Supporting Technologies Optics, Detectors and Data Challenges

Gopal Shenoy

Argonne National Laboratory

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Outline: Challenges in Bridging the New Sources to Future Science

How to Transport X-ray Wavefronts to the Sample without Distorting?

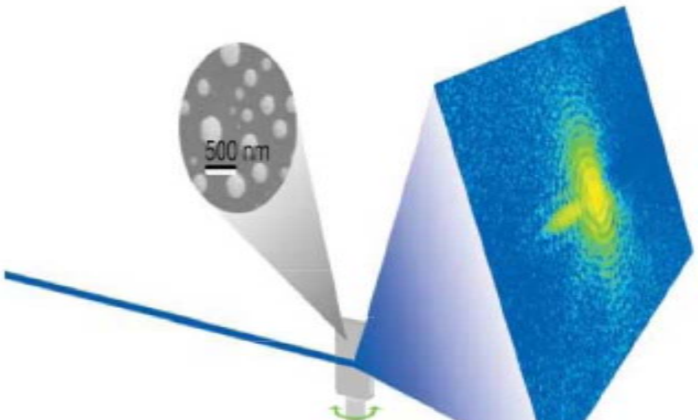
What are the Challenges in Performing Next Generation Experiments?

Which Detector Technologies will Support Future Experiments?

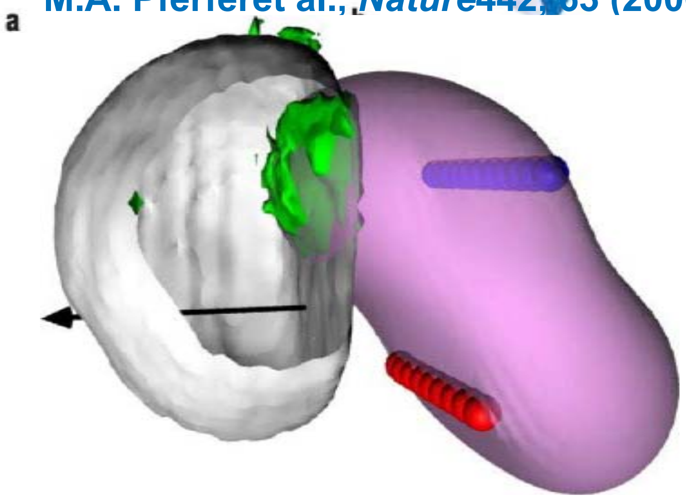
How to Manage and Understand the Data?

Science needing High Coherence Flux

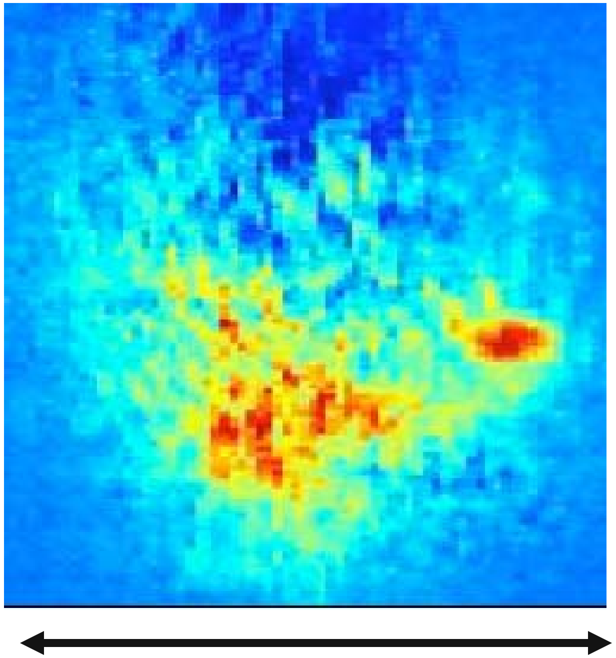
Defects Inside a Nanocrystal



M.A. Pferferet al., *Nature*442, 63 (2006)



Speckle Resolution



$\Delta Q \sim 10^{-2}$ Å^{-1}

Resolution ~ $\pi/\Delta Q$ ~ 50 nm

Improved Resolution Requires Higher Coherent Flux

Science needing Ultra-high Energy Resolution

10 eV
100 meV
1 meV
10 μeV
100 neV
1 neV

Multiphonons & Multimagnons ~ 50 – 500 meV
Pseudogap ~ 30 meV – 300 meV
Optical phonons ~ 40 – 70 meV
Magnons ~ 10 meV – 40 meV

Superconducting gap ~ 1 – 100 meV

Dynamics of disordered and nano systems
Boson peak in Amorphous Solids
Phasons in quasicrystals
Rotational excitations in liquids
Soft phonons

