatin (bottom) to microtubules (top). The increased brightness from the MBA lattice is needed to study crystals such as these kinetochores. Combined with better focusing optics, this will enable focusing down to 0.5 microns, from 5 microns, with a factor of 10,000 increase in flux at the sample decreasing the signal-to-noise ratio. The smaller beam will deposit more of the electron energy outside of the sample spot, reducing primary radiation damage. In addition, the increased brightness combined with room-temperature analysis will decrease the time it takes to collect measurements and thus out run secondary radiation damage. Image courtesy W. Earnshaw, University of Edinburgh.

Large molecular machines such as kinetochore are comprised of many subunits that themselves are composed of many proteins. The current divide-and-conquer approach relies on determining the 3-D atomic-resolution structure of individual proteins and then the protein complexes. Crystallization of the kinetochore for structure determination will be extremely challenging due to the limited amount of each protein, and the difficulty of creating subcomplexes that can be assembled into the full kinetochore. Crystals are likely to be micron sized or smaller and may be very heterogeneous due to the lack of strong contacts between neighboring kinetochores in the crystal. The current APS brightness and large unit-cell parameters of the kinetochore limit the beam and crystal size to five microns or greater. Kinetochore crystals are likely to be significantly smaller than that.

APS MBA Strengths:

To study crystals such as kinetochores, we need the combination of the MBA lattice and better focusing optics to allow the beam to be focused to 0.5 microns, compared to today's 5 microns, and increase the flux by a factor of 10,000. This will significantly improve the signal-to-noise ratio and enable

structure determination from such weakly scattering crystals. The smaller beam will deposit more of the electron energy outside of the sample spot, reducing primary radiation damage. In addition, the increased brightness combined with room-temperature analysis will decrease the time it takes to collect measurements and thus out run secondary radiation damage. Even so, many microcrystals will be required to build a complete crystallography data set from multiple partial data sets.

References

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UNDERSTANDING THE EXCHANGE MECHANISM IN THE NUCLEAR PORE COMPLEX

The nuclear pore complex, NPC, serves as the gateway between the nucleus and the cytoplasm for the selective exchange of macromolecules. Most small molecules can diffuse through the pore. However, larger molecules such as mRNA are actively transported through the pore to the cytoplasm where ribosomes read the mRNA and synthesize proteins. The NPC is also one of the largest supramolecular assemblies in the eukaryotic cell, and is integral to cellular structure (Figure 4.3.3). Although the NPC plays a pivotal role in cellular survival, the exchange mechanism is poorly understood because of its size and complexity. Defects in the NPC structure lead to many diseases such as heart arrhythmia or cirrhosis of the liver [1]. A better understanding of the 3-D atomic resolution structure of the NPC is needed to answer questions such as the mechanism of transport of cargo through the nuclear envelope and the role of the NPC in gene regulation [4]. Understanding these mechanisms will allow the development of more effective drugs to treat disease.

But the size and complexity of the NPC make crystallization difficult [2]. The massive 120-megaDalton assembly measures about 120 nanometers in diameter in the plane of the membrane and about 200 nanometers in length perpendicular to the membrane. The NPC contains a set of multi-protein subcomplexes, each consisting of 30 different nucleoporin proteins that are arranged in a cylindrical structure with eight-fold rotational symmetry. It is estimated that there are 400 to 1,000 proteins in one NPC. Investigators have been systematically determining the structures of the individual nucleoporins and larger subcomplexes [1,3,4]. This “divide and conquer” approach is building towards the structures of larger subcomplex assemblies and introduces the possibility of crystallization of even the intact NPC. However, a multidisciplinary approach may be necessary to dock atomic-resolution structures from X-ray crystallography into electron density maps from cryo-EM reconstructions [4]. Even the subcomplexes are rather large and difficult to crystallize. The crystals often diffract poorly owing to their small size or heterogeneity. Crystals of the NPC are likely to be only two-dimensional and therefore diffract extremely weakly. In addition, the large unit cell parameters will require a highly parallel X-ray beam.

APS MBA Strengths:

The MBA lattice will be essential to study such large structures with X-ray crystallography. The increased brightness will allow delivery of an intense, highly parallel beam that results in a 100-fold improvement in signal-to-noise ratio.

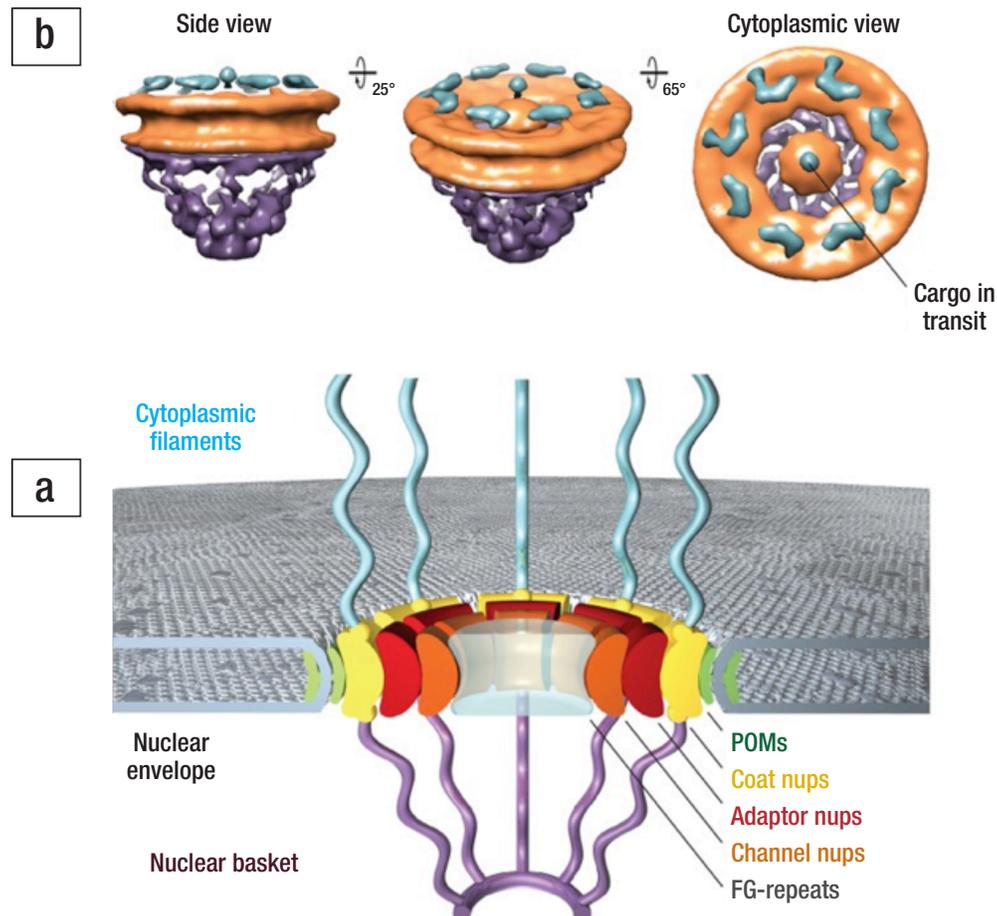


Figure 4.3.3. The overall structure of the nuclear pore complex (NPC). (a) Cryo-electron tomographic reconstruction of the *Dictyostelium discoideum* NPC (Electron Microscopy Data Bank [EMDB] code 1097 [5]). The cytoplasmic filaments, the symmetric core, and the nuclear basket are colored in cyan, orange, and purple, respectively. (b) A schematic model of the NPC. The four concentric cylinders are composed of integral pore membrane proteins (POMs), coat nucleoporins, adaptor nucleoporins, and channel nucleoporins. Natively unfolded phenylalanine-glycine (FG) repeats of a number of nucleoporins make up the transport barrier in the central channel and are indicated by a transparent plug. [1]. The MBA lattice will be essential to study such large structures with X-ray crystallography. The increased brightness will allow delivery of an intense, highly parallel beam that results in a 100-fold improvement in signal-to-noise ratio.

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VIRUSES AND *IN-SITU* ROOM TEMPERATURE CRYSTALLOGRAPHY

A wide variety of viruses cause infectious diseases and several have resulted in pandemics that have killed millions of people. Some of the diseases caused by viruses include influenza, HIV, measles, malaria, and SARS. Understanding the 3-D atomic resolution structure of a virus is essential for developing better drugs that specifically block the virus from infecting a host cell or from replicating.

Virus particles can be quite large, about 100 nanometers in diameter, and have weak intra-crystal contacts, which results in poor order and extremely weak diffraction. Secondary radiation damage to proteins is typically prevented in macromolecular crystallography by cryo-cooling the crystal. Unfortunately, the cryo-cooling process frequently destroys the structural order of virus crystals. Thus, virus crystallography is often performed at room temperature. Diffraction from macromolecule crystals in their growth media and at high temperature (250 to 290 Kelvin), known as “*in-situ* diffraction”, was demonstrated nearly a decade ago [1], and recently has proven valuable for both screening and data collection [2]. The feasibility of the method was beautifully demonstrated by several enterovirus crystal structures solved with diffraction data collected at room temperature from large numbers of crystals in their growth plates [4], and by successful ligand-binding studies of several proteins [5].

APS MBA Strengths:

The new MBA source at the APS will allow experiments with very small crystals of 500 nanometers and should be an ideal source with which to exploit *in situ* diffraction methods. The 100-fold increase in brightness coupled with high-speed detectors [6] and improved optics will allow a reduction in radiation damage at room temperature by exploiting a recently detected effect where secondary radiation damage can be outrun with exposure times less than 100 milliseconds [7]. The high brightness beam will rapidly damage crystals at any temperature, with the result that partial data from many crystals will be merged into complete datasets.

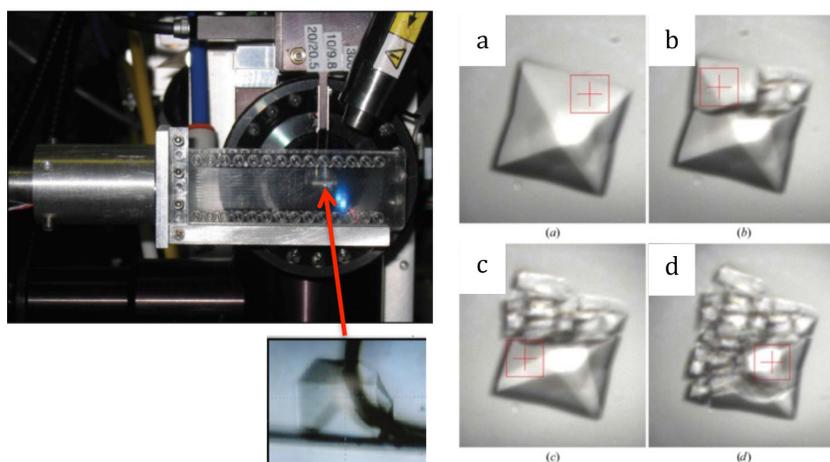


Figure 4.3.4. Left: A microfluidic crystallization card with many crystals mounted on the goniometer of beamline 23-ID-B at the APS. A microcrystal is also shown. Right: Images of an enterovirus crystal after X-ray exposure at room temperature [3]: (a) prior to exposure; and (b), (c), and (d) after successive exposures. The hundred-fold increase in brightness provided by the MBA lattice source, coupled with high-speed detectors, will allow a reduction in radiation damage at room temperatures by “outrunning” secondary radiation damage.

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TRACKING HOW METALS INFLUENCE CELL DEVELOPMENT

Metals and trace elements are essential for life. In any organism, most intracellular processes depend on metals or other trace elements in some form. In fact, it is estimated that one-third of all known proteins contain metal cofactors without which they cannot function. The majority of these proteins function as essential metalloenzymes. The dysregulation of metals in the body causes numerous diseases (e.g., Wilson's disease), and may cause or contribute to neuro-degenerative diseases (such as Alzheimer's); metals are also used as active components in therapeutic or diagnostic agents such as chemotherapeutic drugs (e.g., Pt), or MRI contrast agents (e.g., Gd). While genomics and proteomics have increased our knowledge of how metals and trace elements affect cells, this knowledge remains largely "static" because we lack sensitive approaches to understand how changes in the concentrations and localization of metals influence natural development, differentiation, aging, stress responses, or disease development and progression.

One area of great interest is how trace metals affect life and disease. For example, the role trace metals play in the fertilization and development of mammalian eggs has significant implications for human reproductive health. X-ray fluorescence microscopy has shown that zinc increases dramatically during the final stages of the eggs maturation, making it ready for fertilization (Figure 4.3.5). After that point, the level of zinc drops dramatically. While today's technology is giving us new insight into the previously unknown roles of transition metal in normal egg development, it barely scratches the surface of what researchers need to know. For example, some other questions researchers want to answer are: how is zinc released from the egg and how is it trafficked within the egg? Similarly, we still lack the sensitivity necessary to probe and understand how heavy metal uptake from ground or water contamination can interfere with this signaling and potentially cause the cells to develop improperly, leading to birth defects and cognitive impairment.

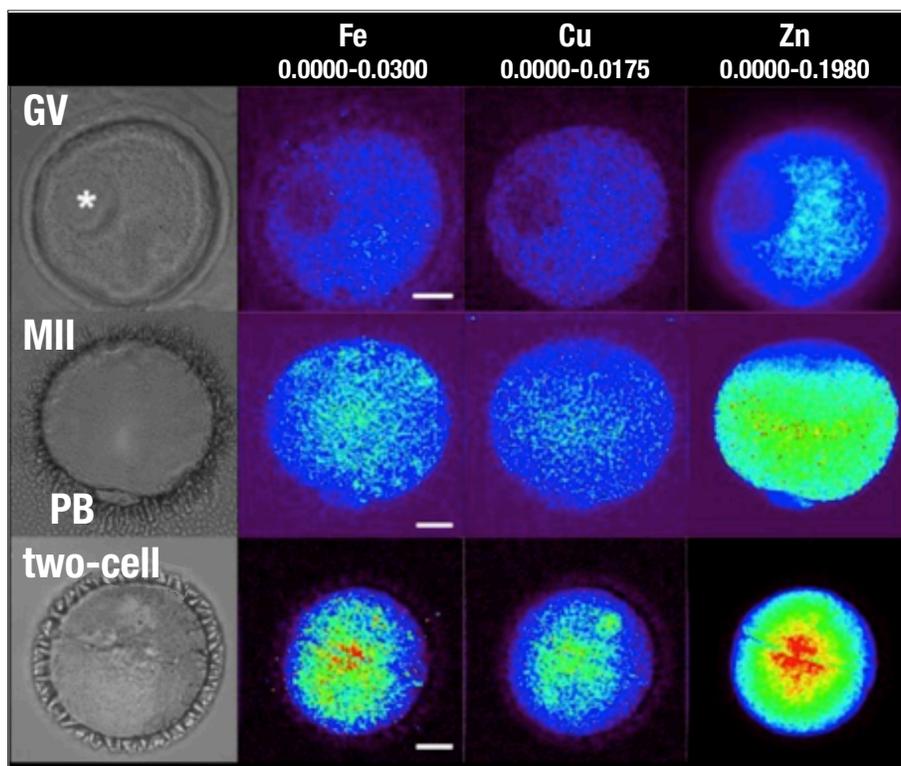


Figure 4.3.5. Elemental images of an immature oocyte (GV), a mature egg (MII) and a two-cell embryo. The germinal vesicle in the immature oocyte largely excludes Zinc; Zn is retained in the mature oocyte, showing an asymmetric distribution, and a polar body (PB) low in Zn. This asymmetry is required for correct oocyte maturation. Scale bar 20 microns. The middle row shows that Zn congregates in the middle of the cell. The increased resolution enabled by the MBA lattice will make visible in 3-D the zinc residing in the inner membrane and how the individual vesicles in the cell emit sparks of Zn to make the egg fertilizable. The increased speed of data collection provided by the MBA also will make it feasible to study dynamics, such as watching the Zn move throughout the layers of the cell. Image courtesy T. O' Halloran, Northwestern University.

At the moment, we cannot effectively probe trace metal content in biological samples at the resolution and sensitivity required to map small clusters of metals as they interact with transporters on cell surfaces and vesicles. We need to increase the spatial resolution, sensitivity, and speed at which we can visualize this trace elemental content in three dimensions in a statistically significant number of cells.

APS MBA Strengths:

The MBA upgrade will provide a 100-to 1,000-fold increase in coherent flux, making this possible – not only for metal interactions within a single cell, but also to map the full 3-D elemental content of hundreds of cells. This would enable statistically relevant conclusions for studies that today are completely out of reach, such as disorders that affect only a few percent of cells. Improved spatial resolution in X-ray microscopy would enable hierarchical imaging at relevant length classes and high spatial resolution within a large field of view. This would allow us to find the proverbial needle in the haystack, such as investigating cytotoxicity of metal-based drugs in animal studies. The high spatial resolution combined with detectors enabling emission spectroscopy and coherent diffractive imaging at high speed promise the ability to probe not only elemental content, but the full chemical state of all

relevant elements and nanoclusters as they interact with cellular content and provide the best picture yet of the dynamic interaction of metal and initial cell development.

UNDERSTANDING METAL-MINERAL REACTIONS TO AID REMEDIATION

Safely storing environmental contaminants such as plutonium requires a deep understanding of how molecular-scale interfacial reactivity and mineral reactions affect its fate and transport. Without an analogue natural mineral to guide predictions, scientists rely on direct observations of near-interface composition and structure.

