Argonne NATIONAL LABORATORY

Update on APS Upgrade Plans

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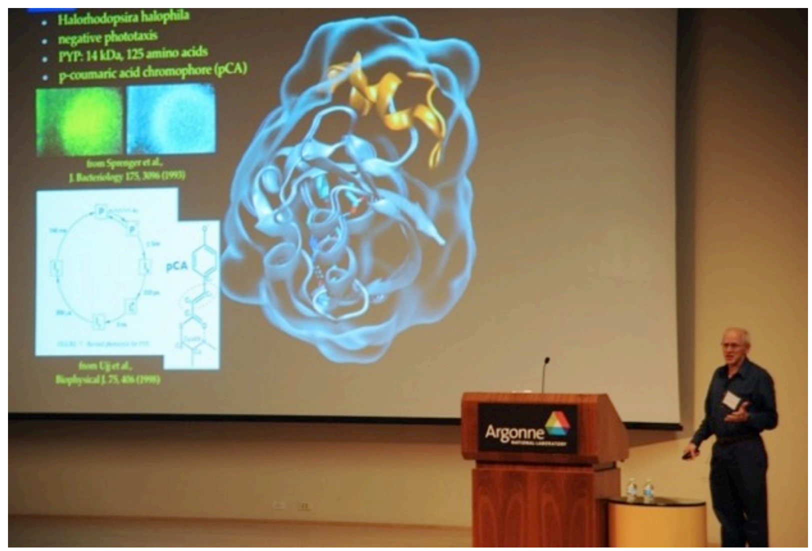
Workshop on Diffraction-Limited Storage Rings

December 9, 2013

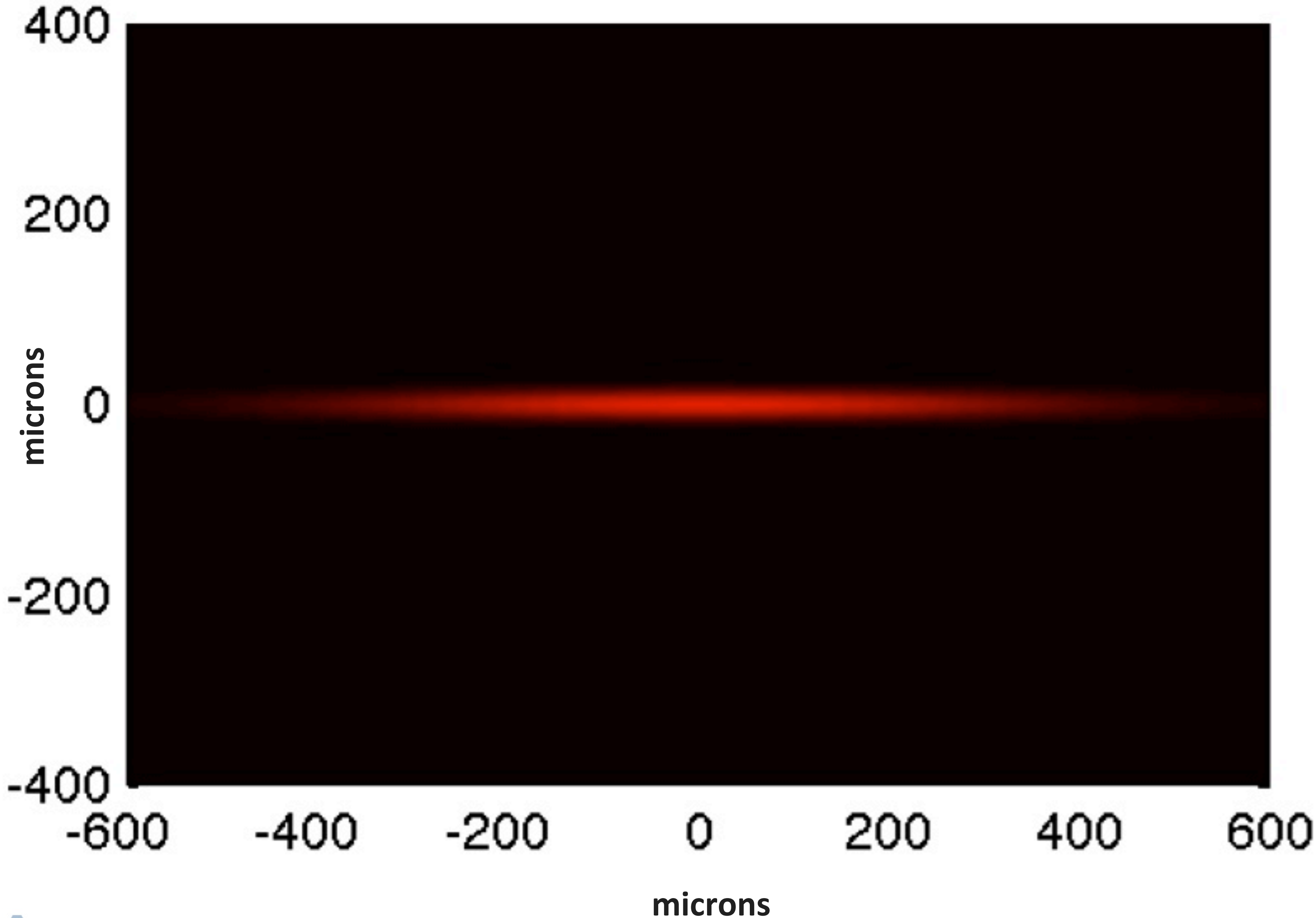
The Advanced Photon Source is an Office of Science User Facility operated for the U.S. Department of Energy Office of Science by Argonne National Laboratory

U.S. DEPARTMENT OF ENERGY | Office of Science

Enthusiastic user workshop on New Science Opportunities Provided by a Multi-Bend Achromat Lattice at the APS