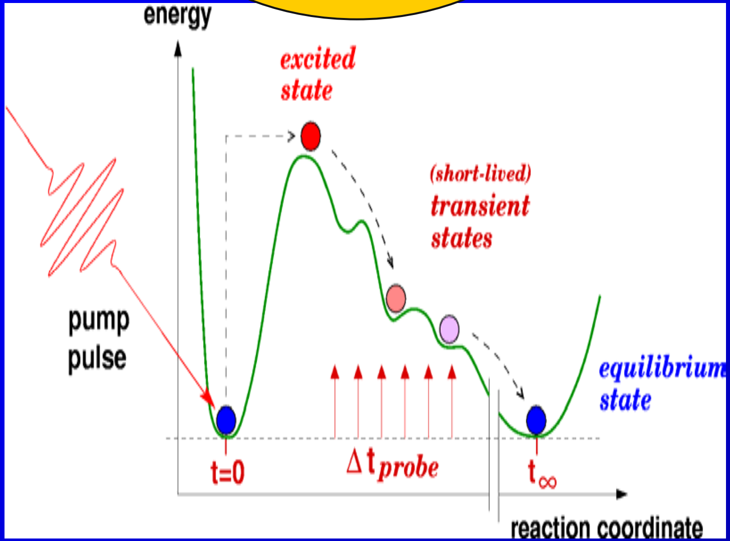
~ 10 -1000 μeV

Relaxation dynamics of fluids ~ 1 – 400 neV

Hyperfine Interactions ~ 1 – 100 neV

Science needing Ultrafast (ps to fs) X-ray Pulses

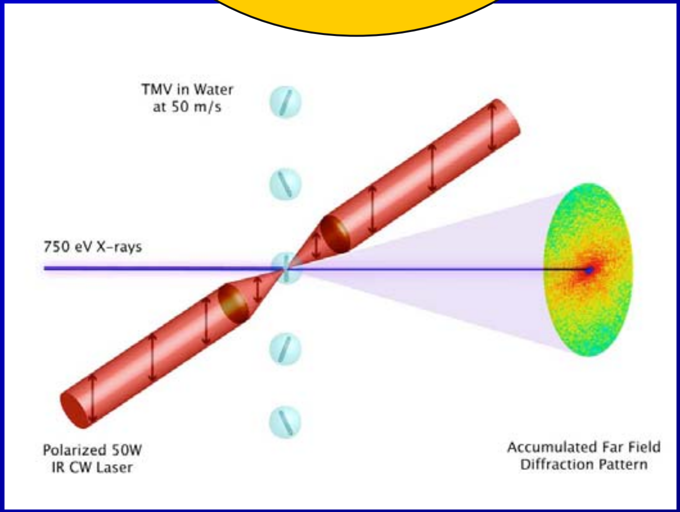
non-equilibrium chemical dynamics



Schematic presentation of transition states in a chemical reaction

Courtesy: Simone Techert

Coherent Diffractive Imaging of smaller molecules



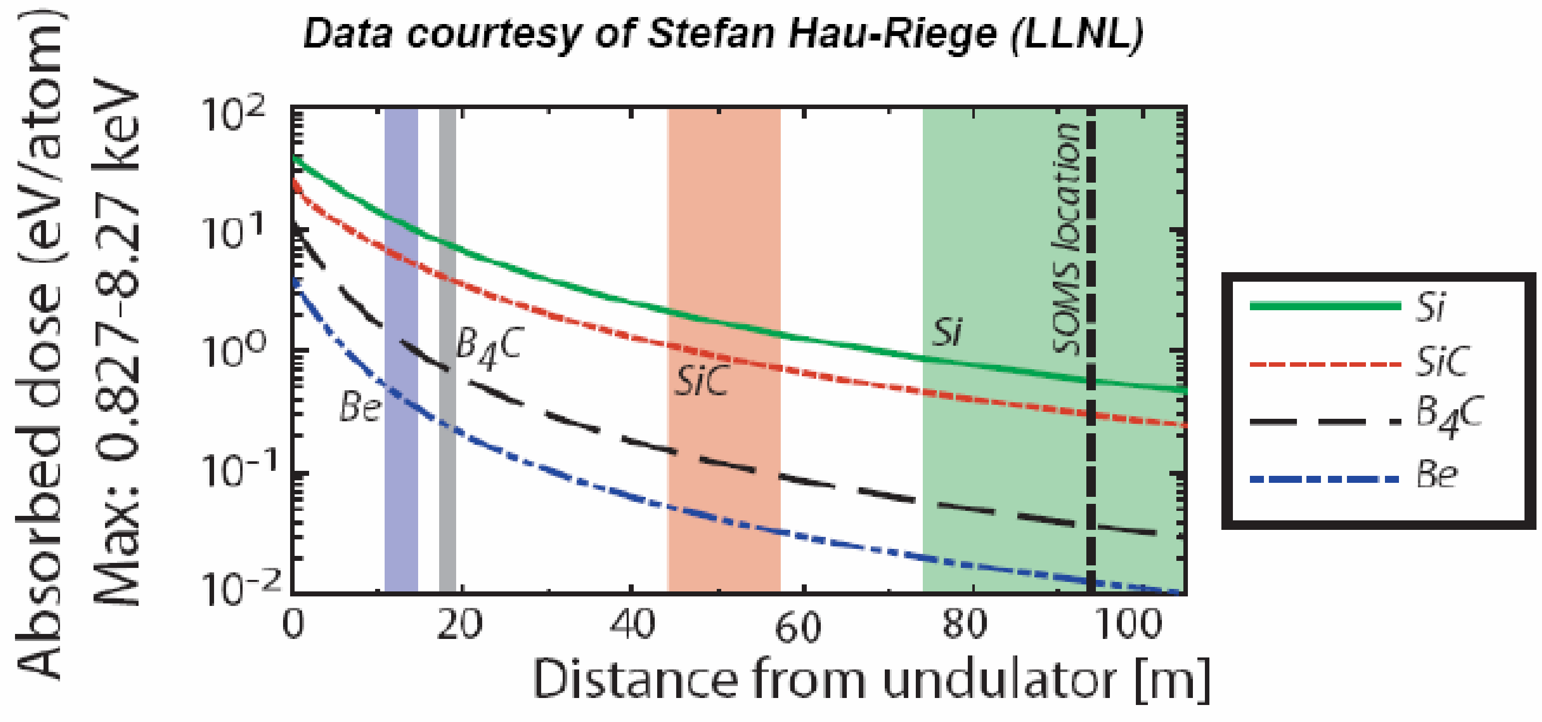
Schematic presentation of laser aligned stream of molecules

J.C.H. Spence and R.B. Doak, Phys. Rev. Lett. 92, 198102 (2004)

Comparison of Source Parameters that Determine the Optics Design

	Storage Rings	ERLs	FELs
Energy (GeV)	3.0 – 8.0	5.0 – 7.0	1.0 – 15.0
Charge (nC/bunch)	0.3 – 14	0.008 – 0.08	1.0
Total Average Power	1 – 35 kW	4 – 35 kW	0.005 – 2 kW
# bunches (Hz)	$0.7 - 34 \times 10^7$	1.3×10^9	$120 - 1.0 \times 10^6$
Peak Power kW/mm^2	0.2 – 5.0 @20 m	0.3 – 3.0 @20 m	0.006 – 200.0 @20 m
Peak Power	1 – 3 MW	8 – 90 MW	9 – 60 GW

Will the First Optic Handle High Peak Power from the FELs?

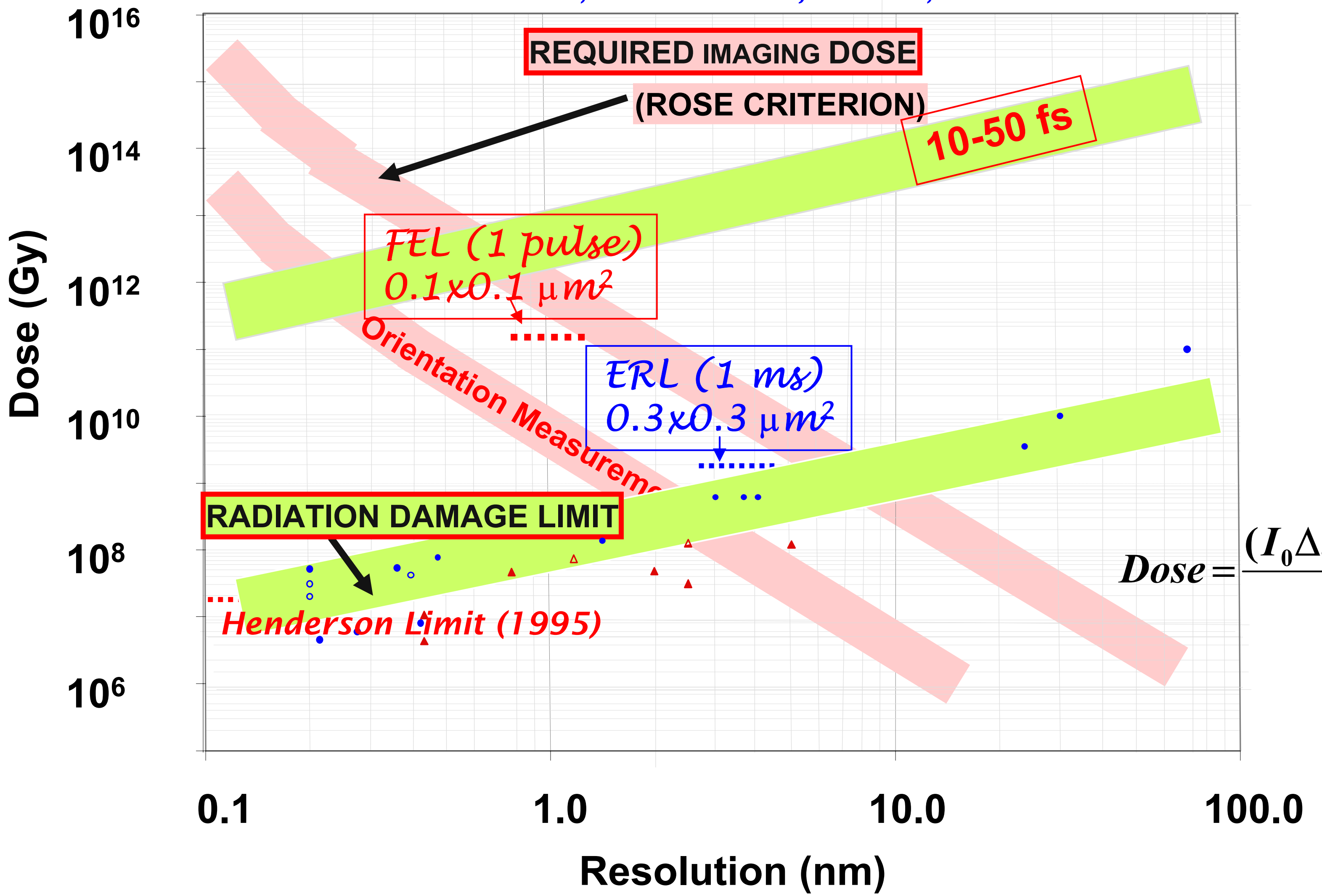


Vertical bands = range of distances over which the absorbed FEL dose will reach melting temperature, or melt each material