Contaminant transport of heavy metals in nature is normally controlled by adsorption of individual ions to charged mineral surfaces. Recent observations by X-ray reflectivity (XR) have revealed a new reaction pathway in which plutonium adsorption to a simple mineral surface accompanies the spontaneous formation of PuO_2 nanoparticles, increasing the adsorption capacity of the mineral surface by a factor of more than 30. But a full picture of this reaction, including the chemical changes, reaction rates, and the rate of this transformation in various environments requires brighter X-rays, a smaller beam and higher angular resolution than is available today.

Today XR measurement probes of this nanoparticle formation requires a sample region of about 1 mm^2 in order to have sufficient signal to observe its occurrence. Consequently, measurements of the behavior are averaged from a collection of nanoparticles. While the average height of the nanoparticles above the surface can now be routinely determined, these measurements do not reveal the in-plane distribution (within the surface plane) or size of individual nanoparticles, nor do they provide an understanding of the specific interfacial mineral surface sites (e.g., steps, defects) that nucleate the reaction. Those key details can only be obtained through measurements of individual nanoparticles forming in real time.

APS MBA Strengths:

The MBA lattice technology will provide a small beam with sufficient X-ray flux to observe the formation and growth of individual nanoparticles at mineral-water interfaces. The nucleation and growth of these particles can be imaged *in situ* and in real-time during their seconds-long formation by using state-of-the-art X-ray optics of X-ray reflection interface microscopy (XRIM).

This new capability provides a robust way to gain a new understanding of the complex interfacial chemistry of plutonium and other heavy metals in the environment. More generally, the ability to watch chemical reactions in real time as they occur at interfaces will greatly enhance our understanding and control of chemical reactions at a wide range of solid-liquid interfaces important for chemical and materials sciences. These key interface behaviors include growth and processing of materials and catalytic reactions.

Reference

1. M. Schmidt, S.S. Lee, R.E. Wilson, K.E. Knope, F. Bellucci, P. Eng, J.E. Stubbs, L. Soderholm, and P. Fenter. Surface-Mediated Formation of Pu(IV) nanoparticles at the Muscovite-Electrolyte Interface. *Environmental Science and Technology*, 2013, in press. DOI: <http://dx.doi.org/10.1021/es4037258>.

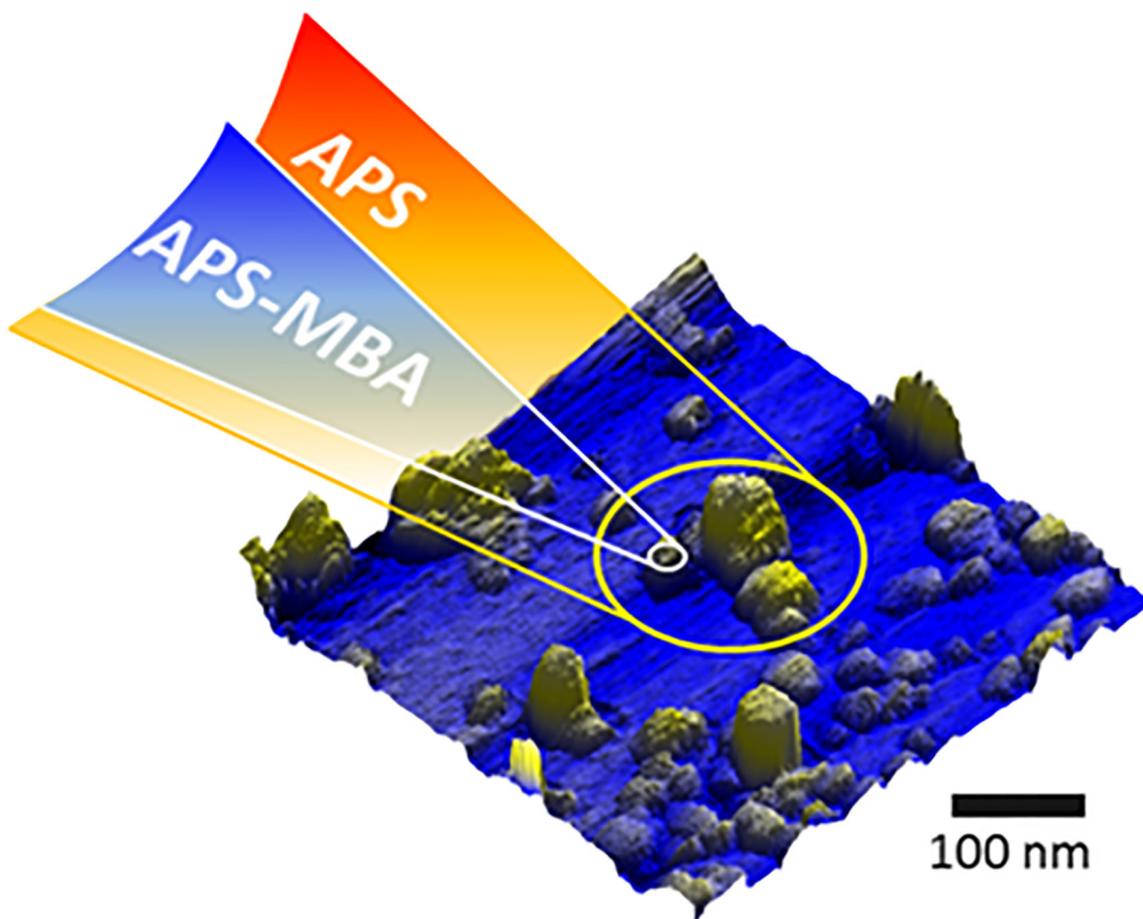


Figure 4.3.6. Ex-situ atomic force microscopy image of PuO_2 nanoparticles formed spontaneously at the muscovite-water interface, illustrating the substantial heterogeneity and complexity of contaminant-mineral reactions in natural systems [1]. Also shown, schematically, is the spatial resolution that can be obtained currently with interfacial X-ray microscopy (~ 100 nm, in orange) and that which will be achieved as a result of the MBA lattice (~ 20 - 30 nm, in blue). The greatly enhanced spatial resolution will enable investigation of the nucleation and growth of individual particles through direct in-situ observations in real time. Image courtesy P. Fenter, ANL.

CHARACTERIZING MICROENVIRONMENTS THAT CONTROL TRANSPORT AND FATE OF POLLUTANTS

Variations in microenvironments, particularly those found in cracks or pores in sediment particles, can dictate the type of remediation needed to remove or stabilize pollutants. Yet the chemistry in these microenvironments is poorly understood, increasing the risk of inaccurately predicting the spread, stability, and lifetime of the pollutant. For highly toxic spills such as the uranium leaking from the Hanford tanks, public and environmental health requires the most precise measurements possible.

But often modeling based on bulk characterization of the sediments fails to match measurements of the excavated soil and sediments. This occurs because the chemistry can be much different in the microenvironments found in confined spaces than in the surrounding soil. Synchrotron methods provide exceptional sensitivity to structure and chemistry and can detect nanoparticles inside the particles. However, to date they have lagged behind the spatial resolution of transmission electron microscopy (TEM).

APS MBA STRENGTHS:

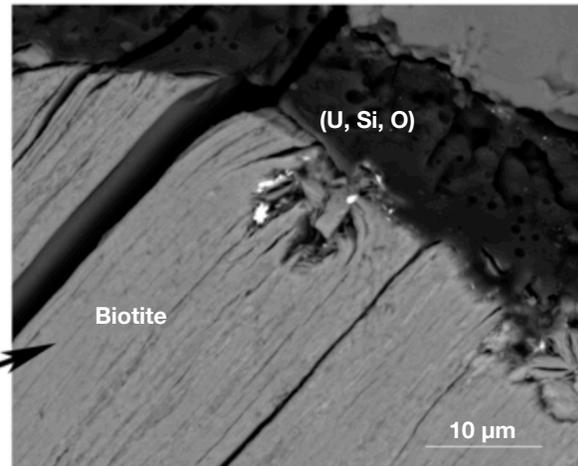
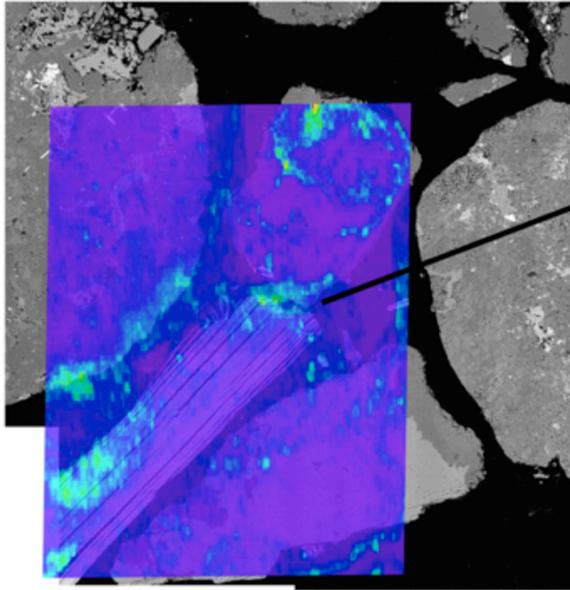
An MBA lattice at the APS would provide the high brightness and small beam needed to characterize micro- and nano-precipitates. TEM-like spatial resolution can be combined with XAFS spectroscopy and micro-diffraction techniques to fully characterize the nano-precipitates, including those buried deep inside grains inaccessible to electron probes. X-ray techniques have the additional advantage that they can be applied under natural conditions, avoiding possible changes as samples are prepared for measurement. This will provide an unprecedented opportunity to study the nano-precipitates. The nanoscale flux should be at least 100 times better, improving spectroscopic sensitivity by a factor of 10 or more.

This will enable a much more systematic investigation of the role of microenvironments on pollutants from a variety of activities including mining, manufacturing, and cold war weapons production.

Reference

J.P. McKinley, J.M. Zachara, C. Liu, S.M. Heald, B.I. Prenitzer, and B.W. Kempshall. Microscale controls on the fate of contaminant uranium in the vadose zone, Hanford Site, Washington. *Geochimica et Cosmochimica Acta*, 70(8):1873–1887, April 2006.

Uranium abundance from x-ray fluorescence
overlay on a backscattered electron image.



Backscattered electron image shows uranium silicate precipitates on the edge of a biotite grain. It does not show precipitates in the grain interior.

Figure 4.3.7. Elemental map of uranium distribution in biotite ore, shown by light blue color. The hundred-fold increase in the flux for the nano-scale beams provided by the MBA lattice will dramatically improve sensitivity to dilute precipitates. This will increase our understanding of how microenvironments impact pollutants from mining and manufacturing and could help shape environmental remediation strategies. Image courtesy J. McKinley, PNNL.



4.4 INSIGHTS INTO EXTREME ENVIRONMENTS

INTRODUCTION

Materials subjected to the extremes of pressure, temperature, and electromagnetic fields often display novel electronic, magnetic, and structural properties. Discovering and understanding these phases of matter provides key insight for designing new materials and improving their functional properties. The most extreme sample conditions, however, can typically be realized only in extremely small volumes. With its intrinsic high brightness, deep-penetrating power, and nano-scale spatial resolution, an MBA synchrotron source provides an ideal probe for revealing the structure, correlations, and dynamics of materials in such extreme environments. For example, the APS MBA lattice will permit studies of materials at pressures beyond one terapascal, more than twice the pressure in the center of the Earth. This will enable studies of such diverse phenomena as metallic hydrogen, pressure-driven complexity in “simple metals” (e.g., Li, Na), and the structure of the interiors of giant gaseous planets. Another exciting research frontier for MBA synchrotron radiation research is offered by the simultaneous application of multiple extreme conditions. Using state-of-the-art technology, it will be possible to include a compact high-pressure cell inside a high-field magnet and cool it to below 300 millikelvin. Such ultralow temperatures combined with high pressures and fields can be used to create and study new states of matter. Lastly, a high-energy MBA source will provide new opportunities for *in-situ* exploration of the physics of “extreme” samples such as irradiated materials and systems under large shock compression, where the sample or interaction volume is extremely small.

UNDERSTANDING THE STRUCTURE AND PROPERTIES OF PLANETARY INTERIORS

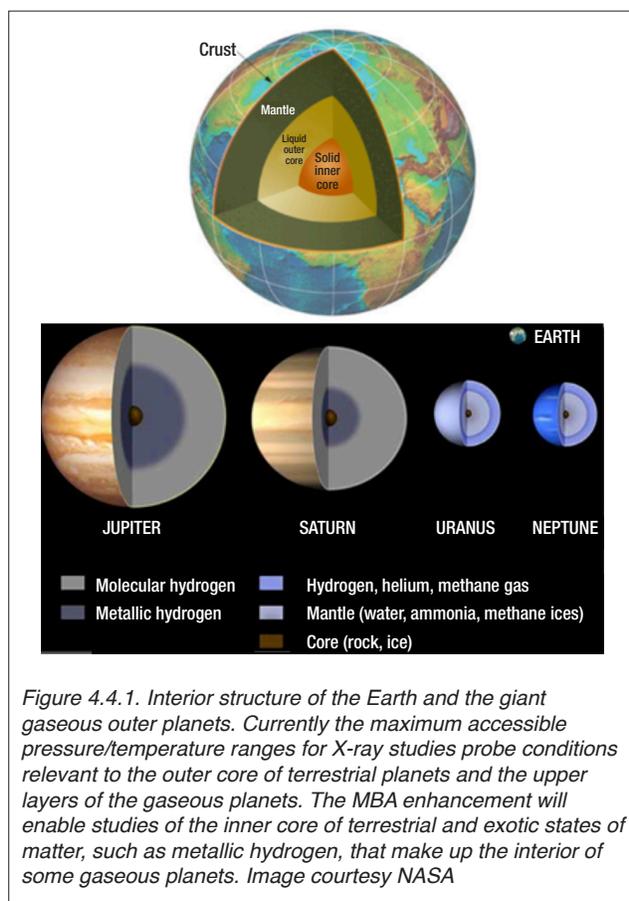
Deciphering the workings of planetary interiors requires creating experimental conditions similar to those found within various strata inside a planet. Our ultimate understanding of the inner structure of planets is directly linked to the maximum accessible pressures and temperatures (P-T) for experiments. The current P-T limits for X-ray studies using state-of-the-art diamond anvil cells and laser heating is about 300 gigapascals (GPa), and about 4,500 Kelvin. These are the conditions encountered at the outer core of terrestrial planets, such as the Earth, and in the top most layers of outer giant gaseous planets in our solar system.

To probe the structure and dynamics of the materials deep inside planetary interiors requires significantly increasing the pressures and temperatures applied to samples. The P-T conditions at the center of the Earth, for example, are thought to be about 400 GPa and about 6,000 Kelvin. Those near the center of the giant gaseous planets extend into the terapascal regime and beyond 10,000 Kelvin. Such extremely high P-T conditions can only be realized in sample volumes on the order of a few-cubic microns.

APS MBA Strengths:

Probing such minute samples with the breadth of X-ray techniques available will require the very intense, tens of nanometer spot size X-ray beams provided by the MBA lattice. These nanometer X-ray beams will not only extend the P-T ranges available for study, but will provide greatly enhanced spatial resolution for better P-T definition, and determining the elemental partition, anisotropy, and phase separation within the material.

One of the most exciting research frontiers that will be opened by the APS MBA upgrade is related to hydrogen, the lightest and most abundant element in the universe. At ultra-high pressures, such as those encountered in the interior of Jupiter and Saturn, hydrogen has been predicted to exhibit exotic properties, such as superfluidity and superconductivity. At these high pressures, electrons disassociate



from the protons and hydrogen is thought to form a metallic phase [1]. Determining the structure and dynamic properties of this metallic phase of hydrogen has been one of the grand challenges in high-pressure science for almost a century, and is critically important for understanding the behavior of giant gaseous planets. The two-to-three-orders of magnitude higher brilliance provided by the MBA lattice at APS only enable the determination of not only the pressure-induced structure of dense hydrogen, but also its electronic structure, which is directly related to metallization, via inelastic X-ray scattering (IXS).

Reference

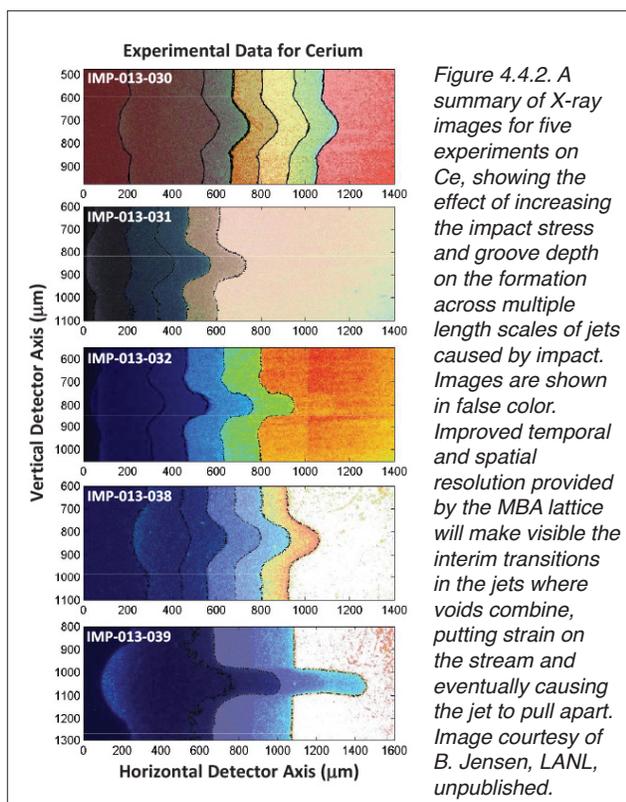
1. P. Loubeyre, R. Letouillec, D. Housermann, M. Hanfland, R.J. Hemley, H.K. Mao, and L.W. Finger, X-ray diffraction and equation of state of hydrogen at megabar pressures, *Nature*, 383: 702, 1996.