October 21-22, 2013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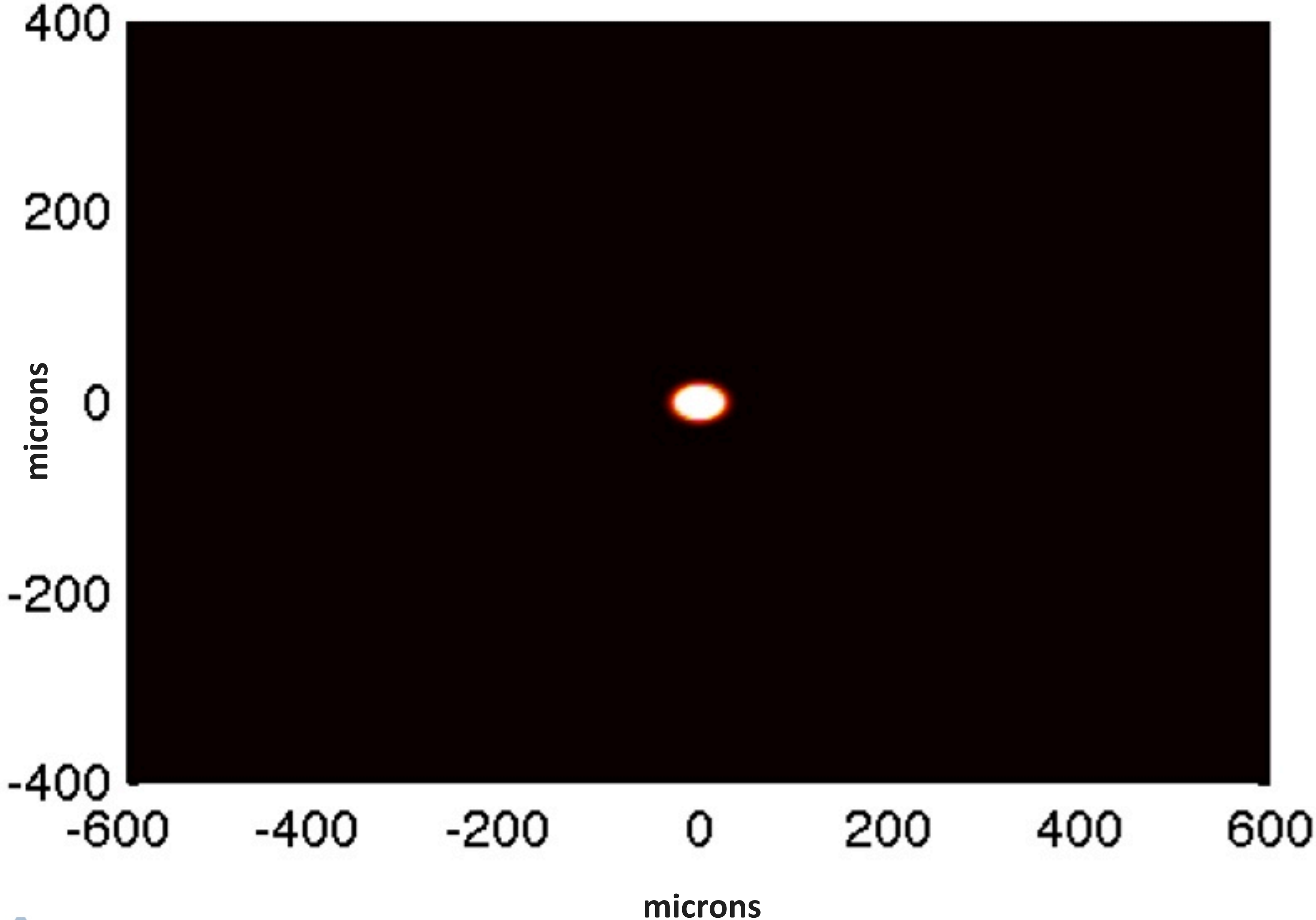
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