Experience from Flash/DESY
At E = 800 eV, 15 mrad on B4C coated mirror at 100 m
0.12 eV/atom < Dmelt = 0.62 eV/atom

Dose-Resolution Relationship for a Frozen-Hydrated Protein Sample

Marchesini et al. 2003; Shen et al, 2004; Howells et al. 2005



$$Dose = \frac{(I_0 \Delta t)\,\mu \cdot E}{\rho}$$

Bridging Science with Optics

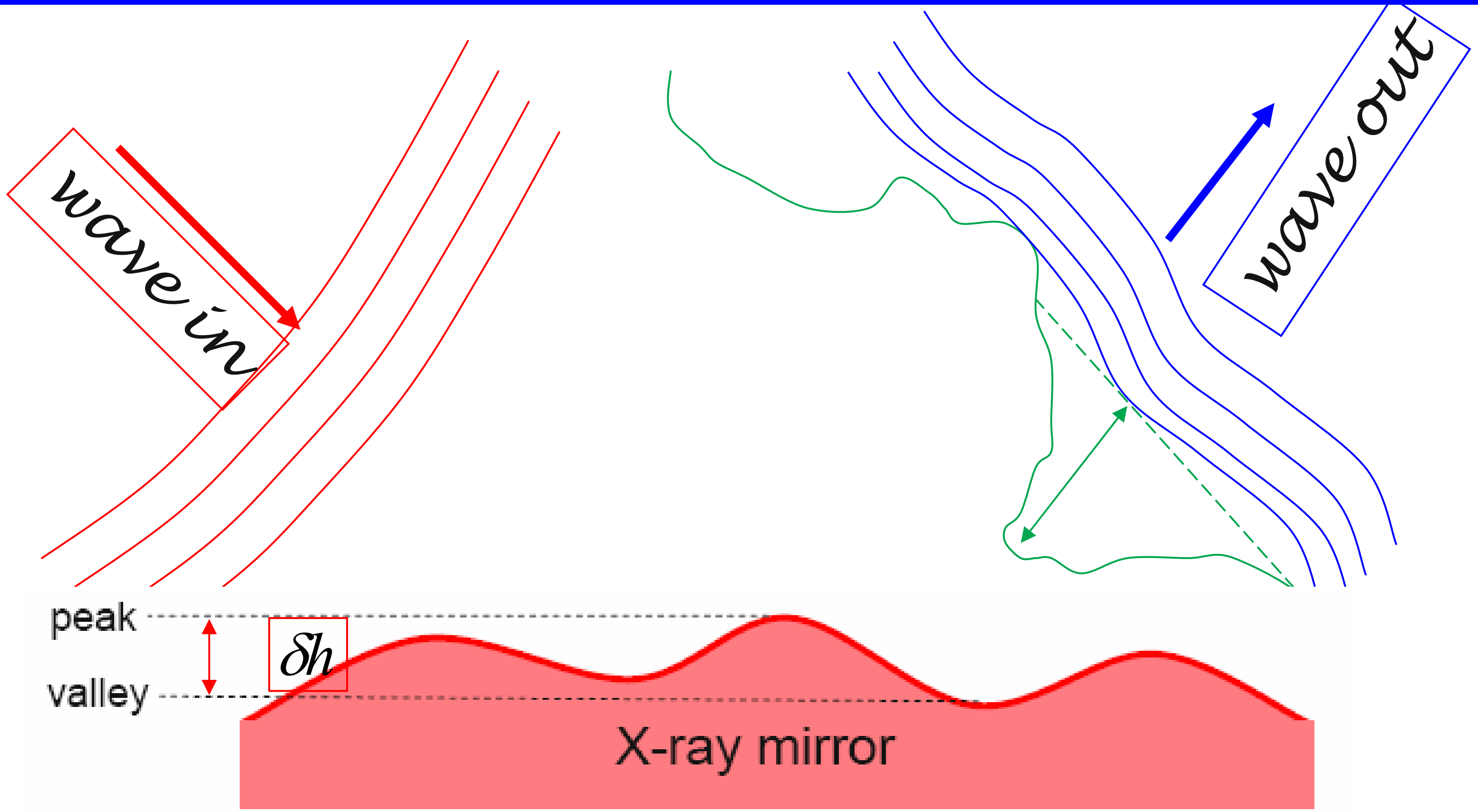
- ***Coherent Diffraction Imaging and 1 nm Spot***
  - *Brightness preserving optics – mirrors, multilayers, etc*
  - *Diffraction-limited K-B optics*
  - *Diffractive and refractive focusing optics*

    - zone plates

    - compound refractive lens

    - kinoform lenses
- ***Ultra-fast (1 fs)***
  - *Compression optics*
  - *Delay lines*
  - *Time response and pulse manipulation optics*
- ***Ultra-high energy resolution (< 100 nV)***
  - *Ultra-high density gratings*
  - *Sub-meV hard x-ray optics*