SHOCKWAVE STUDIES TO PREDICT AND CONTROL MATERIAL AT EXTREMES

Examining the evolution of material properties at dynamic extreme conditions through shockwave physics advances understanding of numerous high-pressure phenomena. These include natural events such as meteorite impacts, general solid mechanics, and fluid flow behavior for applications such as inertial confinement fusion. Dynamic compression techniques provide key information on defects in materials in dynamic situations, and such information can be used to develop strategies to control defects and maximize material performance.

For example, the ability to study the formation of voids and the collapse of fibers in microlattice foam with X-ray phase contrast imaging helped develop the world's lightest metal foam [1]. This foam design can lead to more fuel-efficient and impact-resistant vehicles.

In another example, X-ray diffraction studies of jet formation in metals look at the effects of a shock wave through various sample groove patterns. In these experiments, an impact causes target material to stretch outward in a jet whose shape and height reveal the strength of the material during dynamic deformation. The information is used to understand the origin of material strength across multiple length scales. This helps explain a wide range of phenomena, from the effects of meteorite impacts to improved efficiency of ink jet printers and industrial sprayers.



APS MBA Strengths:

Today, observation of dynamic behavior at the level of microstructure is blurry, if visible at all, and scientists must extrapolate full dynamic behavior from fuzzy periodic snapshots of behavior. The nature of dynamic studies are inherently signal limited, and every improvement in source intensity and detector efficiency leads to new regimes of observation. Brightness increases from the MBA upgrade directly translate into increases in flux density, which in turn directly increases the sensitivity of the experiment. The round beam enabled by the APS MBA upgrade will considerably simplify the interpretation of images since the resolution becomes spatially homogeneous.

The MBA's increased brightness also will enable spatial resolution in X-ray phase contrast imaging to improve from today's one micron to 50 nanometers. For microlattice foam studies, that will make the difference between studying how micro-sized areas of a "rope" of lattice collapse to from a shockwave to seeing with clear resolution how individual fibers collapse.

This combination of improvements will allow engineers for the first time to see clearly the start of defects, including a crack tip and surrounding stresses, and how the collapse of voids in a crystal generate heat to start a detonation reaction. The testing of theories will be possible, vastly improving our ability to predict and control the response of matter at extreme conditions.

Reference

1. B.J. Jensen, S.N. Luo, D.E. Hooks, K. Fezzaa, K.J. Ramos, *et al.* Ultrafast, high resolution, phase contrast imaging of impact response with synchrotron radiation. *AIP Advances*, 2: 012170, 2012.

NEW OPPORTUNITIES FOR X-RAY STUDIES IN HIGH MAGNETIC-FIELDS

Magnetic fields provide a versatile contact-free experimental parameter for exploring novel states in quantum matter that are fundamental to our understanding of a material's potential functional properties. These novel states include superconductors, meta-magnetic phases in correlated-electron systems, exotic ordering in spin-gap and frustrated compounds (Figure 4.4.3), and valence transitions. Frequently, these phenomena arise from an interplay competition among spins, orbital, and charge degrees of freedom in a crystal lattice.

Synchrotron radiation provides an ideal tool for probing these various structural and electronic orderings. Resonant diffraction, for example, can be employed to enhance the signal from particular elements and selectively probe their magnetic and/or multi-polar ordered moments. Polarization dependence, on the other hand, can be applied to directly reveal spin and orbital composition of magnetic moments. Such studies in extremely high magnetic fields, however, have been hampered by the complexity involved in generating these fields with the necessary optical access for X-ray scattering measurements. As a consequence, maximum achievable fields have been limited.

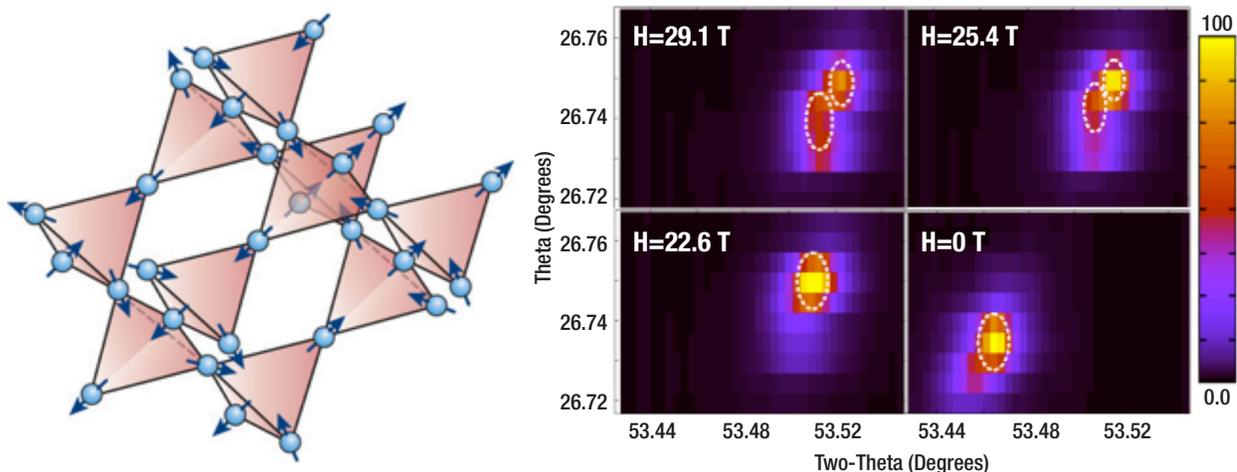


Figure 4.4.3. Frustrated magnets are systems where the atoms lie on a lattice, such as the tetrahedron on the left, where the magnetic interactions cannot be simultaneously satisfied. The figure on the right shows X-ray scattering studies of the magnetostriction (white arrow; $0 < H \leq 25$ T) and subsequent phase-transition (split peak; $H \geq 25$ T) in such a system, $Tb_2Ti_2O_7$ [1]. The MBA lattice upgrade will enable new types of measurements, such as coherent diffractive imaging, at much higher fields with greater flexibility.

APS MBA Strengths:

The nano scale beams provided by the APS MBA source will overcome the optical access limitations to reach much higher maximum fields for X-ray studies upwards of 25-30 Tesla continuous and in excess of 50 Tesla pulsed. This is achieved using novel magnet designs that are matched to the small illuminated sample volume probed by the MBA lattice-generated X-ray beam. In addition, samples of interest for many high-field studies, such as doped complex-oxides, are naturally inhomogeneous on various intrinsic length scales, from nanometer to micrometer. The nano-scale X-ray probe will enable “clean” scattering studies that isolate the contributions from only one particular ordered domain

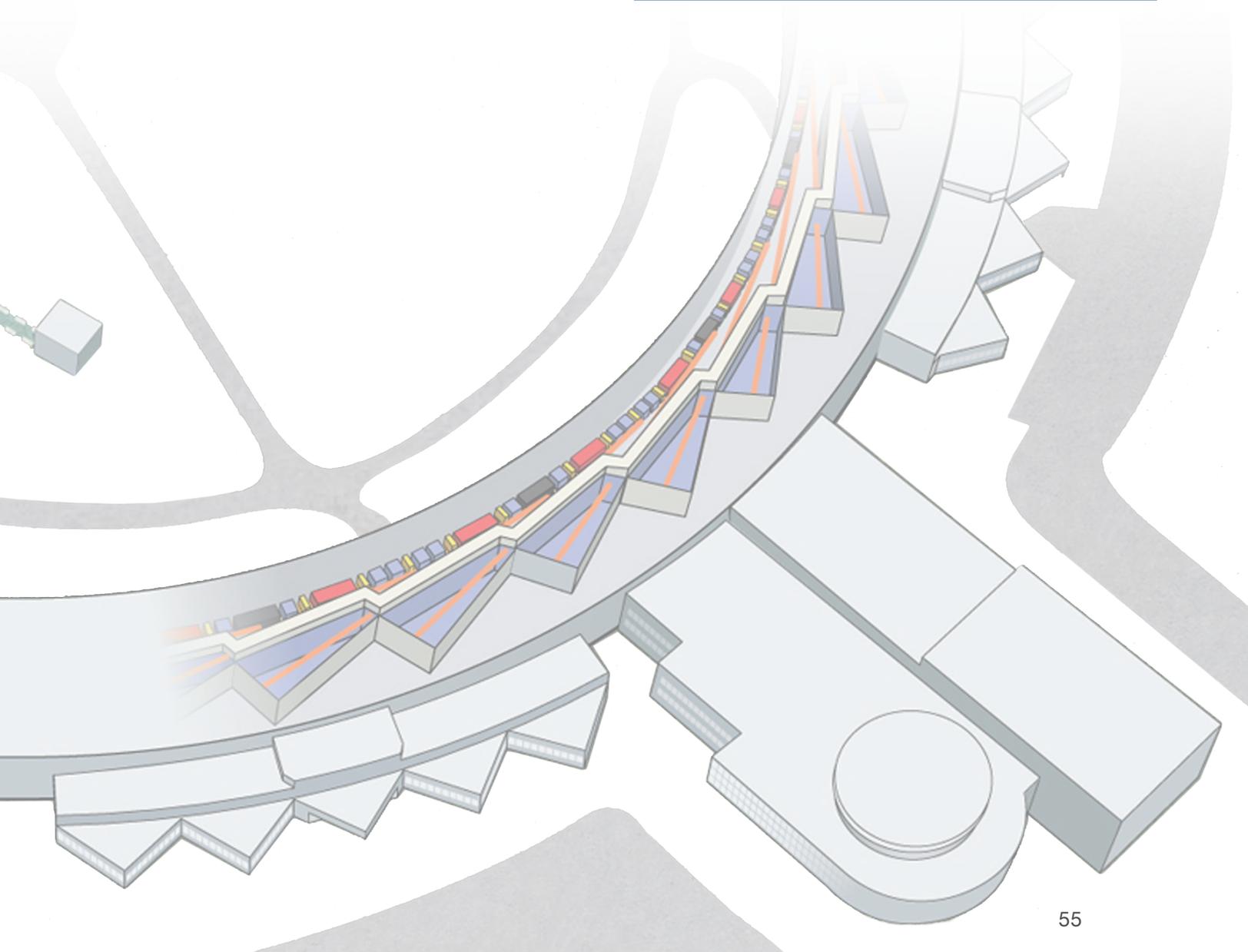
A MBA Lattice at the APS: A New Generation

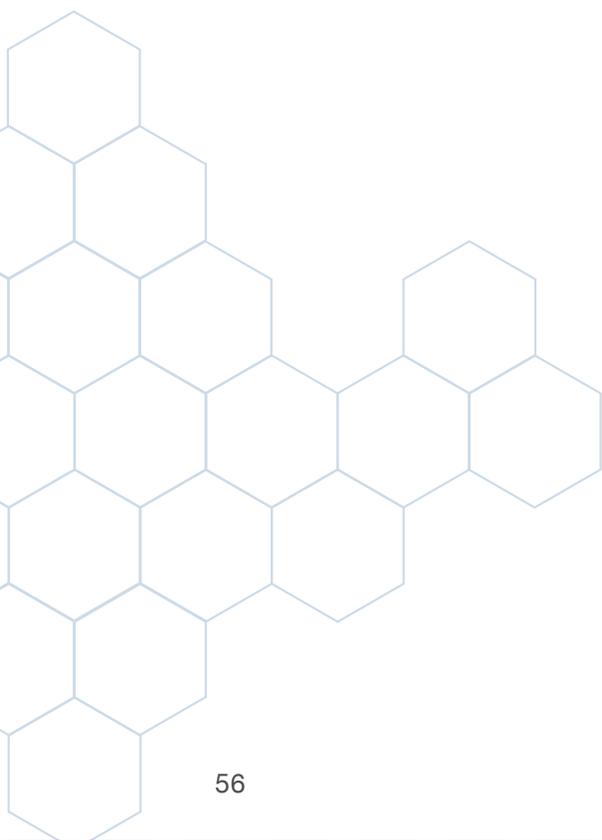
or doping state, rather than yielding the spatially averaged magneto-structural information of current measurements. Furthermore, the increased coherence will open up new possibilities for using coherent diffractive imaging to observe the domain structure (magnetic, charge, and orbital) evolution under applied extreme fields. The morphology of such domains is a critical component in determining the macroscopic electronic properties of a material. Thus, the increased brightness of MBA lattice will open up entirely new avenues for exploring the atomic and mesoscopic structure of materials subjected to extreme magnetic fields. These new capabilities have the potential to truly revolutionize high-field magnetic research.

Reference

1. J.P.C. Ruff, Z. Islam, J.P. Clancy, K.A. Ross, H. Nojiri, Y.H. Matsuda, H.A. Dabkowska, A.D. Dabkowski, and B.D. Gaulin. Magnetoelastics of a Spin Liquid: X-Ray Diffraction Studies of Tb₂Ti₂O₇ in Pulsed Magnetic Fields, *Phys. Rev. Lett.*, 105: 077203, 2010.

5.0 NEW AND IMPROVED TECHNIQUES, CAPABILITIES, AND TECHNOLOGIES





5.1 NEW AND IMPROVED TECHNIQUES TO EXPAND MBA LATTICE SCIENTIFIC IMPACTS

INTRODUCTION

This section provides short descriptions of four techniques that are expected to blossom out of an MBA upgrade to the APS. All are coherence-based techniques, and relatively recent additions to the X-ray toolbox available to scientists.

In addition, the low-emittance photon beam from the MBA APS upgrade enables improvements to the full array of X-ray techniques, which are needed to capitalize on the scientific opportunities described in this workshop report. Diffraction, spectroscopy, and imaging methods all significantly benefit from the properties of a low-emittance beam, often quite dramatically. Both microfocusing and nanofocusing optics become much more efficient, enabling a host of photon-starved experiments at smaller-spatial resolutions. Furthermore, many spectroscopy analyzers will have better resolution with higher throughput as a direct result of the smaller X-ray beams.

PHASE CONTRAST IMAGING (PCI)

X-ray phase contrast imaging (PCI) has capabilities that extend well beyond the familiar technique of absorption imaging. For situations where there is poor absorption contrast (e.g., low-Z materials, high-energy X-rays), phase contrast imaging can increase sensitivity by three orders of magnitude [1, 2].

The decrease in horizontal source size enabled with the MBA lattice will expand the reach of PCI even further (Figure 5.1.2). The small, round source enables development of a projection microscope for full-field PCI [3]. Much finer resolution can be achieved without limits of detector pixel size. Propagation-based PCI can be performed with both image contrast and spatial resolution simultaneously optimized. This is not possible currently at the APS, where the horizontal source size is more than 20 times larger than the source size in the vertical direction.

Propagation-based PCI requires a simple experimental setup. Phase contrast is formed by letting a wave field propagate in free space, after interaction with an object (Figure 5.1.1). Unlike absorption contrast imaging, the detector is not placed immediately behind the sample, but at some distance from it, so the X-rays refracted by variations in electron density can interfere with each other. PCI is a real-space imaging method and can be combined with tomographic techniques to obtain the 3-D distribution of the refractive index of the sample.

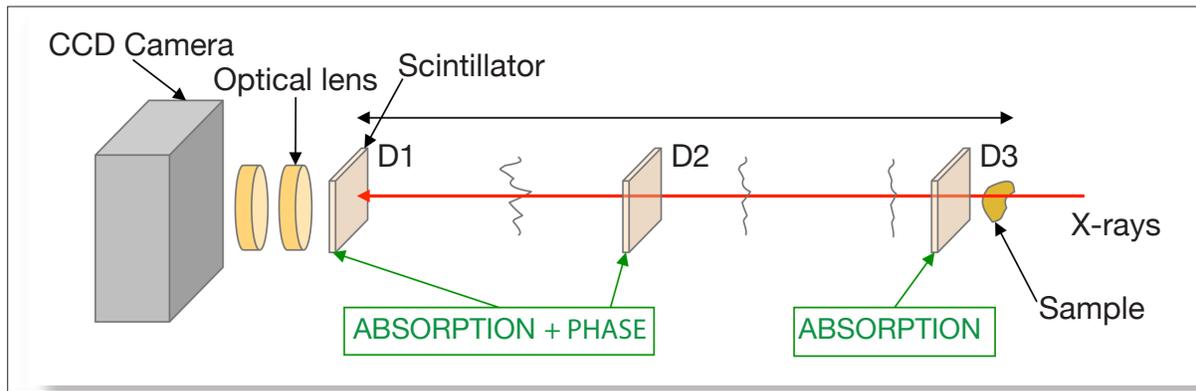


Figure 5.1.1. Schematic of in-line propagation-based full-field phase contrast imaging. Contrast is formed by moving the detector distances $D1$, $D2$, and $D3$ from the sample. The multiple distances of the detector from the sample allows for a range of contributions in absorption and phase contrast.

Another area where PCI will gain large improvements from the MBA lattice is in the “edge-detection” regime where the detector sample distance (D) is adjusted such that the phase contrast is maximized at the edges of an inhomogeneity. This makes PCI particularly sensitive to seeing interfaces in materials. At a given energy, the visibility of interference fringes is determined by the lateral coherence of the beam. Requirements on longitudinal coherence are modest, so polychromatic beams can readily be used [4, 5]. Currently at the APS, PCI performed with broad energy band-pass X-rays achieves exposures down to the single X-ray pulse width of 100 picoseconds. The increased coherent flux for high-energy X-rays provided by the MBA lattice will permit such imaging through high-Z materials with micron-spatial resolution.