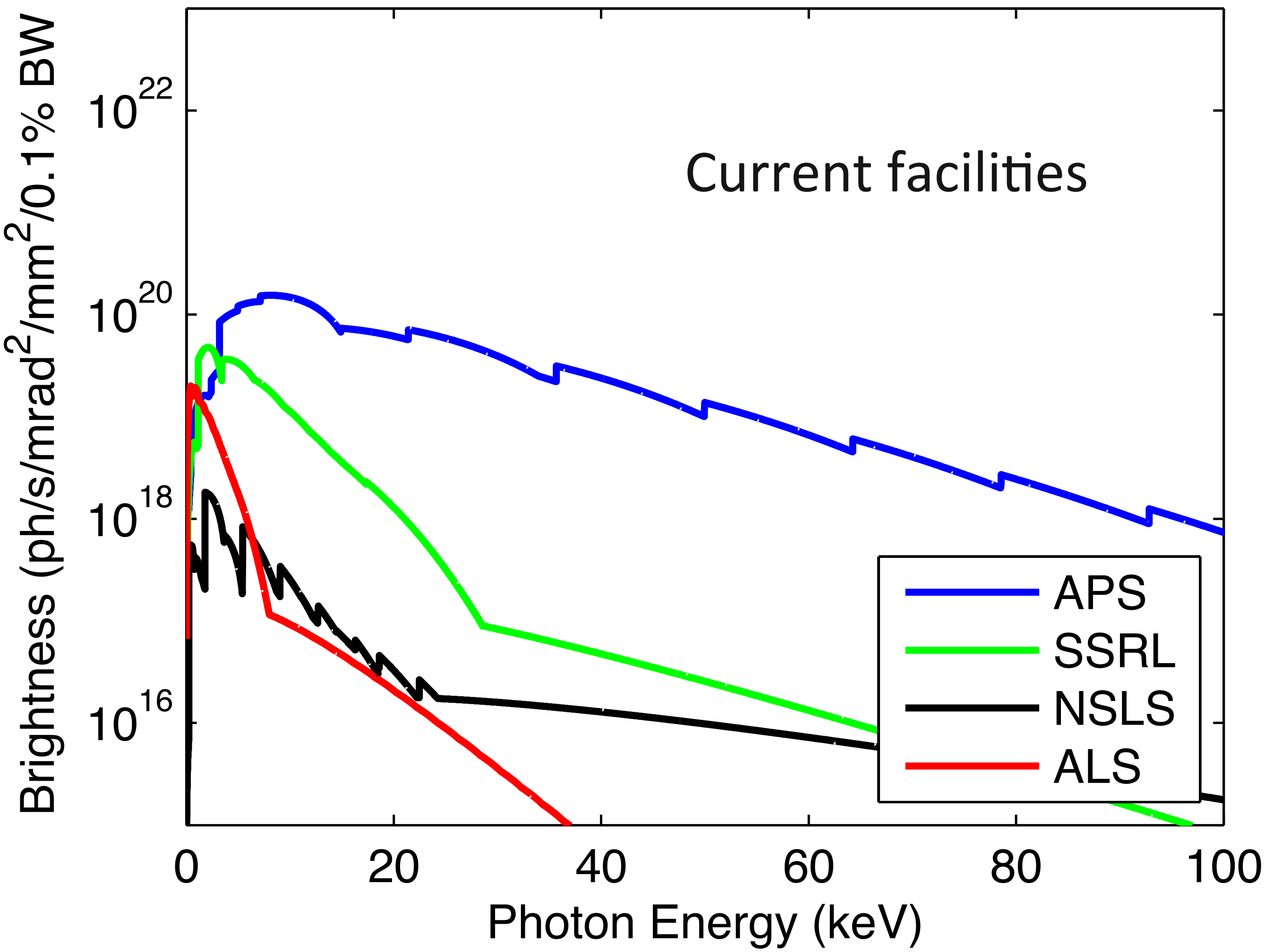
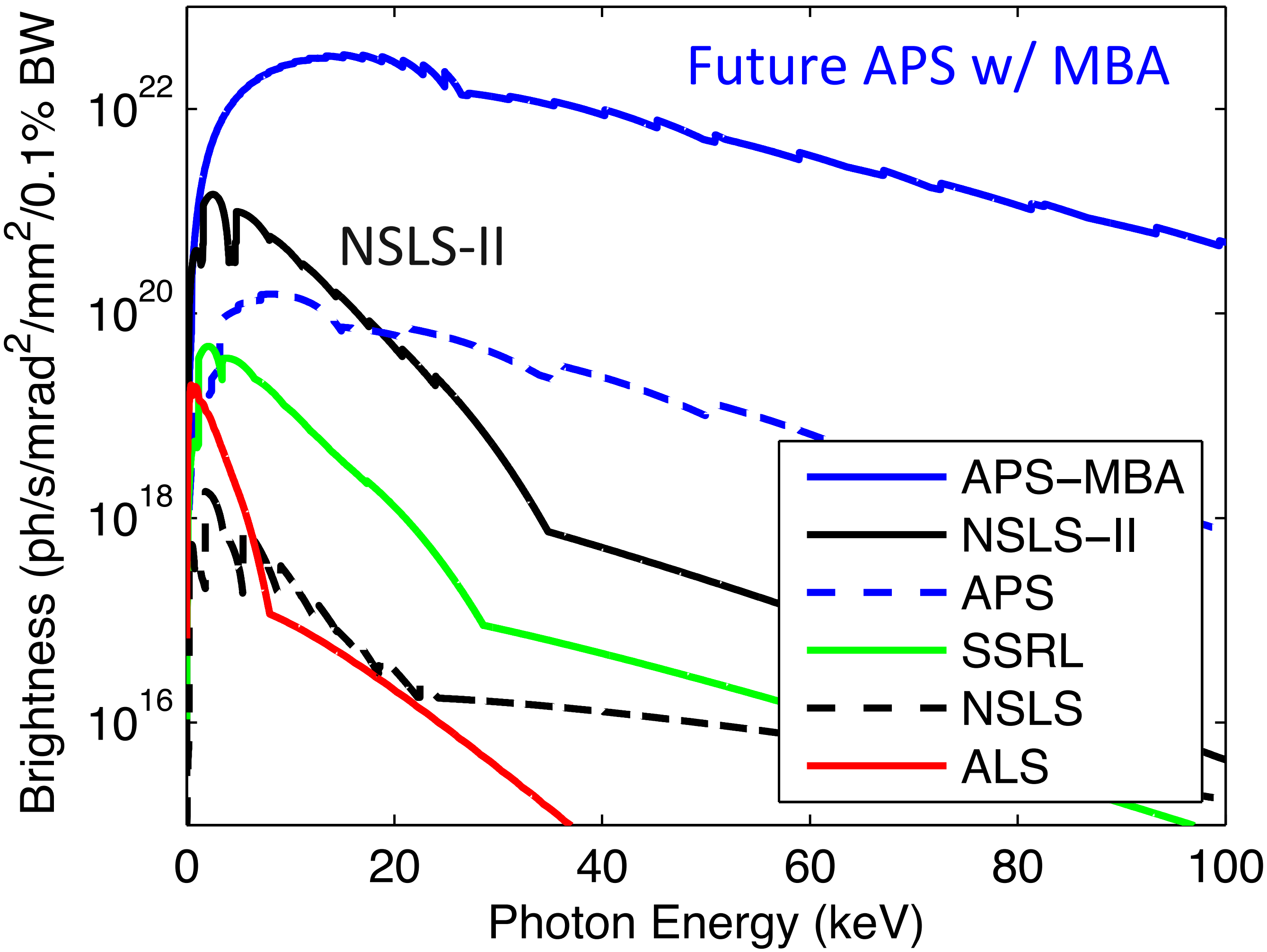
APS: High energy star in US x-ray facility constellation