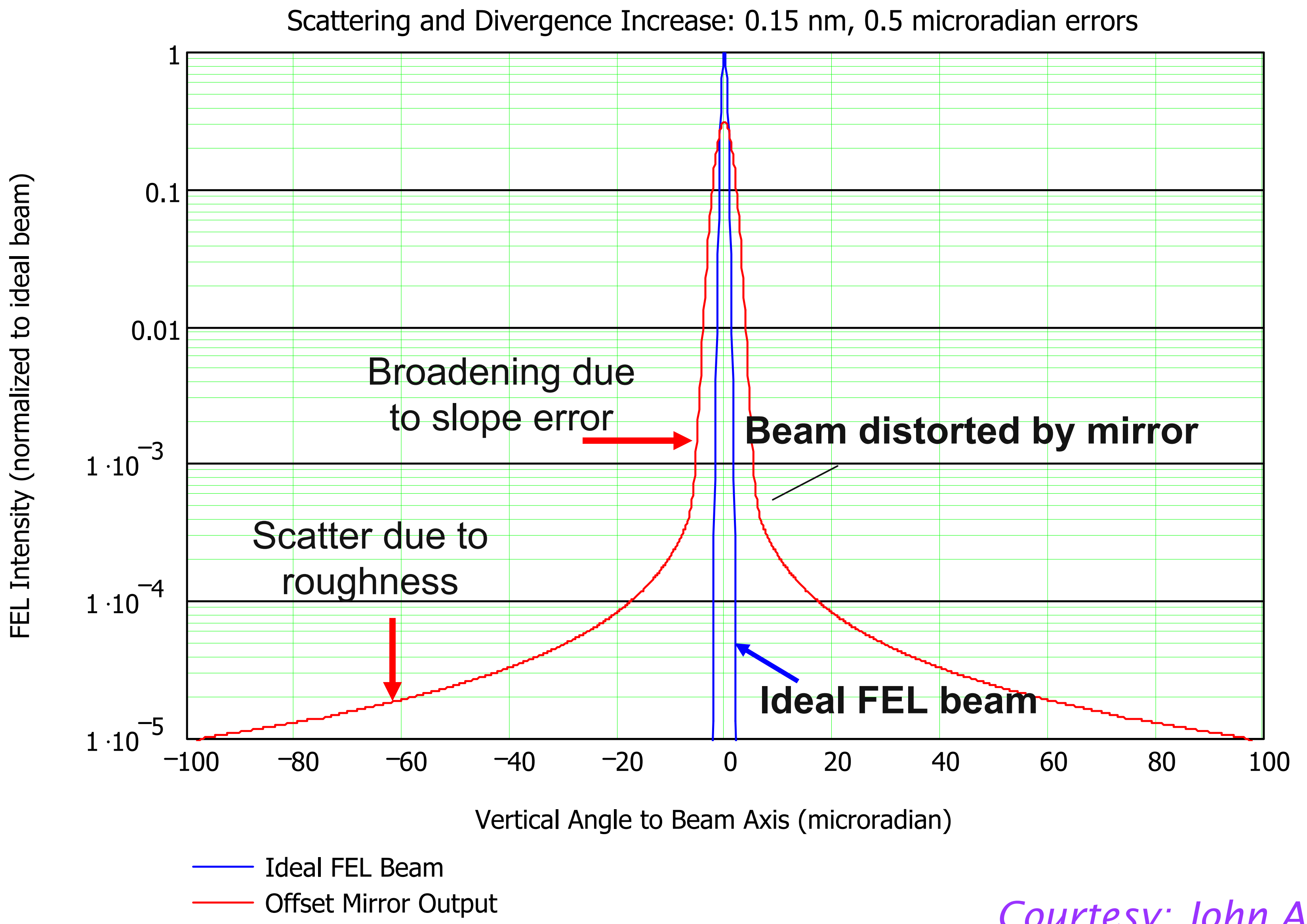
Preservation of Coherence



$$\varphi = \frac{2\delta h \cdot \sin\theta}{\lambda} \le 50 - 100nm$$

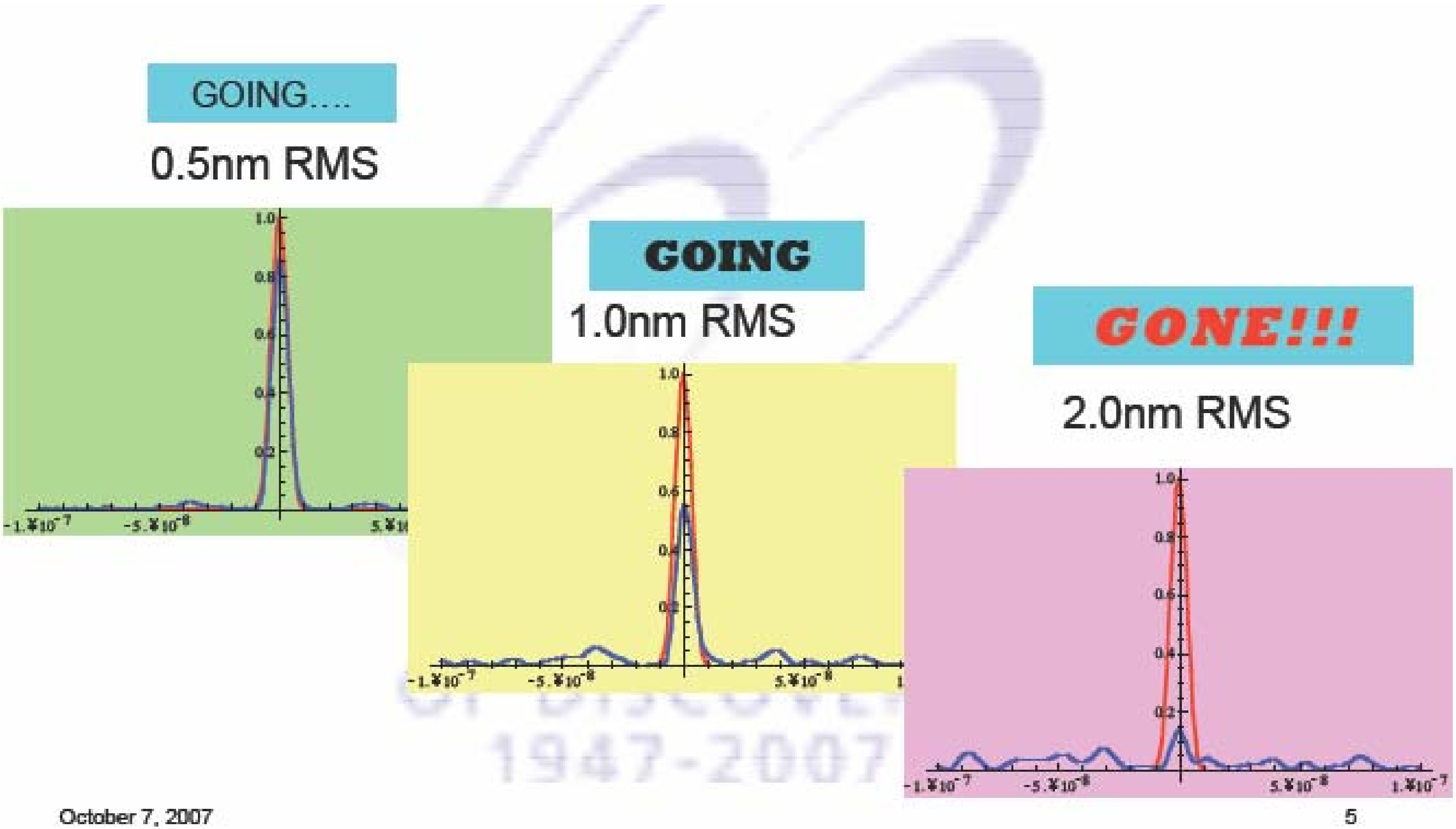
$$\delta h \approx 1.5 - 3.0nm \ \ for\ \lambda = 10nm\ @\ 3^o$$