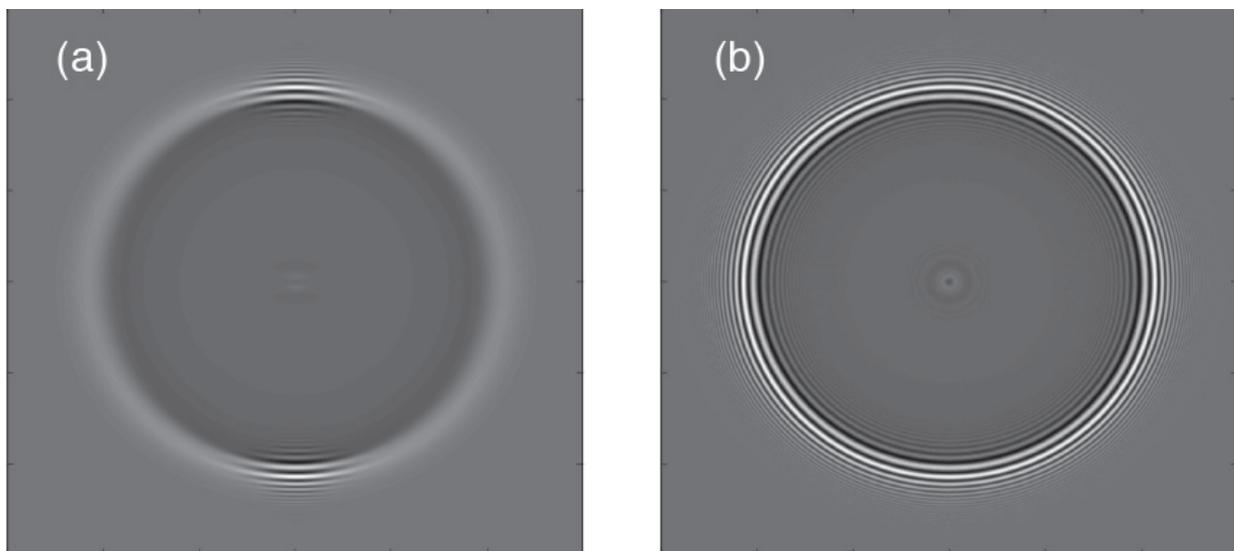


Figure 5.1.2. Source size effects in phase contrast imaging as illustrated by simulated X-ray images of an air bubble ($2\ \mu\text{m}$ diameter) inside water at 15 keV. Bubble (a) is imaged with the current APS lattice, and bubble (b) shows expected imaging with the future MBA lattice at the APS. Image courtesy Kamel Fezzaa, ANL.

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1. A. Snigirev, I. Snigireva, V. Kohn, S. Kuznetsov, and I. Schelokov. *Rev. Sci. Instrum.*, 66: 5486, 1995.
2. K.A. Nugent, T.E. Gureyev, D.F. Cookson, D. Paganin and Z. Barnea. *Phys. Rev. Lett.*, 77: 2961–2964, 1996.
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X-RAY PHOTON CORRELATION SPECTROSCOPY (XPCS)

X-ray photon correlation spectroscopy (XPCS) is a technique that probes the dynamic evolution of the heterogeneity of a sample, such as diffusion of colloidal particles or changes in the morphology of ordered domains. Typical X-ray scattering experiments sample the average structure of a material, since the scattering from various parts of the sample sum incoherently. An XPCS experiment, on the other hand, uses a coherent X-ray beam to provide sensitivity to the exact arrangement of the particles within the coherently illuminated sample volume, yielding a complete picture of the structure in a sample. This information manifests itself as bright and dark intensity modulations in the X-ray scattering called speckle. Fluctuations in the structural, chemical, or magnetic order in the material result in fluctuations in the speckle pattern even while the average diffraction pattern remains unchanged. The characteristic time scales of the fluctuations are recorded and provide a statistical measure of the underlying fluctuations in the sample as a function of length scales over a range from microns to nanometers. XPCS uses at most a few coherent modes of the incident beam. Existing third-generation sources have many coherent modes, which result in low signal levels, limiting the applicability of XPCS. The proposed MBA upgrade to the APS storage ring lattice will be a revolutionary upgrade for XPCS because the applicability of XPCS scales as the square of the source brightness. A 100-fold increase in source brightness will therefore provide a 10^4 -fold increase in dynamic range. This large enhancement will enable XPCS at the MBA-upgraded APS to reach simultaneous nanosecond and nanometer time and space resolutions.

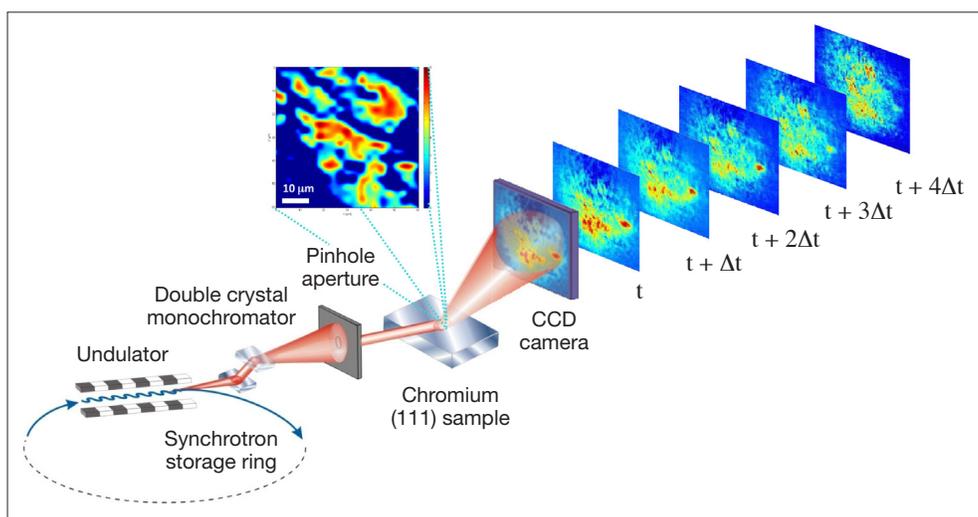


Figure 5.1.3. Schematic of an XPCS diffraction measurement from a chromium single crystal. The modulations in the speckle pattern measure the spatio-temporal evolution of the magnetic domains in the sample [1].

The current APS coherence and brightness limit XPCS usage for studies on time-scales in the seconds range and for strongly scattering particles with sizes greater than 500 nanometers. The APS-MBA upgrade will provide a revolutionary change – a factor of 10^4 increase in time resolution and a factor of 50 reduction in the size of particles that can be studied. By providing higher X-ray energies with enough coherence, X-ray absorption will be reduced and enable studies of industrially important systems in realistic operating environments.

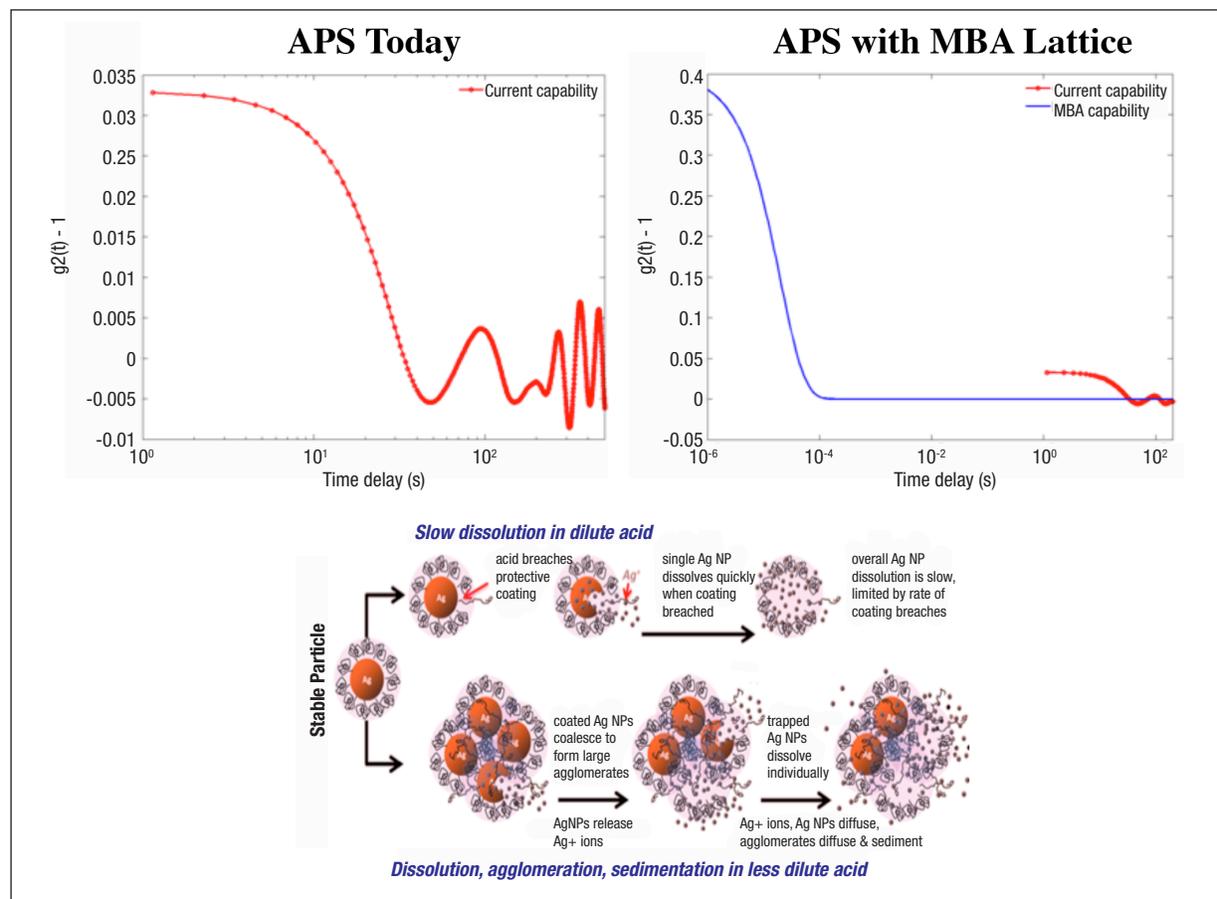


Figure 5.1.4. (Top) $g_2(t)$ represents the normalized intensity auto-correlation function at a particular wave vector q and time delay t . It often follows a form of exponential decay, with the decay rate related to dynamic motion. The MBA lattice will enable access to new time regimes that will allow the differentiation of chemical pathways such as the dissolution of silver nano particles (Bottom). APS MBA upgrade will provide a factor of 10,000 improvement in time resolution and a factor of 50 reduction in the size of particles that can be studied. Image courtesy Fan Zhang, NIST.

References

1. O. Shpyrko *et al.*, Direct measure of antiferromagnetic domain fluctuations. *Nature*, 447: 68, 2007.

COHERENT DIFFRACTIVE IMAGING (CDI) AND PTYCHOGRAPHY

Coherent diffractive imaging is a lensless technique, giving it two significant advantages over traditional X-ray imaging methods. First, the image resolution is not determined by X-ray optics, but rather by the coherent intensity of the incident beam. Second, the constraint of short working distances, inherent to high-resolution X-ray optics, is removed, which leaves ample space for *in-situ* and *in-operando* environmental cells.

Coherent imaging can be done in two ways: one relies on samples being small in size – from a couple of micrometers to less than 100 nanometers. This is typically referred to as coherent diffractive imaging (CDI). The other imaging style relies on an ability to accurately scan a beam across a larger sample, similar to scanning probe microscopy techniques. This style is called ptychography, because the Greek root of the word means “to fold,” and this technique uses measurements from overlapping positions of the sample. Both methods exploit the coherence of the incident beam to measure interference patterns in the scattered beams. Images are formed using special computer algorithms that convert the diffraction patterns to very high-resolution images of the samples.

In CDI, the scattered beam can be measured either in the forward direction or around Bragg peaks of crystalline samples. The measurement in the forward direction is sensitive to electron density, complex index of refraction, and even magnetic structure or electronic states (materials properties). When Bragg peaks are measured there is added sensitivity to strain in a crystalline lattice. The X-rays scattered from the sample are allowed to propagate to the detector and interfere to form complicated diffraction patterns. The relative phases of the interfering waves are retrieved and used to produce an image of the sample. To observe the speckle pattern, the collected data must be sampled on a very fine grid. These algorithms are

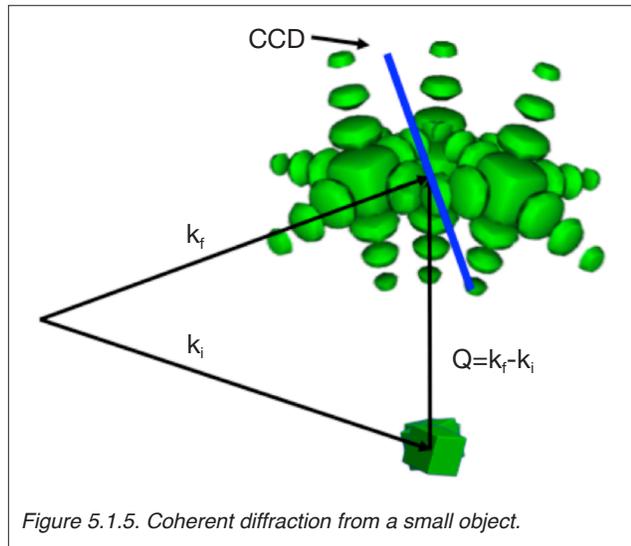


Figure 5.1.5. Coherent diffraction from a small object.

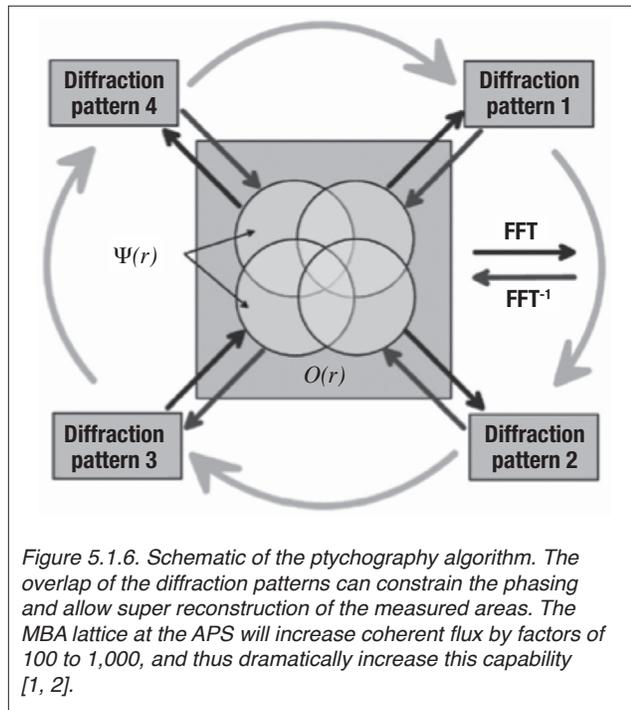


Figure 5.1.6. Schematic of the ptychography algorithm. The overlap of the diffraction patterns can constrain the phasing and allow super reconstruction of the measured areas. The MBA lattice at the APS will increase coherent flux by factors of 100 to 1,000, and thus dramatically increase this capability [1, 2].

A MBA Lattice at the APS: A New Generation

iterative in nature and require fast computers to manage ever-growing data sets and high-resolution images of extended fields of view. Fast computers and efficient algorithms already exist and increased collaboration between APS and Argonne National Laboratory's Mathematics and Computer Science Division will help respond to future needs in these areas.

Ptychography is a relatively new method of extending the reach and use of coherent imaging. A limitation on CDI is that samples need to be compact. Phase retrieval is possible because the sharp edges of the sample place a strong constraint on relative positions of features within the sample. Without sharp boundaries, there are multiple configurations of features in a sample that can give rise to very similar diffraction patterns, making it impossible to image a small field of view within an extended sample.

In ptychography, the use of overlapping of measurements (folding) gives much needed constraints on relative positions of structures in the images. The overlapping regions of the two images are of the same material and must have the same structural information. This can be used to constrain the phasing and allow images to be constructed.

Optimal performance of coherent X-ray imaging requires sufficient coherent flux, and thus the coherence in the incident beam can be preserved to the maximum extent possible. The MBA upgrade to the APS will increase the coherent flux by factors of 100 to 1,000, and hence dramatically increase the capability of coherent X-ray imaging.

References

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5.2 SPECTROSCOPY AND IMAGING, TODAY VS. TOMORROW

The incorporation of an MBA lattice into the APS Upgrade plan will revolutionize the reach of many X-ray capabilities. Below are two examples of the increased spatial and temporal resolutions and expanded chemical and elemental identification expected from the APS MBA Upgrade.

LOOKING AT BATTERY MATERIALS WITH LERIX

Inelastic X-ray scattering is an excellent technique for looking at soft X-ray absorption edges in environments that are inaccessible to low-energy X-rays such as in an operating battery. An upgraded LERIX (low-energy resolution inelastic scattering; currently 20-ID) beamline combined with an MBA lattice will allow charge dependent measurements on such systems with improved spectral resolution and better signal-to-noise ratio. Reduced measurement times on important soft X-ray edges to the desired 20-minute minimum, which eliminates the need to falsely slow down the charging rate to collect data. Overall, capabilities will improve by two orders of magnitude. This incorporates a reduction in signal-to-noise from more and better analyzers, higher flux with optimized undulators, and improvements in energy resolution that stem from the use of collimating mirrors and better analyzers.