Brightness vs. x-ray energy at top beamlines
among BES synchrotron facilities

APS: High energy star in US x-ray facility constellation



Brightness vs. x-ray energy at top beamlines among BES synchrotron facilities

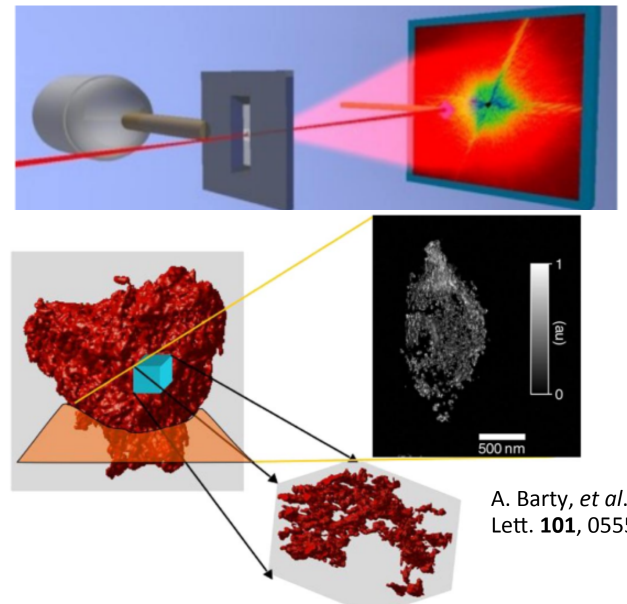
Coherence provides transformation in X-ray imaging

Coherent Diffraction Imaging

- Resolution limited by wavelength and sample stability – not optics.
- Recover real and imaginary parts of refractive index: magnetization, composition, bonding configuration.
- Challenge: reach atomic scale.

Wavelength-Resolution Ptychography

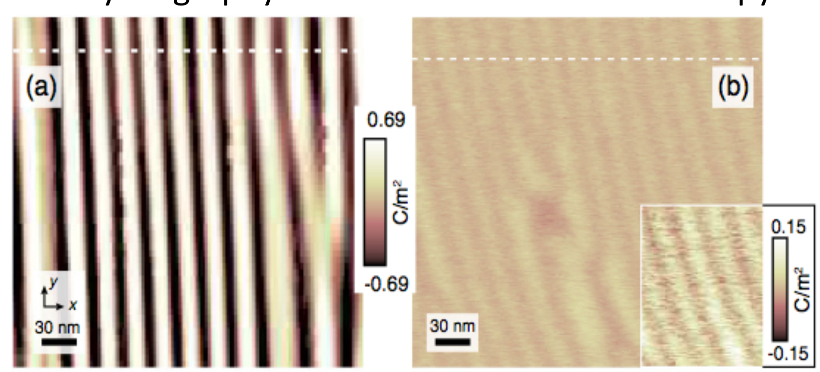
- CDI adapted to continuous samples with scanned-beam **ptychography**, resolution far better than focused X-ray spot size.
- Coherent imaging techniques to approach wavelength resolution from improved coherent flux



Nanofoam Diffraction Pattern/ Reconstruction

A. Barty, *et al.*, Phys. Rev. Lett. **101**, 055501 (2008)

Ptychography   Piezo-force microscopy



Polarization Domains in $PbTiO_3$
Hruszkewycz *et al.*, PRL (2013)

MBA will enable *in operando*, multimodal imaging approaching atomic resolution.

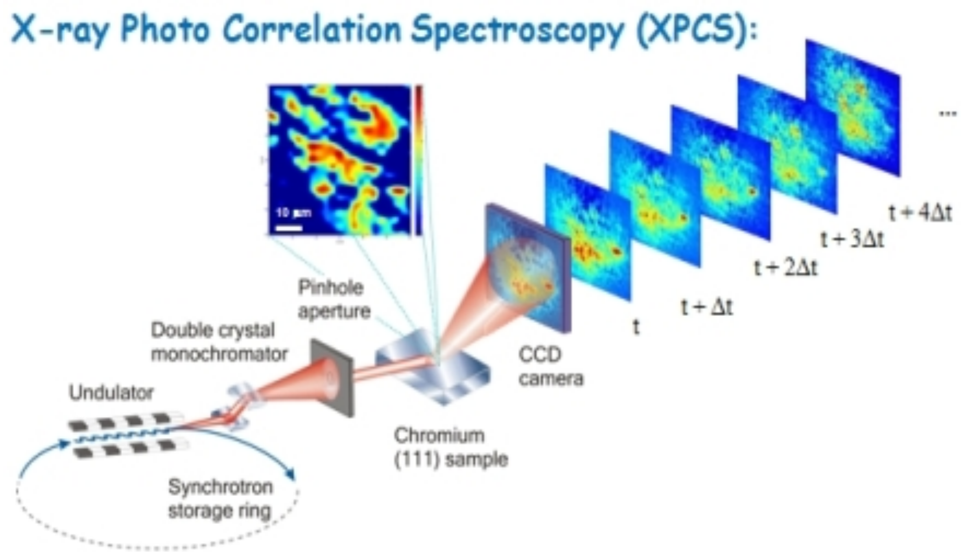
Fast fluctuations with XPCS

X-ray photon correlation spectroscopy

- Chemical, magnetic, and structural fluctuations

Accessible time scale proportional to (coherent flux)^2

- 100 to 1000-fold increased brightness improves time resolution by 10^4 to 10^6



MBA enables ns-resolution studies of nm-scale fluctuations in

- Reaction-diffusion
- Self-assembly
- Domain wall motion
- Complex order parameters

***Time to probe 1 ns fluctuations*:**

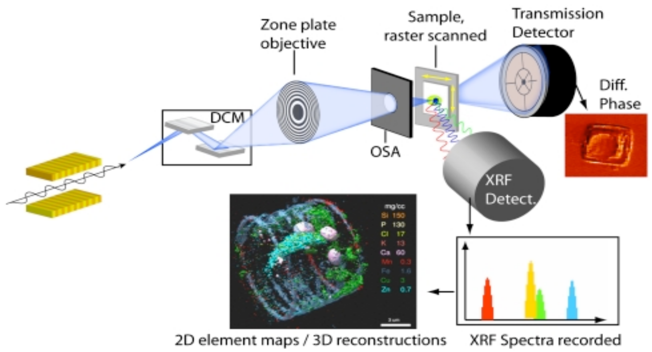
Today:	50,000 hours
MBA + modern BL:	5 hr to 3 min