Beam profile downstream of imperfect mirror



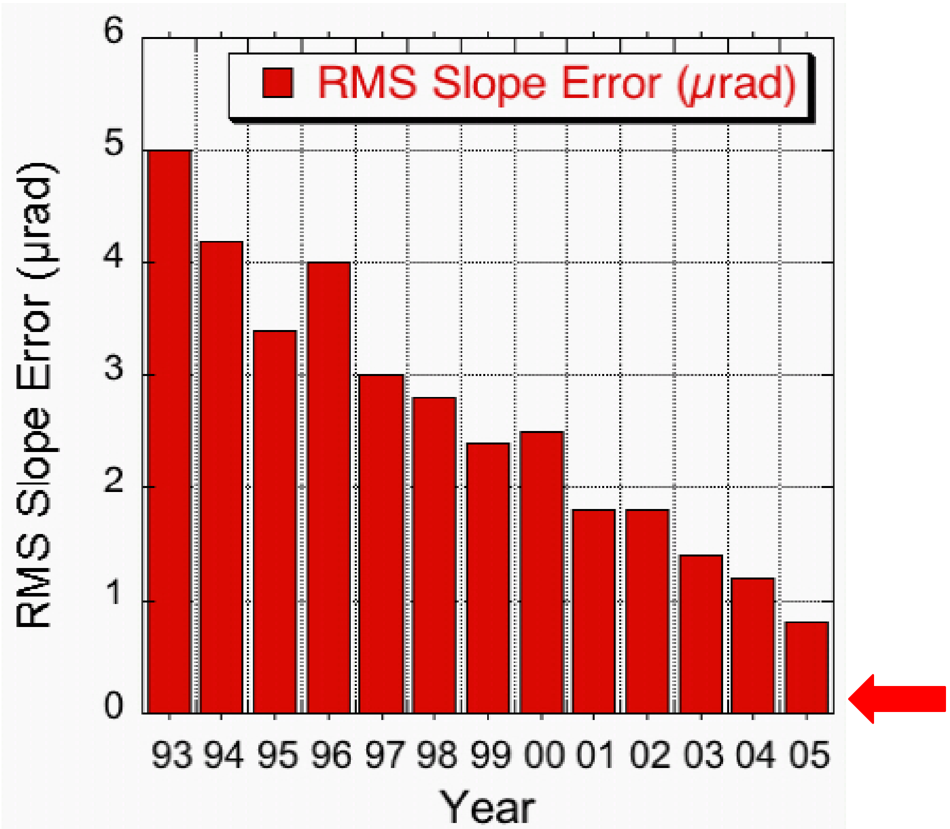
Courtesy: John Arthur

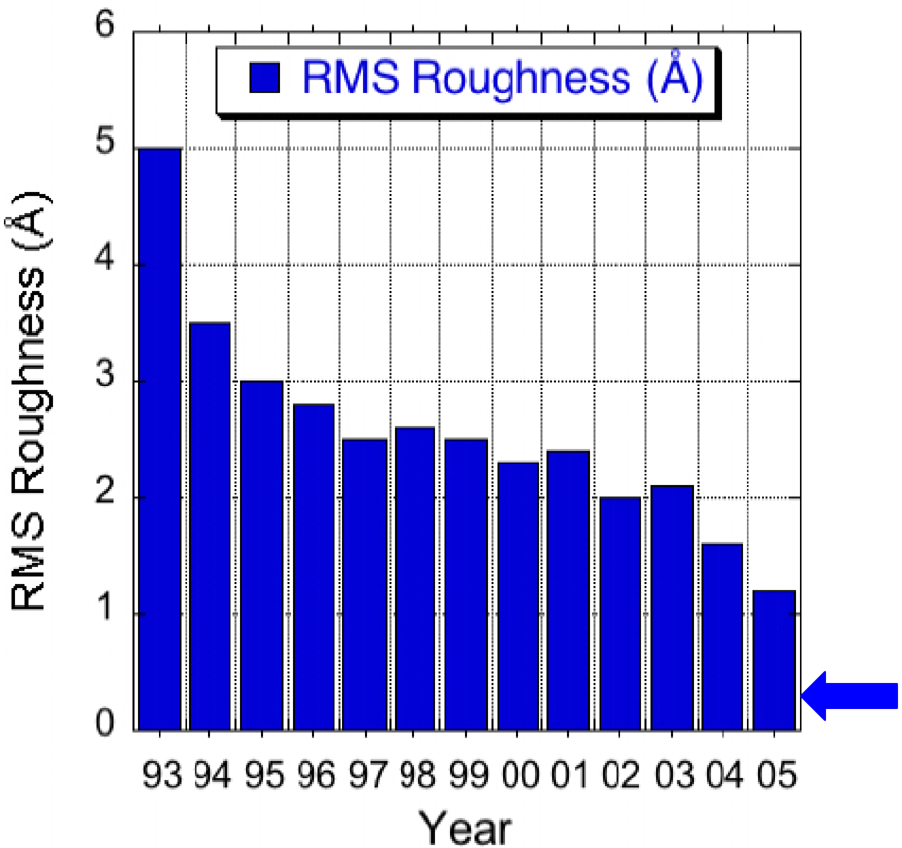
Influence of Roughness
NSLS II Simulation for λ = 0.1 nm