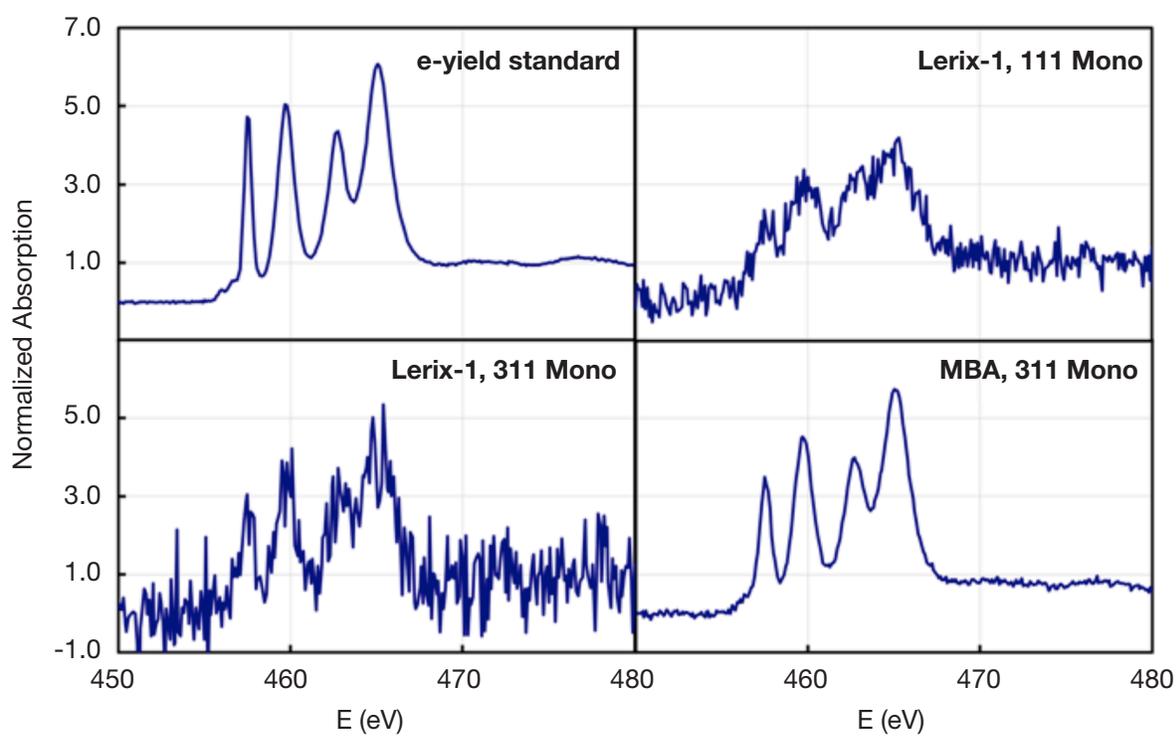


Figure 5.2.1. Simulated 20-minute noise-level scans of Ti L-edge CaTiO_3 . While not a typical battery material, this provides a similar signal to metal oxide battery materials as well as high-quality electron yield data for simulations. Image courtesy S. Heald, ANL.

CHEMICAL AND ELEMENTAL ANALYSIS FOR NEXT-GENERATION NANOPROBES

The MBA lattice at the APS will provide revolutionary capabilities for nanoscale chemical and elemental analysis. The greatly increased X-ray flux in a small focal spot will provide the ability to resolve 5-nanometer W structures; detect and resolve Al structures on thick, 100-micron silicon samples; detect and resolve doping; and determine relative positioning of single atomic-layer W and As structures buried in thick samples.

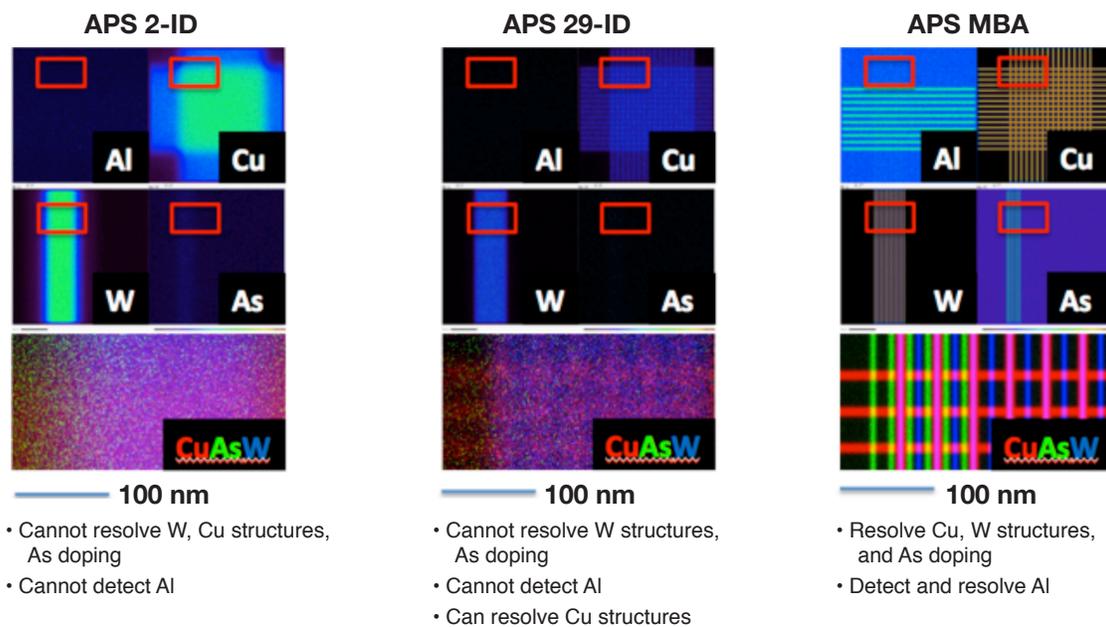


Figure 5.2.2. Left: Simulations of X-ray fluorescence imaging of semiconductor materials. Today's 120-nanometer resolution at the APS's "workhorse" X-ray fluorescence beamline. Middle: Current 35-nanometer spatial resolution at the APS's world-leading nanoprobe. Right: The 5-nanometer spatial resolution made possible with an MBA lattice at the APS. Image courtesy S. Vogt, ANL.

5.3 CRITICAL ENABLING TECHNOLOGIES

The increased brightness of an MBA lattice at the APS will enable a new generation of measurements that could have major impacts across a broad area of science. The extremely low-electron beam emittance (expected to be in the range of 60 to 80 pm) of proposed MBA lattices will produce hard X-ray beams with increased coherent flux that can be focused with high photon densities. These properties will allow the current suite of coherence-based techniques to be extended in temporal resolution and spatial resolutions, and to achieve increased sensitivity. To maximize the benefits of the MBA lattice, APS staff have developed a plan to improve beam stability and will develop a plan to improve sample stability instrumentation installed at the APS. For beamline operations, one of the assets of the MBA lattice technology at the APS is that the benefits can be realized utilizing existing beamline infrastructure, making it an economical upgrade. Even greater benefits that take full advantage of the two-to-three order of magnitude increase in brightness are achievable with relatively modest investments in improved optics, detectors, sample environments, and optimized insertion devices.

X-RAY OPTICS

One of the strengths of the MBA design is that it produces orders-of-magnitude higher brightness without orders-of-magnitude higher flux. This avoids harmful effects such as heating of beamline optics. The heat load will increase only minimally with the MBA lattice. While the current beamlines can benefit without additional investments in optics, even larger benefits can be obtained through modest investments in focusing optics. These improvements can be phased in to keep step with the needs of the community. For example, updated optical systems to transport the high coherent flux for use with coherent imaging and scattering techniques would capture the full benefit of the two-to-three order of magnitude improvement. Likewise, hard X-ray microscopes could go beyond the initial benefits with the use of higher quality focusing optics.

Power Loading on First Optics

Increasing the beam current from the present 100 milliamps to 200 milliamps in a new MBA lattice will minimally increase the heat load on both insertion device (ID) and bend magnet (BM) beamlines optics. This factor of two in current increase is mitigated by the expected decrease in electron energy from 7 GeV to 6 GeV. As a result, expected increases in total-power and peak-power density will be on the order of 30 percent to 60 percent larger than what exists today. Hence the power from a BM and ID source in the MBA lattice is similar to that expected when increasing the APS current from 100 milliamps to 150 milliamps at 7 GeV. For monochromators, this is a value that can be effectively handled by current cooling infrastructures, as proven by several high-current test runs at about 150 milliamps organized to evaluate performance of optical components. However, the requirements for thermally induced slope errors for mirrors will likely be more demanding and so existing cooling schemes may need to be redesigned.

A benefit of having smaller beams is that diamond optics may become a more viable option in the future, if high-quality diamonds are available. This would require further evaluation of the thermal and mechanical stability of all optics, whether cooled or not.

Mirrors and Metrology

To maximize coherence preservation and nanofocusing may require high-quality mirror systems that could necessitate improvements in mirror manufacturing techniques, mechanical mounting, and cooling schemes to meet the expected performance goals of height and slope errors that could reach 0.5 nanometers and 50 nrad, respectively. Metrology tools that work at both optical and X-ray wavelengths will be needed to assess operational performance of these complete systems. The APS metrology facility is equipped with a new Long Trace Profiler (LTP) that has about a 50-nrad noise floor for quality control of mirrors and in-house fabrication of Kirkpatrick-Baez (K-B) mirrors. This facility could be complemented with advanced 2-D metrology tool such as that developed by Osaka University and Jtec Inc., (Japan).

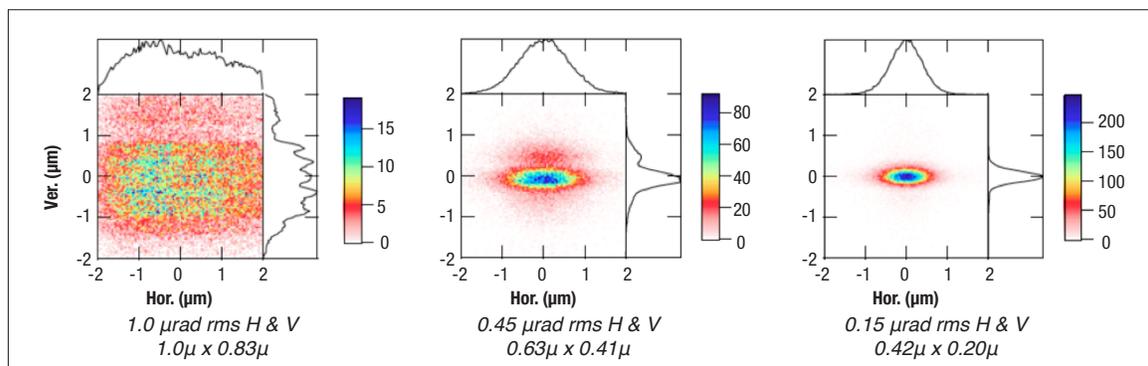


Figure 5.3.1. Ray tracing for a focusing mirrors (mirror 39 meters from the source and with a focus spot 1 meter from the mirror) for three different rms slope errors: 1 microradian (left), 0.45 microradians (middle), and 0.15 microradians (right).

Focusing Optics

Realizing the full potential of the most ambitious science opportunities enabled by the MBA lattice will require higher spatial resolution and higher throughput nanofocusing optics. Several focusing options already exist. Simplicity of alignment of zone plates and their on-axis configuration nature make them attractive for focusing X-rays below 25 keV. However, limitations of present nanolithography constrain the resolution of zone plates for hard X-rays to about 30 nanometers. Multilayer Laue lenses (MLLs) can achieve high spatial resolution with good efficiencies at high energies and are probably the best path for sub-10-nanometer spot sizes above 25 keV. Programs to establish novel fabrication processes for thicker zone plates with finer outer zones will be developed along with continued collaborative work with Brookhaven National Laboratory [1] on multilayer Laue lens fabrication and assembly.

K-B mirror pairs will continue to be used as focusing elements, in part because of their achromatic properties. Steady improvement in fabrication technologies along with new methods to precisely shape

the surface to correct figure errors make K-B mirror systems an attractive solution for focusing of X-ray beams.

The flexibility, ease of implementation and alignment, and long focal lengths of compound refractive lenses (CRLs) make them excellent candidates for secondary source imaging. However, the coherence preserving properties of existing CRLs may not be sufficient. This will need to be further studied, but other alternatives such as single crystal and vapor deposited beryllium to reduce scatter and preserve coherence should be explored as well.

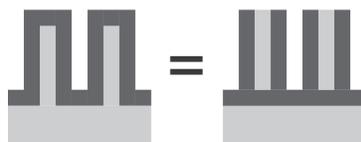


Figure 5.3.2. Improved spatial resolution for high energies provided by thick zone plates using zone doubling [2].

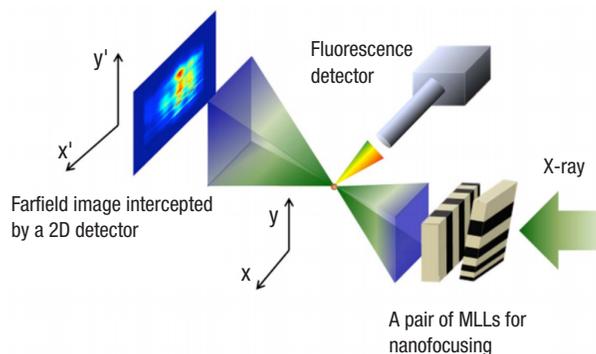


Figure 5.3.3. A schematic of a multilayer Laue lens focusing apparatus for X-ray fluorescence mapping [3].

DETECTORS

Improvements in detectors are required to capitalize on the full benefit of a MBA lattice at the APS. Detecting the X-rays that these improved sources can produce requires advances in sensors, materials, electronics, and interconnect technologies. Technologies already exist to produce a generation of detectors suited for high-brightness sources, such as an MBA lattice.

Area Detectors

Area detectors are a broad class of detectors generally used to record the intensity distribution of X-rays across a two-dimensional surface area. During the past five years, hybrid pixel detectors, such as the Pilatus [3], have grown in importance, replacing charged coupled devices (CCDs) in many applications. The Pilatus pairs basic pulse counting electronics with a pixelated sensor. Every pulse exceeding a discriminator threshold is “counted” as an X-ray incident on a particular pixel. For a variety of reasons, the Pilatus has become a workhorse detector at the APS – it is easy to use, has a fast frame rate (200 Hz for smaller detectors), and its lower level discriminator permits image acquisition with almost no background noise.

The one drawback of photon counting detectors is the inherent rate limitation. A counting detector requires approximately 1 microsecond to amplify, shape, and discriminate an individual photon, so a counting pixel is rate-limited to 1MHz. Attenuating the beam at times or in areas where count rates exceed this limit can mitigate this.

In order to maximize the benefit of the higher brightness of the MBA lattice, for some experiments, a promising approach is to use hybrid pixel detectors with integrating readout logic. Integrating detectors collectively process the charge from multiple X-rays simultaneously incident on a single pixel and so naturally handle higher signal levels without rate limitations. While a counting pixel will properly detect one X-ray every microsecond, an integrating pixel will properly detect 10^4 - 10^5 X-rays from a single APS X-ray bunch. Additionally, techniques exist to achieve MHz frame rates for short bursts with integrating detectors. Adoption of integrating detectors will accommodate the higher brightness of a fourth-generation source, and allow access to the full temporal resolution of the APS.

Plans in the next few years for commercial companies to market second-generation counting detectors with $150\ \mu\text{m}$ pixel size with improved frame rates (to several kHz) and without alleviating count-rate limitations will be appropriate for diffraction techniques. To optimize some coherent techniques that require finer pixels of 50 to $75\ \mu\text{m}$, implementation of integrating area detectors may require in-house detector development.

Spectroscopic Detectors

Currently, the most popular energy dispersive detectors at the APS are silicon drift detectors, usually Vortex detectors from Hitachi [4]. When used with an appropriate shaping amplifier and a multi-channel analyzer, these detectors produce a spectrum of elemental lines with typical resolution of 127 eV (FWHM) for the MnK α line. These detectors can capitalize on the MBA lattice design. However, full optimization of the increased brightness would come from spectroscopic detectors with single-eV energy resolution. At an upgraded APS, such a detector would enable the new scientific technique of chemical mapping at small distance scales. Single-eV energy resolution will permit sensitivity to small energy shifts in K β lines, allowing recovery of the spin and chemical states. Single-eV resolution will also facilitate mapping of heavy elements that often have overlapping lines.

Two new classes of spectroscopic detectors based on superconducting (SC) technologies offer the potential of single-eV energy resolution. Transition Edge Sensors (TES) are SC thin films operated near their critical temperature. A group at National Institute of Standards and Technology (NIST) Boulder has demonstrated single-eV resolution, and produced a detector that is used at the NIST beamline at National Synchrotron Light Source (NSLS). Microwave Kinetic Inductance Detectors (MKIDs) use SC resonators to detect X-ray photons. Absorption of an X-ray produces a change in inductance, which can be used to measure the energy of the incident photon. With the support of a DOE Early Career Award, Nino Miceli of the APS Detectors Group has been adapting MKIDs to synchrotron use. Both options also represent a path to high-energy spectroscopic detectors; both technologies are capable of coupling to absorbers with high atomic number.