MBA will revolutionize our ability to probe fluctuations at molecular length scale and nanosecond time scale

A new regime of scattering and spectroscopy with nanobeams: *nanoXRF*, *nanoXRD*, *nanoXAS*, *nanoRIXS*

X-ray fluorescence nano-tomography

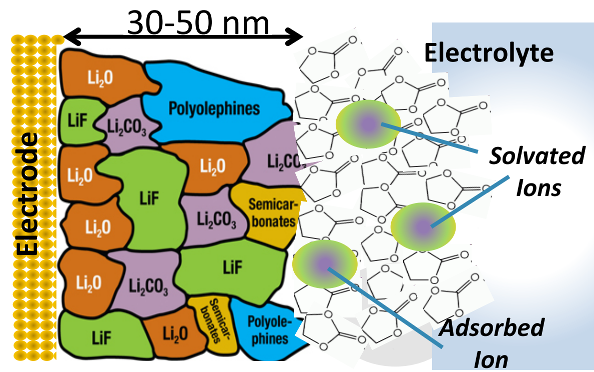
3D elemental mapping of functional mesostructures



de Jonge, et. al., PNAS 107, 15676 (2010).

nanoXRD

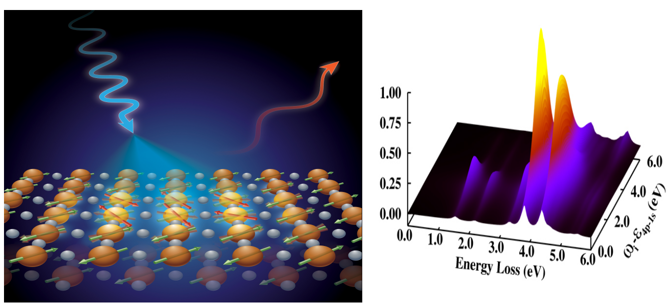
Formation, structure, and function of the solid-electrolyte interface in batteries



JCESR

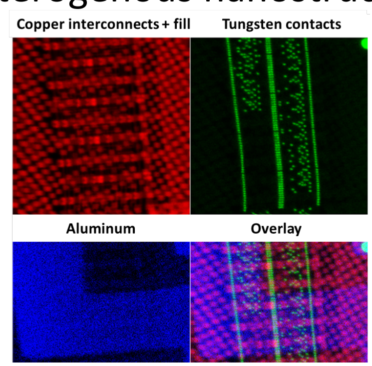
nanoRIXS

understanding coupled excitations in heterogeneous materials and nanostructures



nanoXRF

Understanding elemental composition in heterogenous nanostructures



CMOS semiconductor

MBA will vastly expand the capability and capacity of scanned x-ray probes: high flux at resolution approaching 1 nm.

Observing individual point defects inside functioning devices with single-atom sensitivity

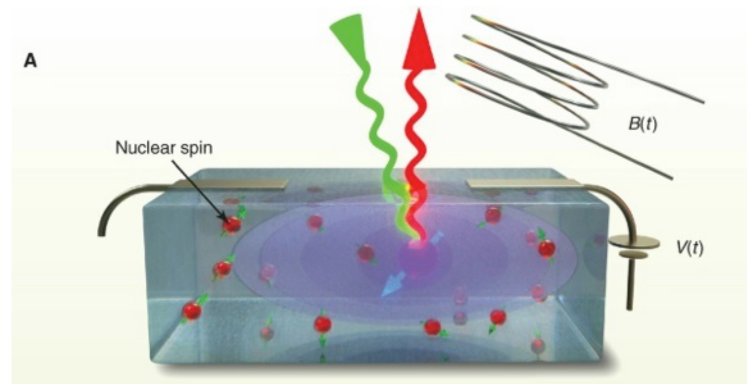
Opportunity

- Quantum spintronics: cryptography, sensing, and quantum computers
- Manipulate interacting arrays of "designer atoms"

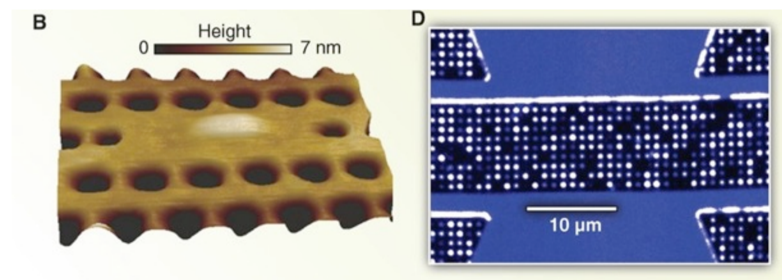
Gains From APS MBA Lattice

- Single-atom sensitivity for fluorescence
- Point defect strain fields at nm resolution; Bragg CDI measurements

Spin states of single point defects in wide-bandgap semiconductors



Why do properties of each defect differ?