Courtesy: Peter Takacs, BNL

Evolution of surface quality of large hard x-ray mirrors during 1993-2005



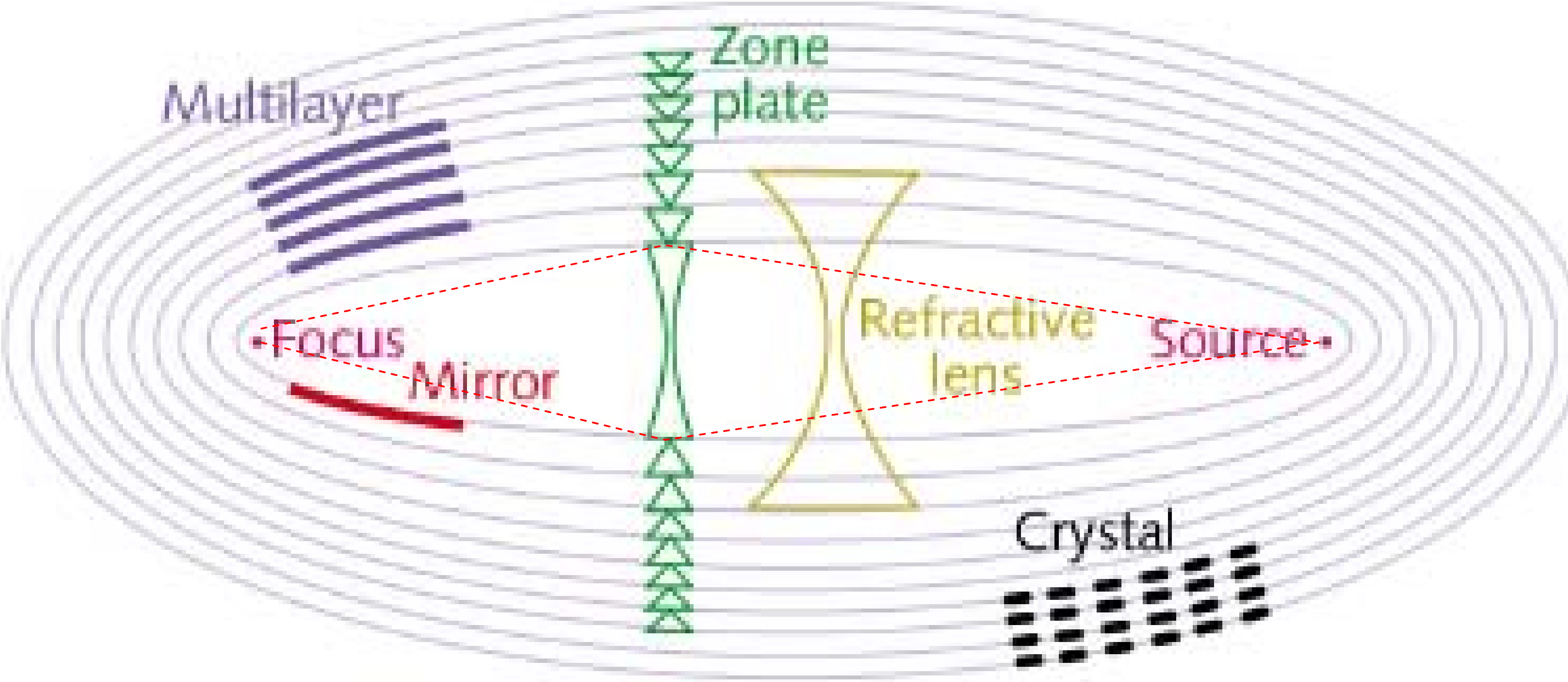


Courtesy: ***Lahsen Assoufid, APS***

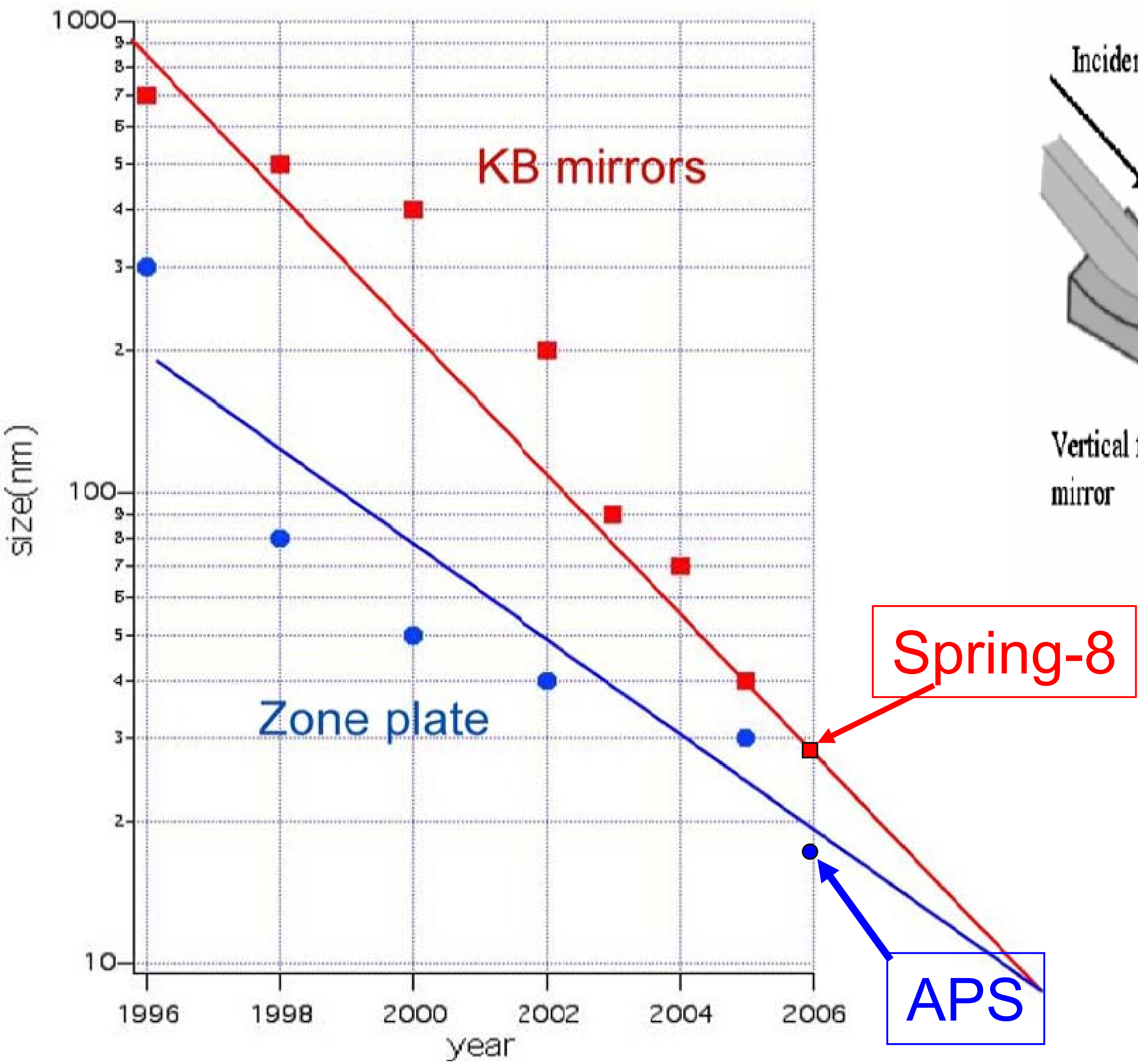
Quality of Mirror Surfaces Presently Achieved and Needs for Future ERLs and FELs

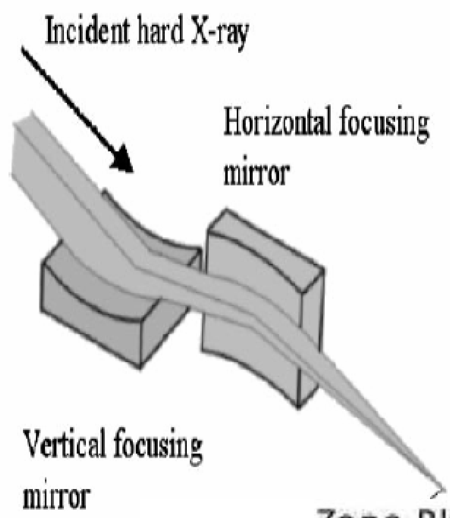
Errors	Best Achieved	Average Achieved	Needs of Future Sources
Slope Error	100 nrad	1000 nrad	20 – 50 nrad
Mid-spatial Roughness RMS	1.5 nm	4.0 nm	< 0.2 nm
High-spatial Roughness RMS	1.0 nm	2.0 nm	< 0.1 nm

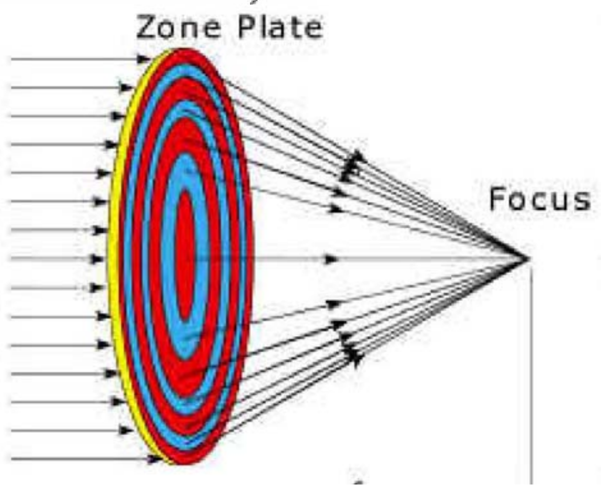
Can we reach 1 nm focus ?