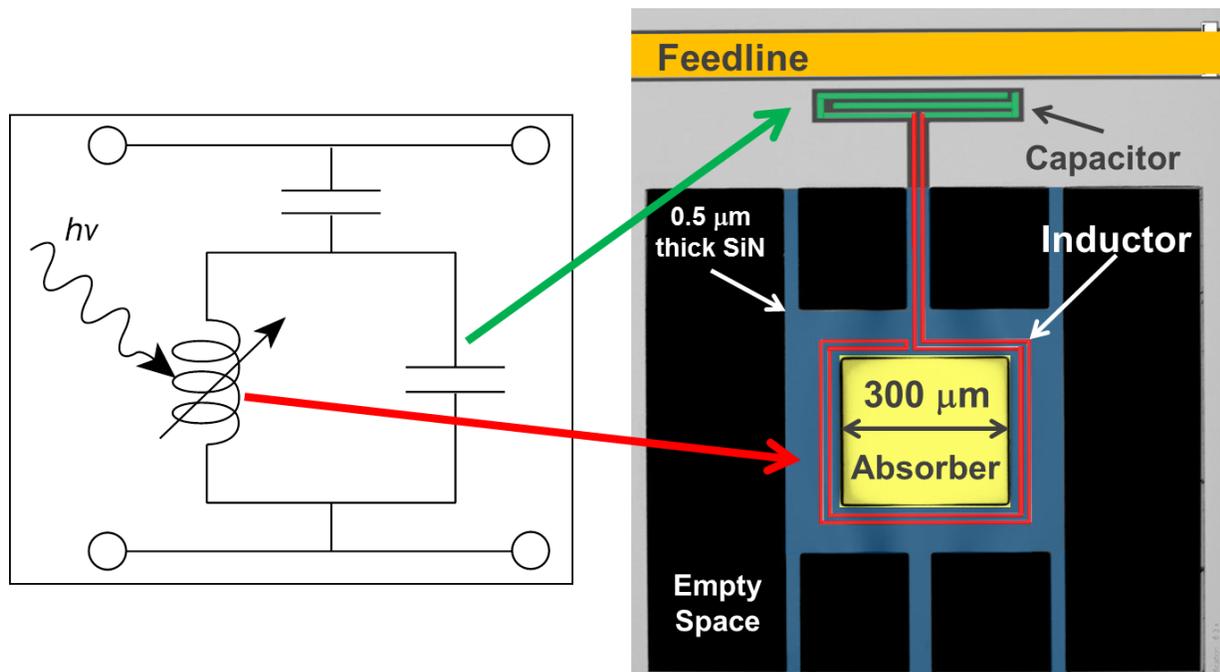


Figure 5.3.4. One pixel microwave kinetic induction detector schematic (above) is shown next to a microscope image of a device designed, fabricated, and tested at APS.

BEAM AND SAMPLE STABILITY

Electron Beam

To maintain the variation in source size and divergence to 10 percent of its nominal values, the APS MBA will require positional and angular stability in the horizontal direction, similar to what has been achieved in the vertical direction, approximately $\Delta\sigma < 1 \mu\text{m}$ and $\Delta\sigma' < 0.5 \mu\text{rad}$, respectively. To achieve this goal, improvements in the physical infrastructure of APS may be required to enhance the temperature stability of the storage ring through improved heating, ventilation and air conditioning and a chilled water system upgrade. Beam stability depends on the temperature stability of the storage ring tunnel and the vacuum chambers. These new requirements are well understood and will be further evaluated with the addition of an MBA lattice.

X-ray Beam and Optics

Vibrations induced by mirrors, monochromators etc. will have to be carefully controlled to maintain the positional and angular stability of the X-ray beam.

Insertion Devices

The MBA lattice, in combination with “swap out” mode for topping of the current, will allow for a smaller, 8.5-millimeter gap versus the 11-millimeter gap that exists today and a more circular cross-section of insertion device vacuum chambers than is permitted in the existing APS storage ring. These two changes in the ID vacuum chamber will have a profound effect on the type of IDs that can be routinely installed in the MBA storage ring lattice.

A smaller ID vacuum chamber will permit the deployment of optimized small-gap insertion devices, such as 13-to-20-millimeter period superconducting planar and helical IDs. Also, superconducting devices will likely become commonplace at the APS with the installation of an MBA lattice.

For permanent magnet devices, smaller gaps may mean increased radiation damage that can be mitigated by tighter beam-loss control and the possibility of using SmCo magnet material, which has higher radiation resistance than NdFeB.

Round ID vacuum chambers may permit permanent magnet planar devices with the magnetic field in the horizontal direction. This geometry could result in a significant reduction in the size of the ID support system and a commensurate reduction in costs. But even more important is the fact that such a device will generate vertically polarized X-rays that will have a profound effect on the simplification of beamline optical components and experimental set-ups. Also, helical IDs will create exciting opportunities for X-ray experiments because they can provide higher brightness and flux than planar devices (first harmonic only) while at the same time suppressing on-axis higher harmonics and reducing on-axis power densities. Further study will demonstrate how these new directions can best optimize IDs for an MBA lattice upgrade of the APS.

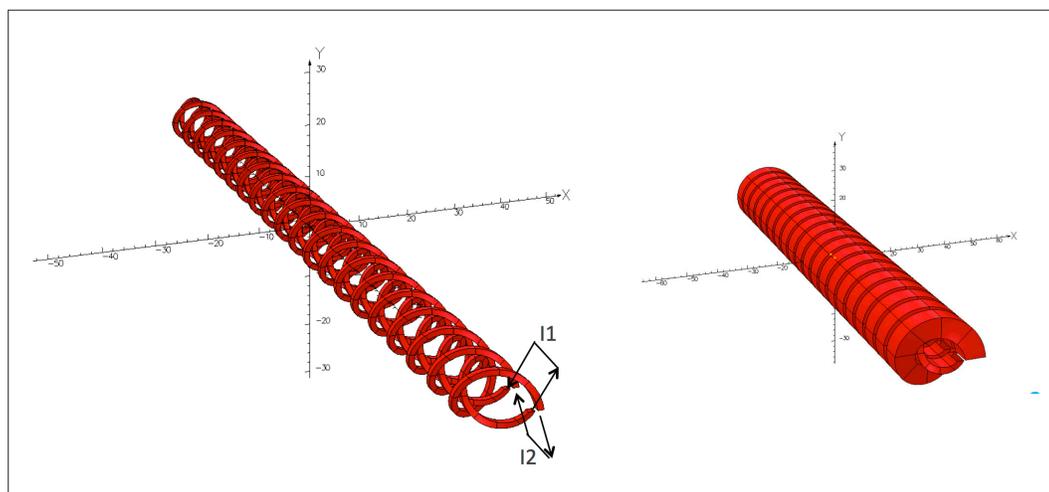


Figure 5.3.5. Initial R&D designs for a universal undulator helical for an APS upgrade with an MBA lattice.

Sample

The low emittance of the source will naturally lead to more stringent requirements on positioning and sample environments. Thermal drift and acoustic and mechanical vibrations will all need to be minimized. The development of innovative sample environments with a particular focus on their integration in the overall design of end-stations will be developed. Use of laser interferometers in feedback loops may be necessary for real-time correction of positioning errors from thermal or vibrational motions, but such systems are limited in correction speed.

Big Data

The MBA upgrade of the APS offers fantastic opportunities for a 10^2 - 10^3 increase in coherent flux for demanding experiments such as nanoprobe imaging. However, this opportunity will lead to challenges for both managing the data produced by the facility and for analyzing this data. The APS already produces in excess of 200 terabytes of data per month, and this amount will increase tremendously with the advent of the MBA source and continued advances in detectors.

In response to this challenge, Argonne has initiated an intra- and inter- lab project to explore new methods for managing these large data volumes, involving the APS, Argonne's Mathematics and Computer Science division, Lawrence Berkeley and Brookhaven National Laboratories, and Stanford National Accelerator Laboratory. The approach being tested involves automated transfer of data from beamline computers to a central data storage system with a tenfold reduction in cost per petabyte, and access to the data automatically configured per experiment with a web-based interface for the principal investigator to add or remove access as project teams evolve. Experimental metadata will be indexed and web searchable using Globus tools developed at Argonne. An initial implementation is now being tested on three APS beamlines to refine the approach for handling such data, and understand the investment required to have a robust, facility-wide system for data management.

Storing, cataloging, and transferring data does not by itself lead to scientific understanding. The exciting scientific opportunities that the MBA upgrade enables will be realized only if methods are also developed to integrate data from multiple detectors and experiments. With this data there must exist an ability to find patterns and automate the analysis so that a user can understand and adjust the experiment as it proceeds. Again, Argonne funding has initiated collaborative work between the APS and the Mathematics and Computer Science division to attack this problem on multiple fronts. This work includes the automatic identification of cells in nanoprobe studies, which leads to statistical measures of their elemental content; real-time analysis in photon correlation studies of phase transitions in materials; pattern recognition approaches, which lead to quantitative analysis of the nanoscale distribution of chemical bonding states in materials; and a Google Earth-like capability to view images of hierarchical materials across all length scales. The U.S. Department of Energy's Office of Basic Energy Science BES and the Office of Advanced Scientific Computing Research are funding additional developments in high-throughput ptychographic imaging. These research projects are pointing the way, and additional

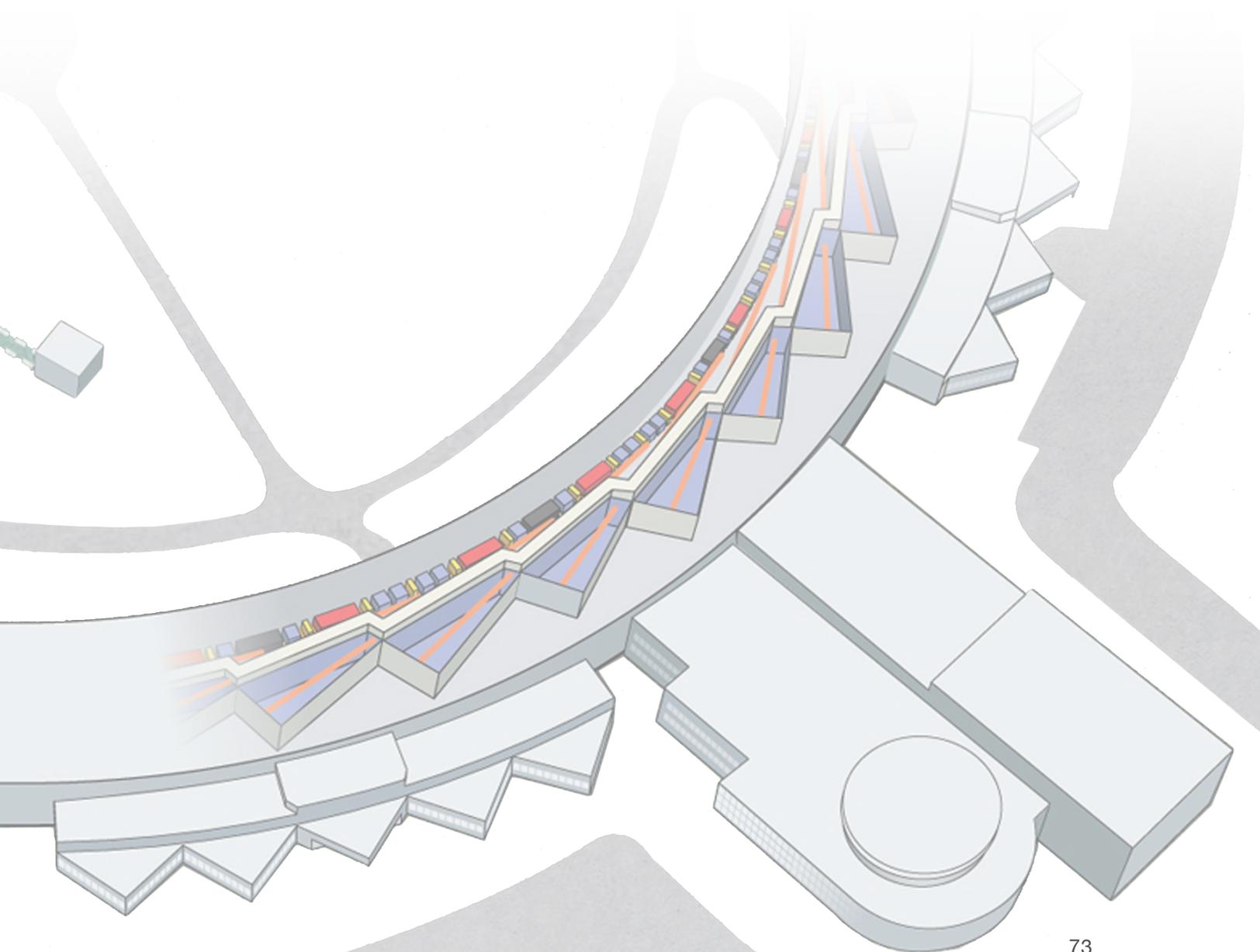
A MBA Lattice at the APS: A New Generation

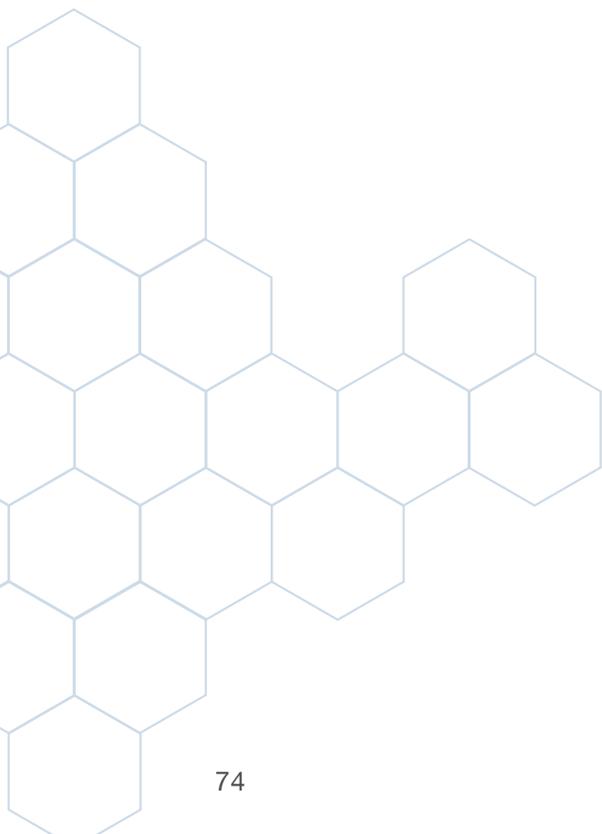
efforts will provide mature, operations-ready software to allow for full scientific utilization of the new capabilities the MBA Upgrade will deliver.

References

1. X. Huang, H. Yan, E. Nazaretski, R. Conley, and N. Bouet. *Nature Scientific Reports*, 3: 3562, 2013.
2. K. Jefimovs *et al.*, Zone-Doubling Technique to Produce Ultrahigh-Resolution X-Ray. *Phys. Rev. Lett.*, 99: 264801, 2007.
3. Pilatus detector: <http://www.dectris.com>
4. Vortex detectors: <http://hitachi-hitec-science.us/vortex.php>

APPENDICES





A.1 WORKSHOP OVERVIEW

The proposal to incorporate an multi-bend achromat (MBA) lattice into the Advanced Photon Source (APS) Upgrade is an exciting prospect that will have a profound impact on a wide variety of science taking place at the APS. It will revolutionize X-ray science by ushering in the nation's first fourth-generation storage ring light source.

To begin to capture the scientific opportunities enabled from the low-emittance lattice, the APS reached out to its community of national and international X-ray users. In a series of small-group meetings with the multitude disciplines that conduct research at the APS, the potential of an MBA lattice was laid out and the community was asked for feedback on how to best optimize this new technology, including identifying R&D needs. These meetings cumulated in the “Workshop on New Science Opportunities Provided by a Multi-bend Acromat Lattice at the APS” on Oct. 21 and 22, 2013. This event drew almost 400 attendees, of which about 40 percent were non-Argonne employees.

The stated goals of the workshop were as follows:

- ▶ *Inform the APS community* concerning the properties of an MBA low-emittance lattice being considered in the APS Upgrade.
- ▶ *Gather input on the new science opportunities* offered by such a source.
- ▶ Address how our current suite of beamlines map onto these envisioned science opportunities, and *what new capabilities are needed*.
- ▶ *Explore the technical advances in optics, detectors, and undulators* that are required to realize these science opportunities.
- ▶ *Identify areas that require R&D efforts* to achieve the ultimate performance from an MBA X-ray source.

To maximize time at the workshop and to ensure users questions were addressed, the community was polled prior to the workshop to help set the agenda, create a list of frequently asked questions (FAQs), and select the speakers and breakout group topics.

The workshop was divided into seven areas, each focused on different X-ray capabilities. An APS staff member and an external non-resident user chaired each session (see Appendix A2). To ensure that the workshop netted the widest selection possible of science opportunities, teams of about a dozen people were assigned to better represent the various scientific goals and technical needs for each area of X-ray capabilities.

In parallel, a series of educational lectures were held on the ramifications of the MBA lattice for optics, detectors, and undulators. All of these lectures were well attended – often with all of the available seats taken and attendees standing in the back of the room. Additionally, to facilitate the evaluation of

A MBA Lattice at the APS: A New Generation

current optics and potential optics for each beamline, tutorials were given on use of advanced computer simulation packages, SHADOW and XOP. To ensure that each participant could have direct, hands on training, several tutorials were held with participation limited to 10 people. More are planned in the near future to meet the continuing demand.

The breakout sessions were designed to encourage participation, and all of the sessions had lively discussion with many participants. On the second day, the chairs or a delegate of each breakout session presented summaries back to the workshop as a whole. Each of these half-hour presentations was packed with highlights of potential MBA related science, and considerable discussion was held on each topic.