D. D. Awschalom et al., *Science*, 2013

Now: structure and composition of point defects are uncharacterized
APS MBA upgrade: gives sensitivity to strain and composition of single atoms through **factor of 100 to 1,000 improvement** in brightness

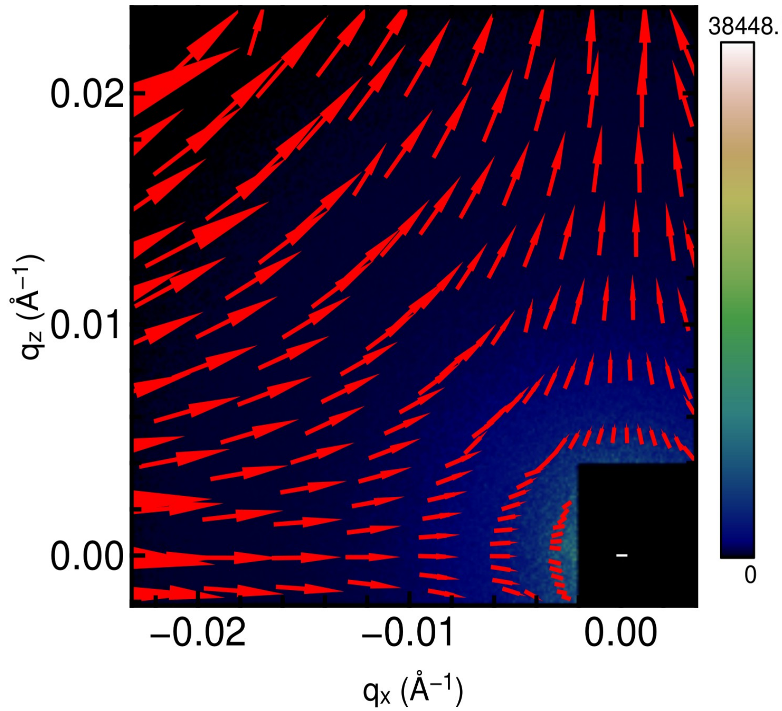
Materials deformation revealed with coherent x-rays

Opportunity

- Strain tensor mapping inside of deforming material, including fluids and glasses, by using space-time cross-correlation analysis of x-ray speckle (XPCS)
- 3-D variation of full strain and stress tensors inside materials evolving in real time under loading

Gains from APS MBA Lattice

- Open up studies into ns range
- Sub-micron spatial resolution



Speckle shifts superimposed on scattering from a 20 micron region of a rubber sample undergoing flow in a stress-strain cell. Shifts are scaled by 200. (M. Sutton, unpublished)

Now: New coherence-based techniques being developed with coarse resolution

APS MBA upgrade: First direct view of molecular flow will be enabled by **factor of 10,000 to 1,000,000 improvement**

Microcrystallography of biological macromolecules

Opportunity
- Nanocrystal studies enabled
- Microcrystals studies routine
- Membrane proteins studies routine

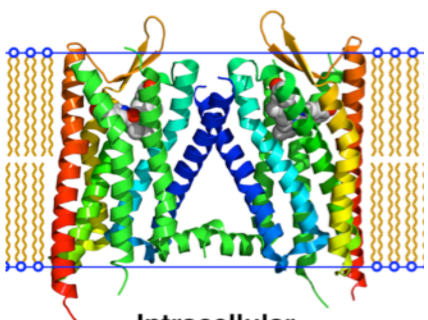
Gains from APS MBA Lattice
- Accelerate drug discovery; 10^2-10^3 increase in brightness opens study of nanocrystals
- Improve S/N and resolution for small (0.5 – 5 µm), inhomogeneous and/or weakly scattering crystals

2012 Nobel Prize in Chemistry

β_2 adrenergic receptor-Gs protein complex

Kobilka & Weis labs

k-opioid GPCR Ray Steven's lab



APS MBA upgrade: mosaicity **factor of 10 improvement;** intensity at sample **factor of 10,000 improvement**

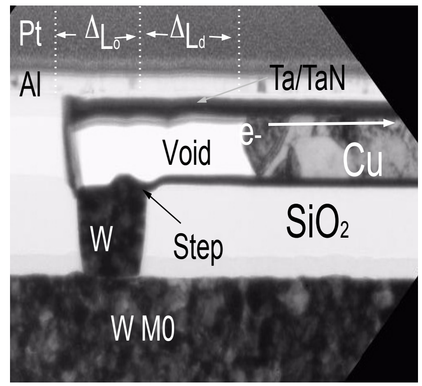
Defect interactions in semiconductor devices

Opportunity

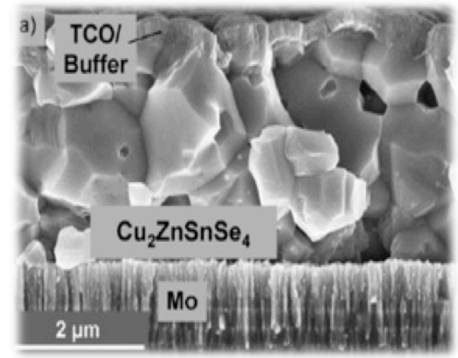
- Accelerate discovery; potential heroic 1.5-year experiments done in 3 days
- Expand semiconductor functionality; remove limiting defects
- Improve performance

Gains from APS MBA Lattice

- Characterize buried nanoscale structure at high sensitivity, *in situ/operando*, with a large field of view, in *real time*



C.K. Hu et al., IEEE 42nd IRPS, 222 (2004)



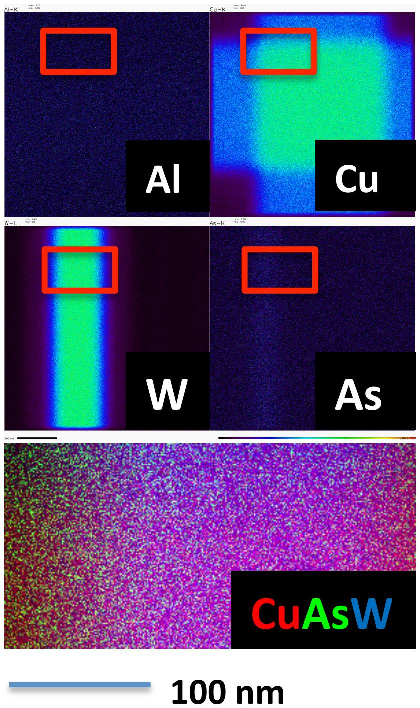
CZTS solar cell
Todorov *et al.*, Adv. Mater. **22**, E156 (2010).