Improvements in X-ray Focusing at 8 keV

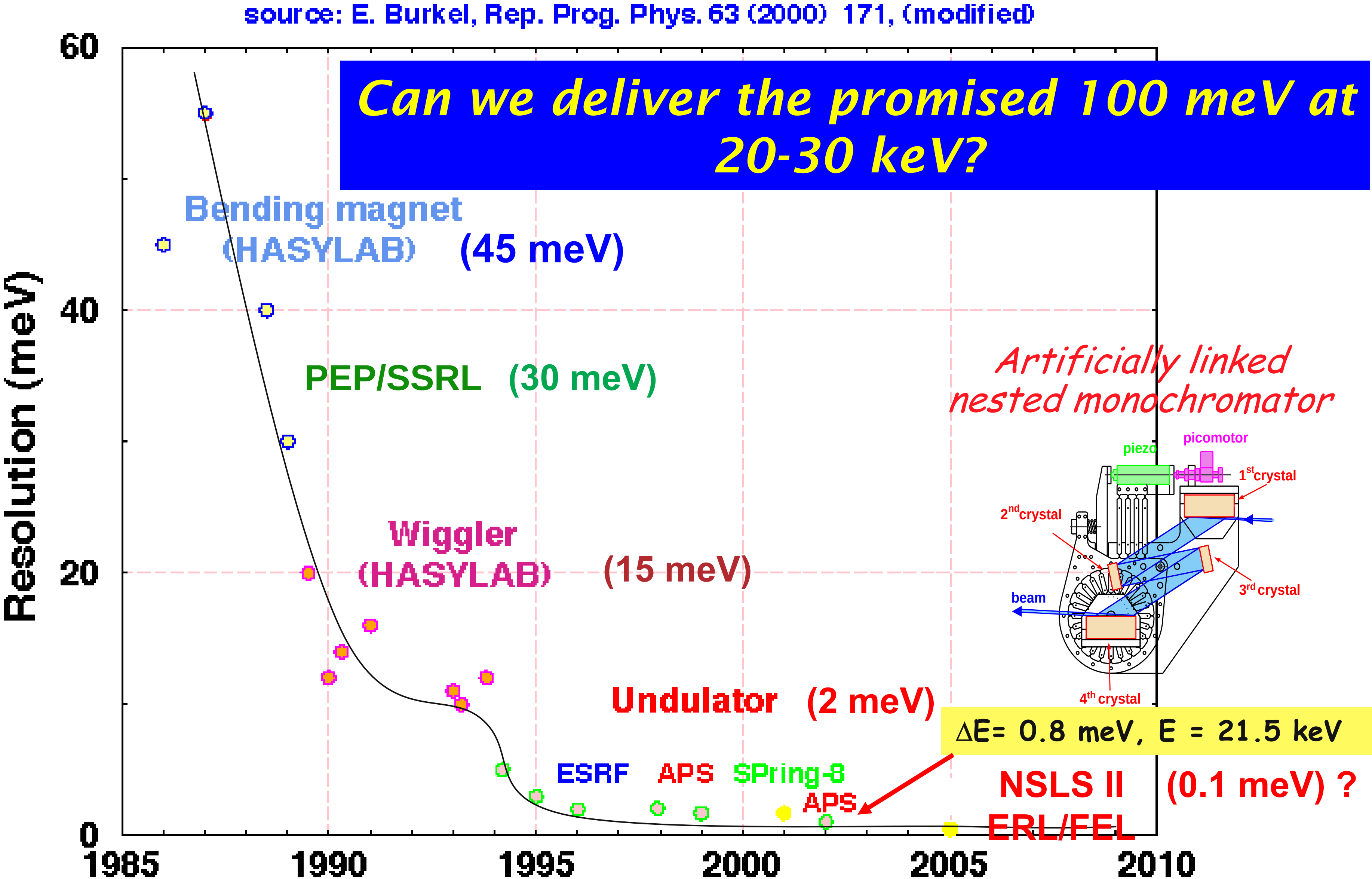






Courtesy: Gene Ice ORNL

Can we deliver the promised 100 meV at 20-30 keV?



Courtesy: Ercan Alp, APS

Past US efforts in optics technology

- Virtual National Laboratory - 1997 - DOE EUV Lithography
  - LLNL, LBL, and Sandia(CA) funded by EUVL LLC consortium CRADA
  - Intel Corporation, Motorola Corporation, Advanced Micro Devices Corporation, Micron Technology, etc

- Optics MODIL - 1988-93 - ORNL - DOD
  - DOD optics technology for StarWars
  - Developed Ion Beam milling process

- LIGO optics - 1997-2003 NSF
  - $1B total project
  - <1nm RMS figure error on 12” dia, 6km radius spherical, not asphere
  - NSF contract went to CSIRO, Australia

- US Synchrotron Radiation Facility Effort
  - Over 10 years old optics fab and metrology facilities (ALS, BNL, APS) with spotty upgrades
    Not adequate to meet the challenges of next generation sources

Compiled by Peter Takacs, BNL

The Nanometer Optic Component Cooperation BESSY

Working Group 1: **surface finishing**

Friedrich-Schiller-Universität Jena
Technisches Institut

ma

Working Group 2: **metrology**

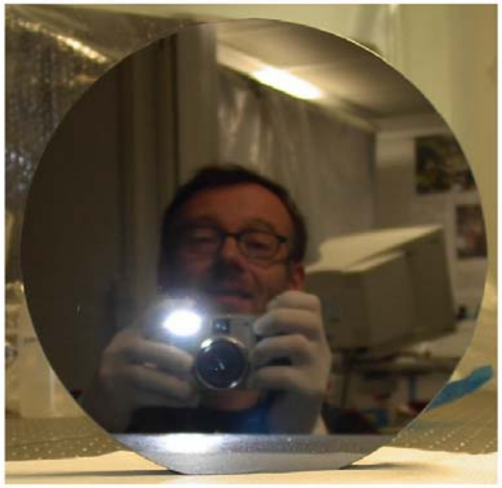


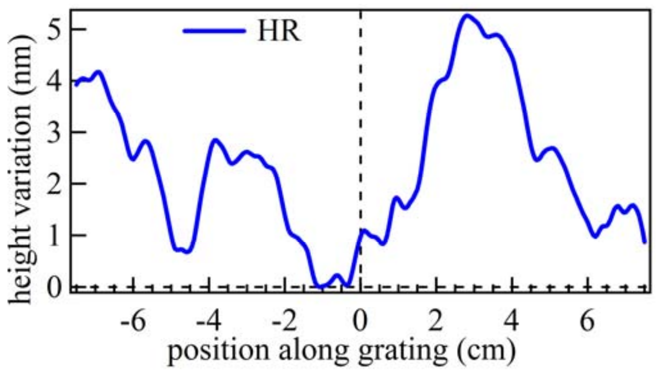
Fig. 1: the substrate at the interferometer table at the BESSY Optics Lab.

Measurement
@ BESSY: 0.25μrad & @ LBL: 0.28μrad

MERLIN Beamline at ALS

Resolving power: E/ΔE ~ 100,000 with 5μm slits
i.e. ~ 1 meV when photon energy below 100eV

Substrate Polishing by InSync Inc. USA
Metrology Measurement by BESSY/PTB
Holographic Ruling By ZEISS



Courtesy: Zahid Hussain ALS

European Approach
X-ray/EUV Optics Fabrication and Metrology Effort

BESSY (Germany)

Nanometer-Optical component measuring Machine (NOM) for 0.05 μrad accuracy metrology – over $5M capital + 15 FTE

PTB (Germany)

Extended Shear Angle Difference (ESAD) instrument with ~0.1 μrad accuracy

And a dedicated storage-ring for metrology

Soleil (France)

Development of metrology using x-rays to 20 nrad (Hartman methods)

CARL ZEISS

Local polishing with a computer controlled polishing robotic arm

Local ion beam figuring

Paul Scherrer Institute (PSI/SLS)

Development of SXR shearing interferometry, < 0.1 μrad

ESRF

Dedicated beamline for in-situ metrology

COST - European Cooperation in the field of Scientific and Technical Research – P7 (2006) collaboration is an investment in optics seen as key technology for ultra-bright light sources and as a technology base for industry

Japanese Approach
Osaka University Center for Atomistic Fabrication Technology

- *Research Center for Ultra Precision Science and Technology*
- *Creation of Perfect Surface (COE) Project with SPring-8 and Industries*

  - **To develop production technologies of optical or electronic devices for practical use**
  - **To continuously develop new "atomistic fabrication technology" based on new physical principles**
  - **To carry out collaborative research in conjunction with laboratories from other field of basic science and advanced industry**
  - **To produce meter-size articles with atomic scale accuracy**
  - **To attract graduate students participate in the forefront of research and to educate research leaders for next generation production technology**

Infrastructure: **Ultraclean Labs with EEM, Plasma CVM, Atmospheric Pressure Plasma CVD, Electro-chemical processing using only ultrapure water, Ultra-precision Aspheric Surface Measurement, SREM/STM, Ultra-weak Light Scattering Surface Measurement, Optical Metrology Tools, Simulation and Modeling, etc.**

Summary

1. *To fully harness the coherence, brightness, and time-structure of proposed VUV/X-ray Sources (ERLs, FELs) a new generation of optics has to be developed along with light sources in the US*

2. *R&D funding should be available immediately to foster new ideas for optics such as liquid metal mirrors, disposable optics, self-assembly DNA optics, kinoform optics, polymide coatings, high resolution diffractive optics, holographic ruling of soft x-ray gratings with $\Delta E/E$ > 100000, new optical schemes leading to sub-mV resolution in the hard x-ray range, nm meter focus, etc.*

3. *An ultra-clean infrastructure for fabrication, and in-situ and ex-situ metrology should be developed with traditional and modern techniques along with simulation and computational tools following the Osaka University model.*

4. *A model similar to Japanese approach would be best suited for NSF stewardship with partnerships between universities, NSF/DOE light sources, and industries. A chosen university will build an ultra-precision optics and dedicated metrology facility using its diverse science and engineering strengths impacting the education, training and economic base for the US during the next decades. This will also stimulate US industries to develop new capabilities required to fabricate next generation atomistic technologies.*

Which Detector Technologies will Support Future Experiments?