A.2 BREAKOUT SESSION TEAM MEMBERS

Spectroscopy and Inelastic Scattering	
Clem Burns (Team co-leader)	Western Michigan University
Steven Heald (Team co-leader)	Argonne National Laboratory
Peter Abbamonte	University of Illinois, Urbana
Dario Arena	Brookhaven National Laboratory
Simon Bare	UOP LLC, a Honeywell Company
Thomas Gog	Argonne National Laboratory
Daniel Haskel	Argonne National Laboratory
John Hill	Brookhaven National Laboratory
Gerald Seidler	University of Washington
Thomas Toellner	Argonne National Laboratory

Coherent Diffraction and Phase Contrast Imaging, XPCS	
Ian Robinson (Team co-leader)	University College London
Jin Wang (Team co-leader)	Argonne National Laboratory
Francesco De Carlo	Argonne National Laboratory
Kamel Fezzaa	Argonne National Laboratory
Ross Harder	Argonne National Laboratory
Stephan Hruszkewycz	Argonne National Laboratory
Larry Lurio	Northern Illinois University
Ian McNulty	Argonne National Laboratory
Paul Nealey	University of Chicago and Argonne National Laboratory
Alec Sandy	Argonne National Laboratory
Oleg Shpyrko	University of California, San Diego
Sunil Sinha	University of California, San Diego
David Vine	Argonne National Laboratory

Interface and Single Crystal Diffraction	
Paul Fuoss (Team co-leader)	Argonne National Laboratory
Jonathan Tischler (Team co-leader)	Argonne National Laboratory
Tai Chang	University of Illinois, Urbana-Champaign
Paul Fenter	Argonne National Laboratory
John Freeland	Argonne National Laboratory
Hawoong Hong	Argonne National Laboratory

Interface and Single Crystal Diffraction	
Zahirul Islam	Argonne National Laboratory
Christian Schleputz	Argonne National Laboratory
Fred Walker	Yale University

Scattering, Diffraction and Small-Angle Scattering	
Jan Ilavsky (Team co-leader)	Argonne National Laboratory
Lyle Levine (Team co-leader)	National Institute of Standards and Technology
John Budai	Oak Ridge National Laboratory
Mark Rivers	Center for Advanced Radiation Sources, University of Chicago
Guoyin Shen	High Pressure Collaborative Access Team, Carnegie Institute of Washington
Stanislav Sinogeikin	High Pressure Collaborative Access Team, Carnegie Institute of Washington
Jonathan Almer	Argonne National Laboratory
Karena Chapman	Argonne National Laboratory
Matthew Suchomel	Argonne National Laboratory
Robert Suter	Carnegie Mellon University
Randall Winans	Argonne National Laboratory

Scanning Probe Imaging	
Tonio Buonassisi (Team co-leader)	Massachusetts Institute of Technology
Rafael Jaramillo (Team co-leader)	Massachusetts Institute of Technology
Stefan Vogt (Team co-leader)	Argonne National Laboratory
Conal Murray	IBM
Martin Holt	Argonne National Laboratory
Joerg Maser	Argonne National Laboratory
Steve Sutton	University of Chicago
Barry Lai	Argonne National Laboratory
Gayle Woloschak	Northwestern University
Wenjun Liu	Argonne National Laboratory

Timing and Dynamics	
Paul Evans (Team co-leader)	University of Wisconsin, Madison
David Keavney (Team co-leader)	Argonne National Laboratory
Ercan Alp	Argonne National Laboratory
Philip Anfinrud	National Institutes of Health
Bill Bailey	Columbia University
Lin Chen	Argonne National Laboratory and Northwestern University
Eric Dufresne	Argonne National Laboratory
Tim Graber	Washington State University
David Reis	Stanford University
Steve Southworth	Argonne National Laboratory

Macromolecular Crystallography	
William Weis (Team co-leader)	Stanford University
Robert Fischetti (Team co-leader)	Argonne National Laboratory
Keith Brister	Northwestern University
Malcolm Capel	Cornell University
Stephen Harrison	Harvard University
Andrzej Joachimiak	Argonne National Laboratory
Keith Moffat	University of Chicago
K. Rajashankar	Cornell University
Janet Smith	University of Michigan
Bi-Cheng Wang	University of Georgia
Steve Wasserman	Lilly Research Labs

A.3 BREAKOUT SESSION AGENDAS

Workshop on New Science Opportunities Provided by a Multi-bend Achromat Lattice at the APS				
Start	Finish	Time	Description	Speaker
October 21 & 22, 2013				
Day 1 (October 21, 2013)				
			Plenary Session Location – 402 Auditorium	
9:00	9:10	0:10	Welcome	Eric Isaacs
9:10	9:55	0:45	The MBA Lattice – Building the Next Generation Storage Ring	Brian Stephenson
9:55	10:10	0:15	Break	
10:10	10:20	0:10	Workshop Organization and Breakout Session Logistics	Dean Haeffner
10:20	11:00	0:40	Source Properties of a Potential MBA Lattice at the APS	Glenn Decker
11:00	11:30	0:30	Optics, Detector, and Instrumentation Developments for High Brightness X-ray Sources	Dennis Mills
11:30	13:00	1:30	Working Lunch: Q&A Discussions from the Plenary Session Location – Lower Gallery	
13:00	17:00	4:00	Breakout Sessions	See Breakout Sessions for Room Location
Breakout Sessions				
Scanning Probe Imaging – Location – 401/A5000				
13:00	13:45	0:45	Technical Opportunities Enabled by the MBA APS Upgrade	Stefan Vogt
13:45	14:30	0:45	Opportunities for Energy Sciences	Rafael Jarmillo/Tonio Buonassisi
14:30	15:15	0:45	Visualizing the Opportunities of Next-Generation Nanoelectronics Using Scanning Probe Imaging	Conal Murray
15:15	15:30	0:15	Break	
15:30	16:15	0:45	Scientific Opportunities in Earth, Planetary and Environmental Sciences	Steve Sutton
16:15	17:00	0:45	Unique Opportunities for the Life Sciences	Gayle Woloschak
17:00	18:00	1:00	Discussion and “Open Mic” Presentations – Opportunity for all to present an idea with one slide.	All

Workshop on New Science Opportunities Provided by a Multi-bend Achromat Lattice at the APS				
Start	Finish	Time	Description	Speaker
Coherent Diffraction and Phase Contrast Imaging, XPCS – Location – 401/E1100				
13:00	13:30	0:30	Future Perspectives of Coherent Diffraction with a Brighter Storage Ring	Ian Robinson
13:30	14:00	0:30	Using Coherent X-rays to Study Disordered Materials	Mark Sutton
14:00	14:30	0:30	High Resolution <i>In-vivo</i> Phase Contrast Micro Tomography for Developmental Biology	Ralf Hoffman
14:30	15:00	0:30	Prospects for XPCS on Biophysical System	Larry Lurio
15:00	15:15	0:15	Break	
15:15	17:00	1:45	Short Presentations	
			CNM Science	Ian McNulty & Martin Holt
			Fluid Dynamics and Fast Dynamics in Solids	Kamel Fezzaa
			Nano Particles and Dynamics	Ross Harder
			Nano-Rheology in Complex Fluids	Suresh Narayanan
			Dynamics in High-Q Range	Alex Sandy
			Laser Initialized Mesoscopic Dynamics in Multiferroics	Haiden Wen
			High Pressure	Wenge Yang
			Science Opportunities for MBA Lattices with Ptychography & Coherent Imaging	David Vine
Timing and Dynamics – Location – 402 Auditorium				
13:00	13:15	0:15	Welcome and Overview – Timing on MBA Machine	David Keavney
13:15	13:45	0:30	Update on Picosecond Science with X-rays	Linda Young
13:45	14:15	0:30	Bunch Structure and Nuclear Resonant Scattering: Challenges and Opportunities	Ercan Alp
14:15	14:30	0:15	Mesoscale Dynamics in Complex Systems	Haidan Wen

Workshop on New Science Opportunities Provided by a Multi-bend Achromat Lattice at the APS				
Start	Finish	Time	Description	Speaker
14:30	14:50	0:20	Magnetization Dynamics and X-Ray Spectroscopy: Opportunities and Challenges at Low Emittance Storage Rings	Dario Arena
14:50	15:10	0:20	Discussion	
15:10	15:30	0:20	Break	
15:30	16:00	0:30	Combining Coherence and Dynamics to Probe Novel Electronic Materials	Paul Evans
16:00	16:30	0:30	Picosecond Photobiology: What Can We Do Today and What Would We Like To Do Tomorrow?	Phil Anfinrud
16:30	17:00	0:30	Time Resolved Coherent Diffraction Imaging	Ian Robinson
17:00	17:30	0:30	Discussion	
Interface and Single Crystal Diffraction – Location – 438/C010				
13:00	13:30	0:30	Introduction	Jon Tischler
13:30	14:00	0:30	XRIM	Paul Fenter
14:00	14:45	0:45	Coherent Diffraction from Surfaces	Hoydoo You
14:45	15:30	0:45	Crystal Growth	Jeff Eastman
15:30	16:00	0:30	Scientific Opportunities Using High Brightness Sources	Joel Brock
16:00	16:30	0:30	Coherence for Critical Behavior & Thin Film Growth	Tai C. Chang
16:30	17:00	0:30	Diffuse Scattering	Ray Osbourne/ Sephan Rosenkranz
Structural and High Energy Scattering, SAXS – Location – 431/C010				
13:00	13:15	0:15	Introduction	Jan Ilavsky
13:15	13:40	0:25	Nanoscale X-ray Diffraction for Ultralight Elements in Ultrahigh Pressures	David Mao
13:40	14:05	0:25	Scientific Opportunities for High Energy X-ray Diffraction with an MBA Lattice	Robert Suter
14:05	14:30	0:25	In-Situ Study of Dumbbell Nucleation	Elena Shevchenko
14:30	14:55	0:25	New Opportunities for Solar Fuels and Electrochemical Energy Conversion Analysis Using In-Situ Hard X-ray Scattering	Dave Tiede

Workshop on New Science Opportunities Provided by a Multi-bend Achromat Lattice at the APS				
Start	Finish	Time	Description	Speaker
14:55	15:10	0:15	Break	
15:10	15:35	0:25	In-Situ Diffraction and Imaging Studies of Transient and Irreversible Phenomena in Materials	Todd Hufnagel
15:35	16:00	0:25	Prediction and Accelerated Laboratory Discovery of Heterogeneous Catalysts	Kenneth Poeppelmeier
16:00	17:00	1:00	Discussion and Report Writing	
Spectroscopy and Inelastic Scattering – Location – 401/Lower Gallery				
13:00	13:15	0:15	Opening Remarks	Steve Heald
13:15	13:45	0:30	Catalyst and Energy Science	Simon Bare
13:45	14:30	0:45	Inelastic Scattering	Clem Burns - NIXS
13:45	14:30	0:45	MBA and RIXS	Young-June Kim
14:30	15:00	0:30	Nuclear Resonant Scattering	Ercan Alp
15:00	15:15	0:15	Break	
15:15	16:00	0:45	Science at Extreme Conditions	David Mao and Daniel Haskel
16:00	17:00	1:00	Other Topics and General Discussion	Steve Heald
Macromolecular Crystallography – Location – 401/A1100				
13:00	13:30	0:30	Overview of Committee Recommendations, and Beamline Performance	Bob Fischetti
13:30	14:00	0:30	Mitigating Radiation Damage	Gerd Rosenbaum
14:00	14:30	0:30	Sampling, Handling, and Alignment Techniques	Malcolm Capel
14:30	15:00	0:30	Ultra-High Multiplicity to Detect a Weak Phasing Signal	Janet Smith
15:00	15:30	0:30	How to Think About Diffraction Data From Tiny Crystals	Steve Harrison
15:30	16:00	0:30	Town Hall Discussion	All
16:00			Adjourn	
Day 2 (October 22, 2012)				
9:00	11:00	2:00	Breakout Discussion and Report Preparation Location – See Monday Breakout Session	
11:00	11:00	0:00	Workshop Reports and Plenary Discussion Location – 402 Auditorium	

A MBA Lattice at the APS: A New Generation

Workshop on New Science Opportunities Provided by a Multi-bend Achromat Lattice at the APS				
Start	Finish	Time	Description	Speaker
11:00	11:30	0:30	Timing and Dynamics	David Keavney/Paul Evans
11:30	12:00	0:30	Coherent Diffraction and Phase Contrast Imaging, XPCS	Jin Wang/Ian Robinson
12:00	13:30	1:30	Working Lunch: Q&A Discussions from Breakouts Sessions Location – Lower Gallery	
13:30	13:30	0:00	Workshop Reports and Plenary Discussion (cont.) Location – 402 Auditorium	
13:30	14:00	0:30	Scanning Probe Imaging	Stefan Vogt/Tonio Buonassisi and Rafael Jaramillo
14:00	14:30	0:30	Interface and Single Crystal Diffraction	Jon Tischler/Paul Fuoss
14:30	15:00	0:30	Structural and High Energy Scattering, SAXS	Jan Ilavsky/Lyle Levine
15:00	15:30	0:30	Spectroscopy and Inelastic Scattering	Steve Heald/Clem Burns
15:30	16:00	0:30	Macromolecular Crystallography	Robert Fischetti/Bill Weis
16:00	16:30	0:30	Workshop Closeout	Workshop Committee

A.4 WHITE PAPER ON MBA LATTICE AT THE APS

Preliminary Expected Performance Characteristics of an APS Multi-Bend Achromat Lattice

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ANL/APS/LS-337

CVS revision 1.28: Tue Oct 1 00:11:54 CDT 2013.

1 Introduction

The Advanced Photon Source is the brightest storage ring synchrotron radiation source in the western hemisphere. It is presently in the midst of an upgrade to deliver even higher performance and powerful new capabilities for scientific research using hard x-ray techniques. Recently, it has become accepted that a new avenue for creating high brightness x-ray beams is opening up, based on technology that enables the use of multi-bend achromat (MBA) magnet lattices in the storage ring.

In July, a report by the Basic Energy Sciences Advisory Committee (BESAC) [1] recommended considering the incorporation of this new technology to enhance research facilities such as the APS. Hence, the APS Upgrade is exploring how the incorporation of an MBA lattice into the on-going project can optimize the scientific capabilities.

To facilitate discussion of the scientific impact and design optimization of such a lattice, this document describes the expected performance characteristics calculated for an initial “straw-man” design. Since the design is still being developed, these characteristics may change in the future as they are optimized with community input.

A primary benefit of the MBA lattice is to dramatically increase x-ray brightness, which is achieved by implementing four improvements, listed here in order of importance:

- Reducing the electron beam emittance from the present value of 3.1 nm (or nm-rad) to under 100 pm.
- Tuning the beta functions at the insertion devices closer to the optimum values of L_u/π , where L_u is the undulator length.
- Deploying optimized small-gap insertion devices.
- Increasing the beam current to 200 mA.

Additional design goals include enhancing the x-ray flux and the per-pulse brightness and flux, which are further characteristics that benefit the scientific capabilities.

1.1 Electron Beam Properties

The zero-current natural emittance in an electron storage ring is governed by [2, 3]

$$\epsilon_0 \sim C_\epsilon \frac{E^2}{N_s^3 N_d^3}, \quad (1)$$

where C_ϵ is a constant, E is the beam energy, N_s is the number of sectors (40 in the case of APS), and N_d is the number of dipole (or bending) magnets per sector. The present APS lattice runs at $E = 7$ GeV and has $N_d = 2$. The MBA lattice design described here has $N_d = 7$, which implies an approximately 40-fold reduction the natural emittance. In this initial design, we have chosen a beam energy of 6 GeV, which appears necessary to make the magnet strengths tractable. However, the choice of beam energy is a complex matter and has yet to be fully explored.

Typically, we expect that $\epsilon_0 = \epsilon_x + \epsilon_y$, where ϵ_x and ϵ_y are the emittances in the horizontal and vertical planes, respectively. This is often parametrized by the emittance ratio κ

$$\begin{aligned} \epsilon_y &= \frac{\kappa}{1+\kappa} \epsilon_0 \\ \epsilon_x &= \frac{1}{1+\kappa} \epsilon_0 \end{aligned} \quad (2)$$

These equations are strictly correct only in the limit of zero current. For non-zero current, particularly when the natural emittance or κ are very small, the emittance and energy spread of the bunch may increase as a result of intra-beam scattering. This effect is more severe when the current in a bunch is higher and when the bunch is short. Increasing κ and stretching the bunch are effective methods of reducing the impact of intra-beam scattering.

1.2 X-ray Brightness

With some simplifying assumptions, the x-ray brightness B of an undulator source in an electron storage ring is governed by

$$B = \frac{F_s}{4\pi^2 \Sigma_x \Sigma_{x'} \Sigma_y \Sigma_{y'}}, \quad (3)$$

where F_s is the spectral flux (typically stated in units of photons/second/0.1%BW), $\Sigma_{x,y}$ are the total rms photon beam sizes for the horizontal and vertical planes, and $\Sigma_{x',y'}$ are the total rms divergences. The total rms beam sizes are obtained by convolving the electron beam distribution with the radiation distribution emitted by a single electron traversing an undulator. Assuming uncorrelated gaussian beams, these convolutions give

$$\Sigma_q = \sqrt{\epsilon_q \beta_q + \epsilon_r \beta_r}, \quad (4)$$

for the sizes, while the divergences are

$$\Sigma_{q'} = \sqrt{\frac{\epsilon_q}{\beta_q} + \frac{\epsilon_r}{\beta_r}}, \quad (5)$$

where q is x or y , ϵ_q is the electron beam emittance, and β_q is the electron beam beta function. The quantities ϵ_r and β_r are the emittance and beta function of the monochromatized undulator radiation emitted by a single electron. For photons of wavelength λ from an undulator of length L_u , these are roughly given by

$$\epsilon_r = \frac{\lambda}{2\pi} \quad (6)$$

and

$$\beta_r = \frac{L_u}{\pi}, \quad (7)$$

giving

$$\sigma_{r'} = \sqrt{\frac{\epsilon_r}{\beta_r}} = \sqrt{\frac{\lambda}{2L_u}} \quad (8)$$

and

$$\sigma_r = \sqrt{\epsilon_r \beta_r} = \frac{1}{2\pi} \sqrt{2\lambda L_u}. \quad (9)$$

(Note that these values assume detuning of the undulator to maximize flux [4] and are in any case only approximate.)