Interfacial defects dictate performance, both in nanoelectronics and photovoltaics

Now: 35 nm spot size with $1x10^9$ ph/s
APS MBA upgrade: 5 nm with $5x10^{11}$ ph/s by improvements in brightness and optics

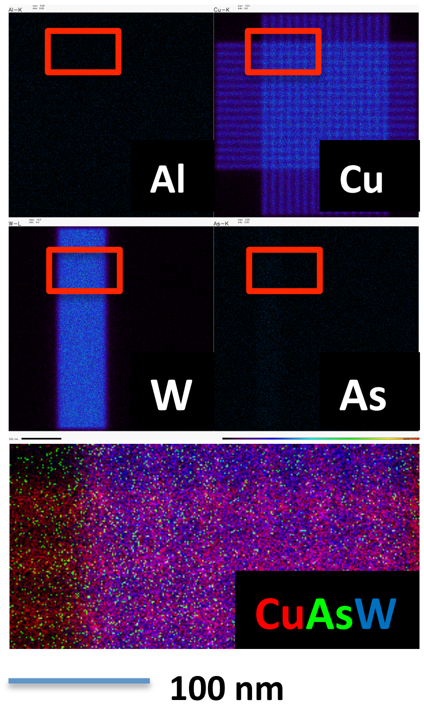
APS MBA upgrade, 5 nm spatial resolution: revolutionary

2-ID-D today, 120 nm spatial resolution: "work horse"



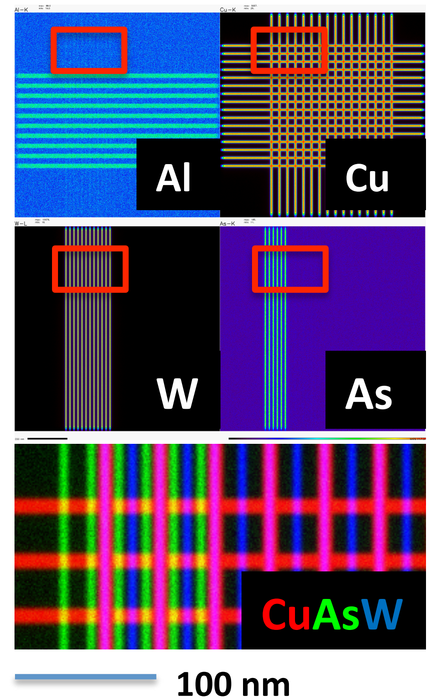
- Cannot resolve W, Cu structures, As doping
- Cannot detect Al

26-ID nanoprobe today, 35 nm spatial resolution: "cutting edge"



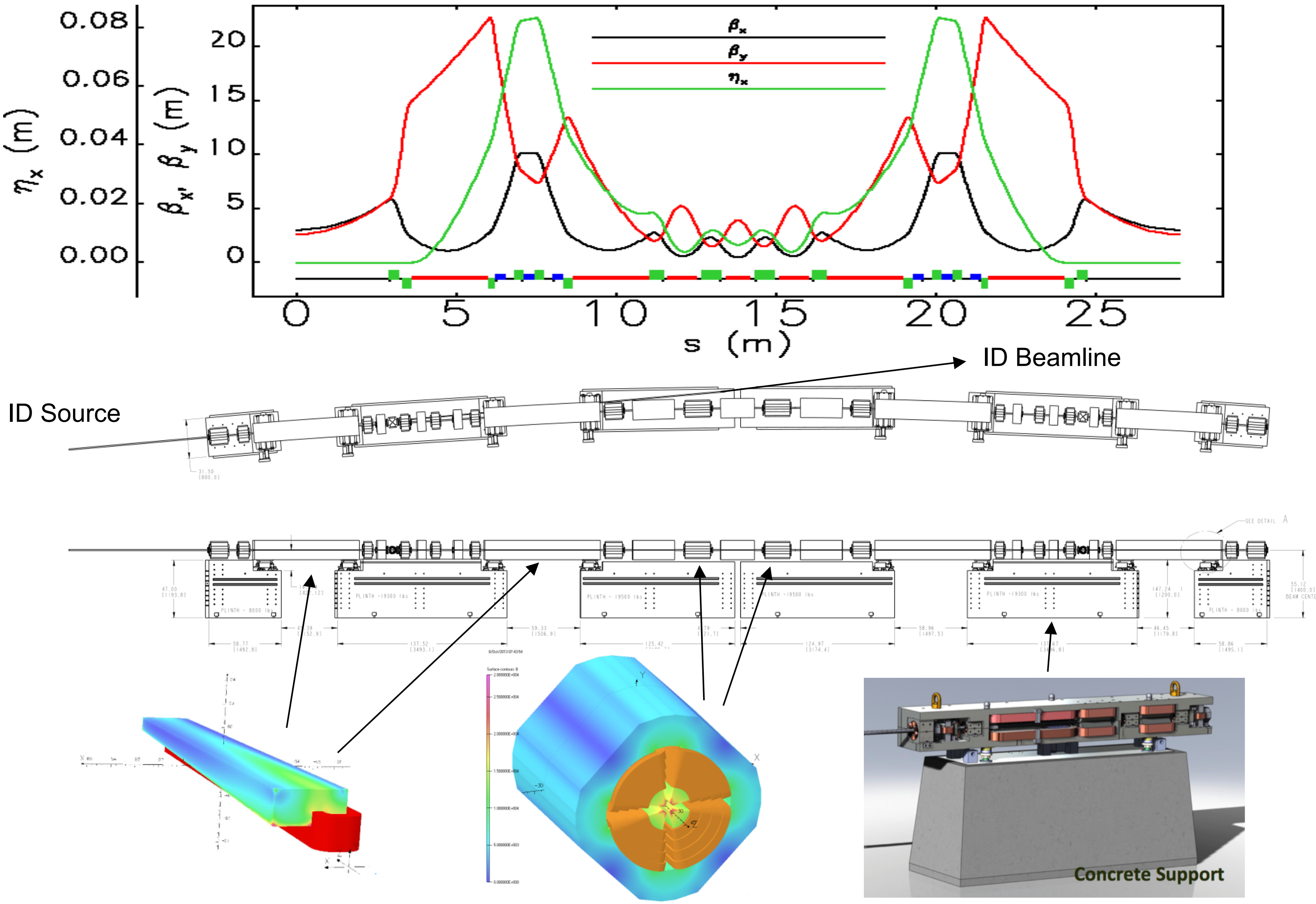
- Cannot resolve W structures, As doping
- Cannot detect Al
- Resolve Cu structures