- *Examples of Experiments Requiring 2D X-ray Detectors*
  - *Pump Probe crystalline diffraction*
  - *Pump-Probe non-crystalline diffraction*
  - *Coherent Diffraction Imaging*
  - *Single Particle Imaging*
  - *X-ray Photon Correlation Spectroscopy*
- *Detector types include gas, Si, GaAs, Ge, HgI, InP, ThBr, CZT/CdTe, electron spectrometer and ion recoil detectors*
- *Detectors for diagnostics*

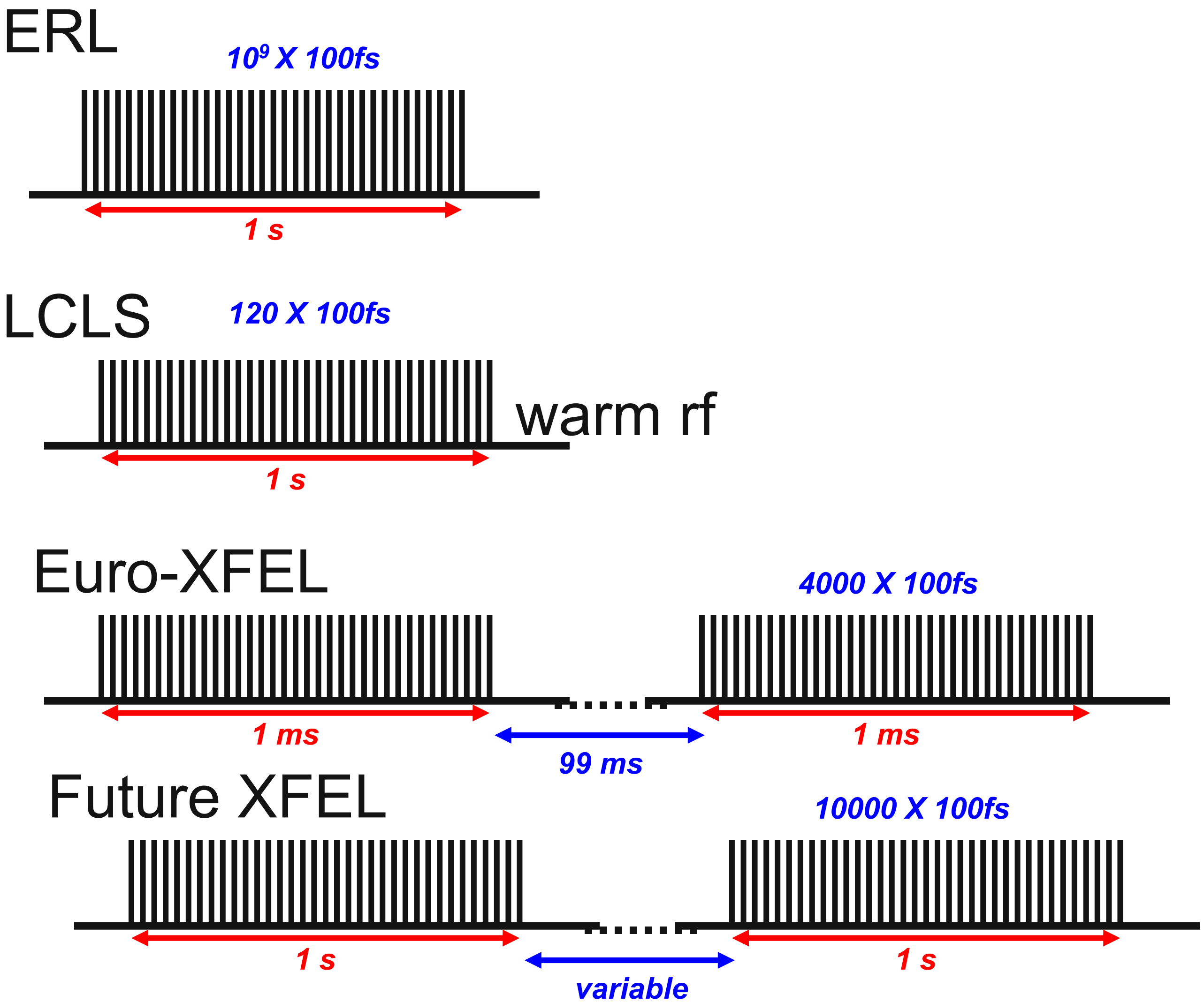
Each Experiment needs a Unique Set of Detectors

Example: 2D X-ray Detector Characteristics

Pixel Size ~ 0.1mrad or < 100 microns
Read out noise < 1 to 10^{-2} photons
Signal rate/pixel/pulse ~ 10^2 to 10^4
S/N ~ 10^4 beyond current detector technology
Number of Pixels ~ 10k x 10k
Single photon resolution – may be difficult
Sample-detector subtended angle ~ 120°
Detector tiling ~ acceptable
Photon energy range few eV to 8-12 keV
Quantum efficiency > 0.8
Radiation Hardness 10^{16} X-rays per pixel (~ 3 years)

Can't be met by commercially available CCD detector technology

Detector Readout Time - Matching Source Pulse Sequence



	Pulse-to-Pulse Separation	
	Micro	Macro
ERL	0.8 ns (1.3 GHz)	--
LCLS	8.3 ms (120 Hz)	--
Euro-XFEL	0.25 μs (4 MHz)	99 ms (10 Hz)
Future XFEL	0.1 ms (10 kHz)	variable

Typical Detector Development Activities

- *Detector specification, design, materials R&D, radiation damage*
- *Micro- nano-fabrication, R&D foundry at a university or an industrial lab (semiconductor/materials technologies)*
- *Front-end integration*
- *ADC, data storage*
- *Data compression*
- *DAQ, slow control, mechanical and thermal integration, calibration, readout*
- *Instrument and analysis*

Ideally all activities must be co-located

Dedicated Detector Activities and Expertise

US:

BNL – X-ray Active Matrix Pixel Sensors (XAMPS) for LCLS
Cornell University – Integrating Analog Pixel Array Detectors

Europe:

European Consortium for high speed X-ray Imaging (ECI) (MPI-Halbeiterlabor, Politecnico di Milano and INFN, Fraunhofer Institut-IMS, Uni Mannheim, Uni Bonn, Uni Hamburg, DESY) – Silicon Drift Detectors

Paul Sherrer Institute (PSI) – Hybrid Pixel Detectors (Pilatus II)

DESY - XFEL Project Team for Detectors

CCLRC - Council for the Central Laboratory of the Research Councils – Rutherford Lab

Summary on Detector Development

- US institutions have sub-critical effort
- There is a need for an updated roadmap focused on detectors for the next generation light sources
- US is lagging behind in the detector R&D on the world science scene
- European institutions are working collectively integrating foundry capabilities with detector designs
- European model centered around a lead institution seem to work well (e.g., DESY)
- A university with semiconductor design foundry and EEE R&D capability is ideal to steward an NSF detector program in the US

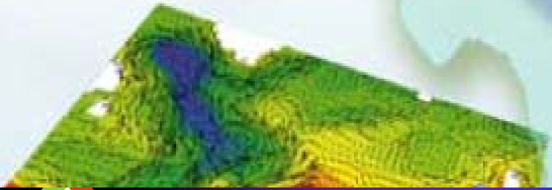
BES Science Network Requirements

Report of the Basic Energy Sciences Network Requirements Workshop

Conducted June 4-5, 2007

ESnet

Energy Sciences Network



Conclusions

- *Performing R&D on optics, detectors, instrumentation, and data processing is imperative in order to harness the unprecedented capabilities of next-generation light sources*
- *The funding of long-term R&D and creating associated infrastructure is of utmost urgency in the US to remain competitive in science and technology during next decades*
- *NSF is well positioned to create centers of excellence focused around unique and diverse knowledge base at the universities*
- *For example, centers on optics with atomic perfection, ultra-fast 2D detectors, and nano-instrumentation will educate and train science- and technology-leaders for the 21st century.*