To maximize brightness, we must minimize the denominator of Equation (3). This entails minimizing the products $\Sigma_x \Sigma_{x'}$ and $\Sigma_y \Sigma_{y'}$. While ϵ_q should ideally be small compared to ϵ_r , this is not always possible, particularly for short wavelengths. In practical units,

$$\epsilon_r [\text{pm}] \approx \frac{200}{E_p [\text{keV}]} \approx 16 \lambda_p [\text{\AA}] \quad (10)$$

For example, for 10 keV, we have $\epsilon_r = 20$ pm. The virtue of the MBA lattice is that we can approach this value much more closely than is possible with the present lattice. Note that when ϵ_r and ϵ_q are comparable, it is important to have $\beta_q \approx \beta_r$.

2 Global Accelerator Properties

Some global properties of the accelerator design described here are listed in Table 1. The circumference and number of sectors are, of course, unchanged from the present machine, although in fact the circumference would change slightly to accommodate the change in geometry that results from having bending in different locations. Although there are many more dipoles in a sector, we anticipate only a single bending magnet beamline in each sector, as in the present machine. The average pressure is expected to be quite low in spite of the narrow vacuum pipe, owing to the use of NEG-coated chambers. This should ensure similar bremsstrahlung radiation levels as seen at present.

Quantity	Symbol	Range	Units
Circumference	C	1104	m
Number of sectors	N_s	40	
Number of dipoles per sector	N_d	5-8	
Arc beam pipe outside diameter	D_p	26	mm
Average pressure	P_{ave}	< 2	nT

Table 1: Global accelerator properties

3 Basic Electron Beam Properties

The basic properties of the electron beam in this design are listed in Table 2. The major changes from the present-day APS are the dramatic drop in horizontal and vertical emittance, as well as a decrease in the beam energy from 7 to 6 GeV. The expected fractional rms energy spread would be very similar to the present value.

The natural emittance is expected to be in the range of 60 to 80 pm, which would be closely realized only for fill patterns with small single-bunch charge. Due to intra-beam scattering (IBS), the emittance would grow somewhat for fill patterns with few bunches. It is thought that the maximum single-bunch charge would be similar to that of the present APS 24-bunch mode (~ 15 nC or 4.2 mA per bunch). Typically in cases with higher single bunch charge we would increase κ to reduce the impact on beam lifetime.

Quantity	Symbol	Range	Units
Beam energy	E	6	GeV
Natural emittance	ϵ_0	60 - 80	pm
Rms energy spread	σ_δ	0.09 - 0.12	%
Emittance ratio	$\kappa = \epsilon_y/\epsilon_x$	0.1 - 1.0	
Emittance increase due to IBS	-	< 25	%
Horizontal emittance	ϵ_x	30 - 91	pm
Vertical emittance	ϵ_y	40 - 5	pm

Table 2: Basic electron beam properties

4 Fill Pattern

Table 3 shows the timing parameters for simple fill patterns consisting of uniformly spaced single bunches, using a maximum current per bunch of 4.2 mA (15 nC bunch charge). For uniformly spaced single bunches, the 48 bunches needed for 200 mA would have a spacing of 77 ns. Many other fill patterns are possible, such as uniformly spaced multiplets, with larger times between multiplets (and 2.8 ns between bunches within a multiplet), or hybrid fills with part of the ring filled with widely spaced singlets and the remainder of the bunches grouped more closely. Note that improved opening speeds for choppers to separate bunches for timing applications should be possible because of the smaller beam sizes.

As noted above, because of intra-beam scattering these few-bunch patterns will have increased coupling compared to many-bunch fills. Table 7 shows more detailed parameters.

Quantity	Symbol	Range	Units
Total current	I	200	mA
Number of bunches	N_b	48-324	
Bunch rate	f_b	13-88	MHz
Rms bunch duration	σ_t	70-18	ps

Table 3: Parameters of simple uniform fill patterns

5 Insertion Device Sources

Ranges of insertion device source points of this design have the properties listed in Table 4. These values are stated for the centers of the straight sections. Devices offset from this position would see somewhat different parameters. Although ranges of values are given, this should not be interpreted as indicating that individual straight sections would have different values from others. The intention is to deliver the same values at all straight sections, in order to maintain the symmetry of the lattice. Detailed properties for the latest revision are given in Section 7.

Quantity	Symbol	MBA Range	Present-day	Units
Horizontal beta function	β_x	1-4	19.5	m
Horizontal dispersion function	η_x	< 3	170	mm
Horizontal beam size	σ_x	5 - 19	275	μm
Horizontal beam divergence	$\sigma_{x'}$	3 - 10	11	μrad
Horizontal size-divergence product	$\sigma_x\sigma_{x'}$	30 - 91	3100	pm
Vertical beta function	β_y	1-4	2.9	m
Vertical dispersion function	η_y	0	0	mm
Vertical beam size	σ_y	2 - 13	10	μm
Vertical beam divergence	$\sigma_{y'}$	1 - 6	3.5	μrad
Vertical size-divergence product	$\sigma_y\sigma_{y'}$	5 - 40	35	pm

Table 4: Insertion device source point characteristics

Insertion device straight sections would accommodate insertion devices with properties listed in Table 5. Note that the maximum *magnetic* length for superconducting undulators (SCUs) would be

significantly shorter than the value listed; a magnetic length of 3.7 m is a reasonable assumption for SCUs.

Quantity	Symbol	Range	Units
Maximum length	L_u	4.8	m
Vertical chamber inside gap	g_v	≥ 6	mm
Horizontal chamber inside gap	g_h	≥ 6	mm
Vertical magnet gap	m_v	≥ 8.5	mm
Horizontal magnet gap	m_h	≥ 8.5	mm

Table 5: Insertion device properties

Figures 1 through 4 show calculations of the x-ray brightness and flux (both average and per pulse) anticipated from this MBA lattice design, compared with those for the present-day APS. All insertion devices were assumed to be the maximum possible length of 4.8 m for permanent-magnet devices and 3.7 m for SCUs. The devices were chosen to represent the potential improvements, rather than exhaustively catalog the possibilities. Other choices of undulator period should provide similar improvements of two or more orders of magnitude in brightness at hard x-ray energies above a few keV. For the present APS, we used 100 mA beam current with 4.8-m-long 33-mm-period and 27-mm-period devices with 10.75-mm magnetic gaps. For the MBA lattice, we used 4.8-m-long 25 and 28-mm period permanent magnet devices and 3.7-m-long 15.5- and 20.5-mm period devices, all with 8.5-mm magnetic gaps. In all cases, we assumed 200 mA stored current in the MBA lattice with $\epsilon_0 = 80$ pm. For the average brightness computation, we assumed $\kappa = 0.1$, while for the pulse brightness and flux we assumed $\kappa = 1$, since this will be needed to minimize IBS effects. All calculations assume the use of the existing APS high-heat-load front-end design [5].

Unlike the present-day APS ring, we expect that an MBA lattice would be operated in on-axis injection mode (“swap-out” instead of “top-up”) [6, 7]. Because of this, we should not be restricted to traditional insertion devices with small vertical gaps and relatively large horizontal gaps. Instead, we should be able to use devices with small horizontal gaps as well, opening the possibility of vertical and helical undulators. For example, superconducting helical devices producing circular polarization may be workable for the first time in a lightsource storage ring. (Note that impedance considerations will limit the number of devices with small gaps in both planes.)

Despite the higher current and dramatically higher brightness of this design, the total power and power density from optimized undulators would be less than or comparable to the power and power density from existing APS undulators. This may be understood by noting that the angular spread of the white beam from an undulator is K/γ , with no dependence on the beam emittance [8].

6 Bending Magnet Sources

Because of the decreased electron beam energy, a high-field insertion must be used to increase the critical energy of bending magnet radiation. Details are yet to be determined. Goals for bending magnet source properties are listed in Table 6.

Quantity	Symbol	Range	Units
Critical energy	E_c	15-20	keV
Radiation fan width	θ_B	>5	mrاد

Table 6: Goals for bending magnet source properties

7 Details for Latest Lattice Revision

Table 7 shows detailed ID source point properties as a function of the number of bunches N_b . Listed are the emittance ratio κ , the rms horizontal and vertical emittances $\epsilon_{x,y}$, the rms horizontal and vertical beamsizes $\sigma_{x,y}$, the rms horizontal and vertical divergences $\sigma'_{x,y}$, the rms bunch duration σ_t , the rms energy spread σ_δ , the 10th-percentile predicted Touschek lifetime $\tau_{10^{th}}$, and the approximate injection interval ΔT_{inj} . In most cases, several bunch durations are listed, including a minimum duration plus durations of approximately 35 and 70 ps. κ is adjusted to attempt to maintain the 10th-percentile predicted lifetime $\tau_{10^{th}}$ above 3 hours.

Table 7: Parameters for ID source points for H7BA-TwoSector-60pm-nux105-nuy34

κ	σ_t ps	ϵ_x pm	ϵ_y pm	β_x m	β_y m	σ_x μm	σ'_x μrad	σ_y μm	σ'_y μrad	σ_δ 10^{-4}	$\tau_{10^{th}}$ hour	ΔT_{inj} s
$N_b = 48$ $f_b = 13.0\text{MHz}$												
1.00	70	41.7	41.7	1.3	2.9	7.4	5.7	10.9	3.8	9.95	1.38	10.4
$N_b = 81$ $f_b = 22.0\text{MHz}$												
1.00	35	42.5	42.5	1.3	2.9	7.4	5.7	11.0	3.9	1.00×10^1	1.19	5.3
1.00	69	39.6	39.6	1.3	2.9	7.2	5.5	10.6	3.7	9.77	2.23	9.9
$N_b = 162$ $f_b = 44.0\text{MHz}$												
1.00	21	41.6	41.6	1.3	2.9	7.3	5.7	10.9	3.8	9.95	1.41	3.1
1.00	35	39.6	39.6	1.3	2.9	7.2	5.5	10.6	3.7	9.77	2.23	5.0
0.24	68	56.1	13.3	1.3	2.9	8.5	6.6	6.2	2.2	9.74	3.00	6.7
$N_b = 216$ $f_b = 58.7\text{MHz}$												
1.00	20	40.7	40.7	1.3	2.9	7.3	5.6	10.8	3.8	9.86	1.72	2.9
1.00	34	38.8	38.8	1.3	2.9	7.1	5.5	10.5	3.7	9.70	2.91	4.9
0.11	68	61.4	6.5	1.3	2.9	8.9	6.9	4.3	1.5	9.79	3.00	5.0
$N_b = 324$ $f_b = 88.0\text{MHz}$												
1.00	18	39.5	39.5	1.3	2.9	7.2	5.5	10.6	3.7	9.76	2.32	2.6
0.22	35	56.6	12.6	1.3	2.9	8.6	6.6	6.0	2.1	9.74	3.00	3.3
0.10	68	59.8	5.9	1.3	2.9	8.8	6.8	4.1	1.4	9.69	4.31	4.8

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- [1] Report of the BESAC Subcommittee on Future X-ray Light Sources, July 2013. [sci-ence.energy.gov/~media/bes/besac/pdf/Reports/Future_Light_Sources_report_BESAC_approved_72513.pdf](http://science.energy.gov/~media/bes/besac/pdf/Reports/Future_Light_Sources_report_BESAC_approved_72513.pdf).
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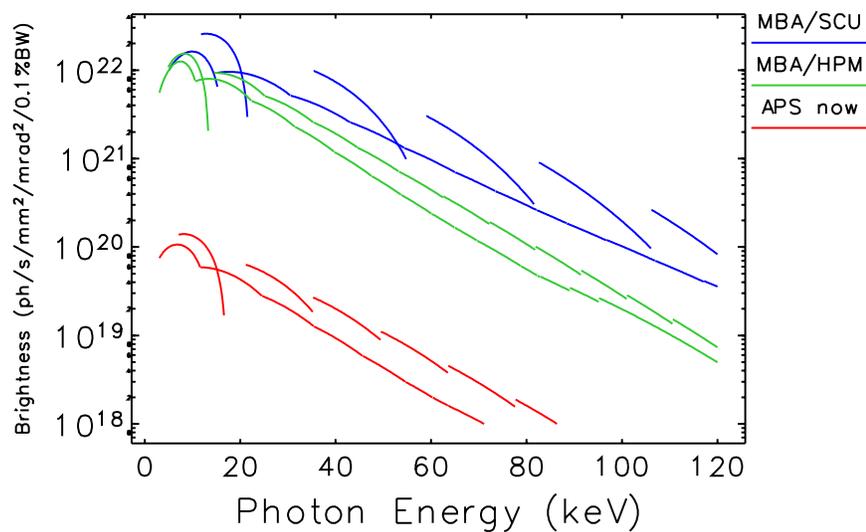


Figure 1: Comparison of brightness from the present APS to selected hybrid-permanent magnet and superconducting undulators in the MBA lattice design described here. See text for details.

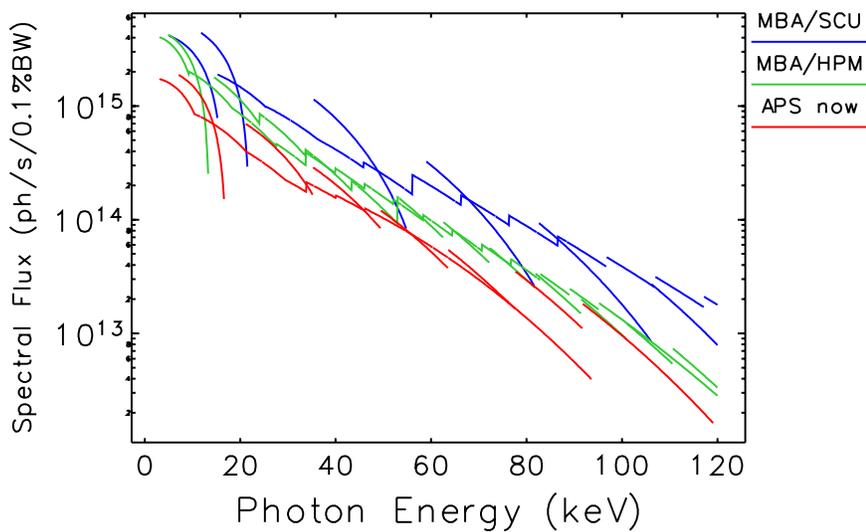


Figure 2: Comparison of flux from the present APS to selected hybrid-permanent magnet and superconducting undulators in the MBA lattice design described here. See text for details.

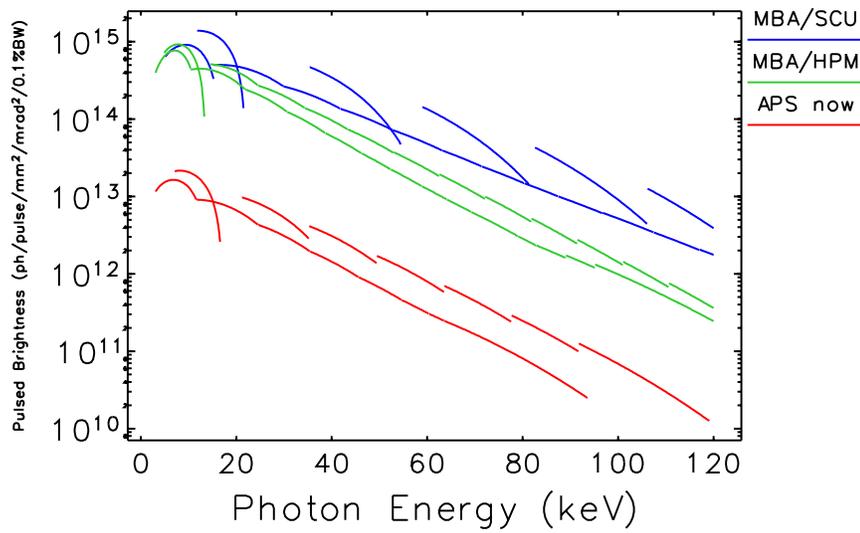


Figure 3: Comparison of pulsed brightness from the present APS to selected hybrid-permanent magnet and superconducting undulators in the MBA lattice design described here. See text for details.

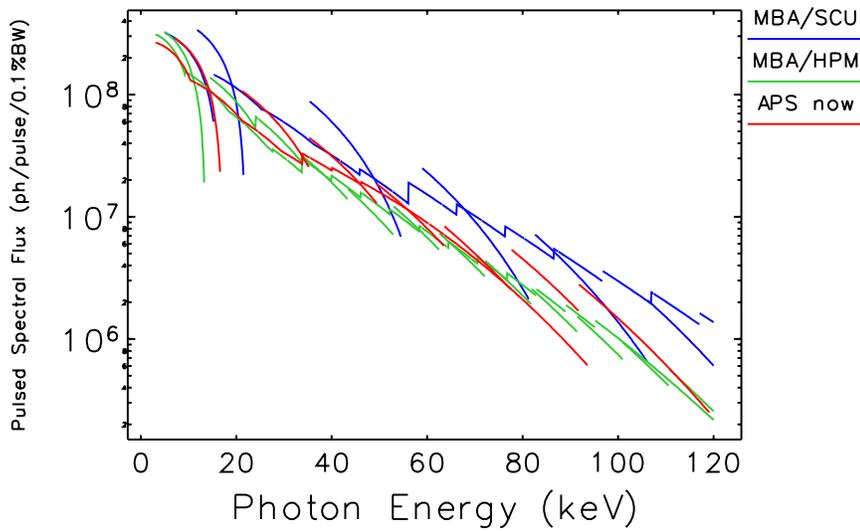


Figure 4: Comparison of pulsed flux from the present APS to selected hybrid-permanent magnet and superconducting undulators in the MBA lattice design described here. See text for details.