Simulation of MBA upgrade, 5 nm spatial resolution: "revolution"



- Resolve Cu, W structures, and As doping
- Detect and resolve Al

MBA accelerator design development



Longitudinal-gradient dipoles Quadrupoles Multi-Magnet Concept (MAX-IV)

Preliminary APS MBA parameters

- Preliminary parameters for a possible APS MBA lattice

Quantity	Symbol	APS	MBA	MBA	Units
Beam energy	E	7	6	6	GeV
Effective emittance	ϵ_0	3100	60	60	pm
Beam Current	I	100	200	200	mA
Number of Bunches	N_b	24	48	324	
Emittance ratio	$\kappa = \epsilon_y/\epsilon_x$	0.016	1.0	0.1	
Horizontal emittance	ϵ_x	2500	30	60	pm
Vertical emittance	ϵ_y	40	30	6	pm

Note that intrabeam scattering has been ignored

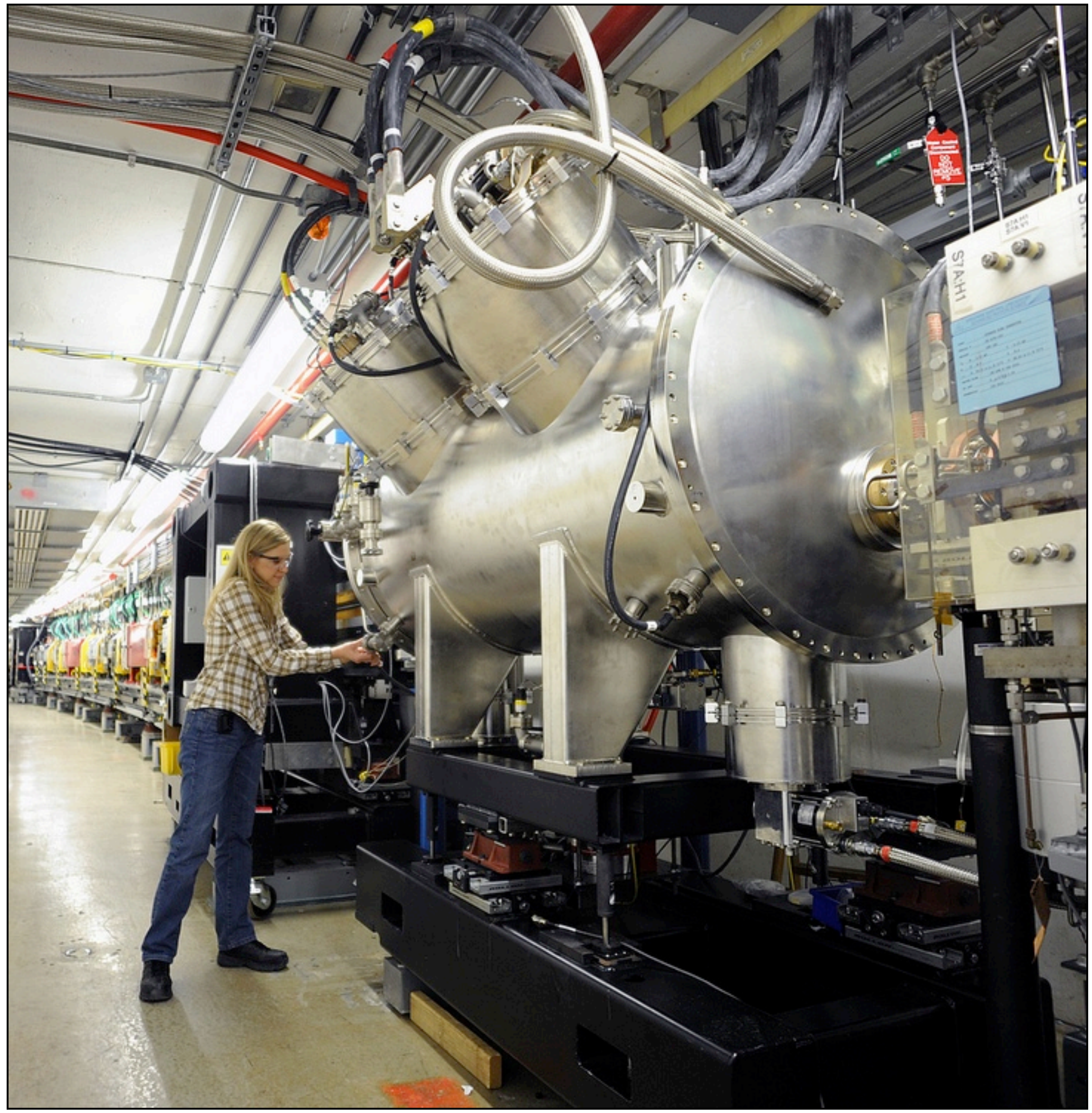
Preliminary APS MBA fill patterns

- Total beam current is expected to be 200 mA
- Fill patterns with 48 to 324 bunches will be possible
- Various timing patterns should be possible with up to 4.2 mA/bunch

Total current	I	200	200	mA
Number of bunches	N_b	48	324	
Bunch current	I_b	4.2	0.6	mA
Bunch rate	f_b	13	88	MHz
Rms bunch duration	σ_t	70	18	ps

Prototype superconducting undulator operational

- 30-cm prototype SCU has been providing beam to users at Sector 6 ever since it was installed
- Exceeds design specs, very reliable, and already outperforms our standard undulator A at 85 keV
- 1-m SCU under construction



Prototype superconducting undulator installed in APS, December 2012

An MBA lattice at APS: a new generation