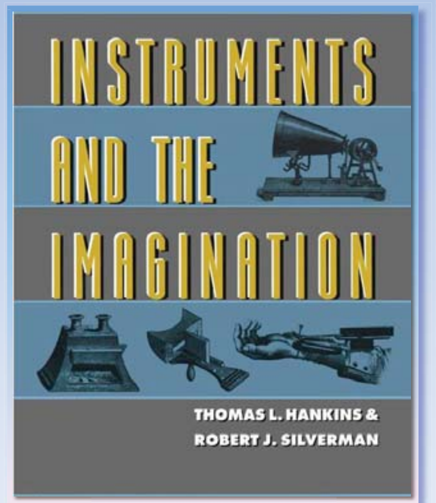
Advanced Experiments using Accelerator Based X-ray Sources

J. Hastings SLAC
Oct. 2, 2012

Remarks of Prof. J. Etchemendy, Stanford University Provost, at the LCLS Groundbreaking, Oct. 20, 2006.



Quoting from Tom Hankins and Robert Silverstein in *Instruments and the Imagination*

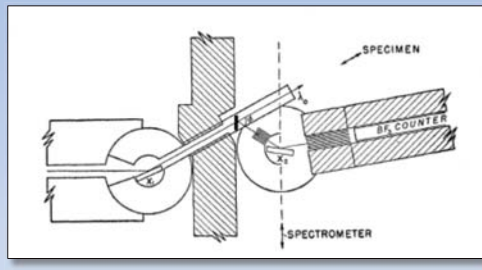
"Instruments have a life of their own. They do not merely follow theory; often they determine theory, because instruments determine what is possible, and what is possible determines to a large extent what can be thought.

The telescope, the microscope; the chronograph, the photograph: all gave rise to a blossoming of theoretical understanding not possible before their invention."

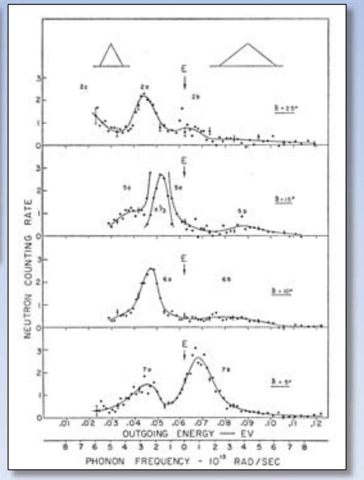
High resolution x-ray scattering

- Components of an experiment:
  (1) Incident beam
  (2) Sample environment
  (3) Detector system/Data Acquisition System
- A look back at neutrons
- High Q resolution scattering with x-rays: 8 keV and 100+ keV
- Powder diffraction
- *To see small signals: REDUCE THE BACKGROUND*
- Nuclear resonant scattering
- XFELS
- A spontaneous precursor: SPPS
- Multi-photon effects in clusters
- Nano-crystallography
- X-ray laser mixing
- The future

A look back at neutron scattering



B. N. Brockhouse, "Energy Distribution of Neutrons Scattered by Paramagnetic Substances", Phys. Rev., **99**, 601 (1955)



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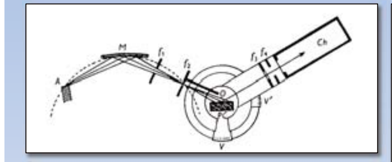
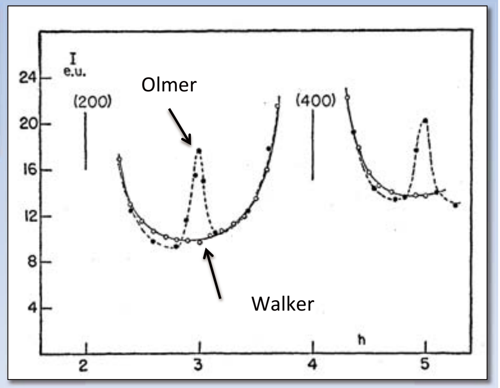
From X-ray tubes to storage rings





P. Olmer, "Dispersion des Vitesses des Ondes Acoustiques dans l'Aluminium", Acta Cryst., 1,47 (1948)

C. B.Walker "X-Ray Study of Lattice Vibrations in Aluminum", Phys. Rev., **103**, 547 (1956)

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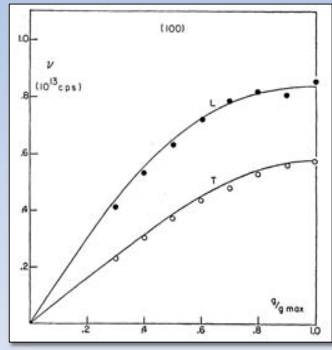

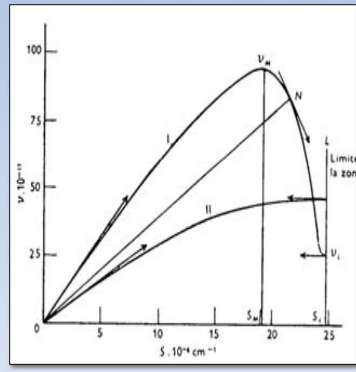

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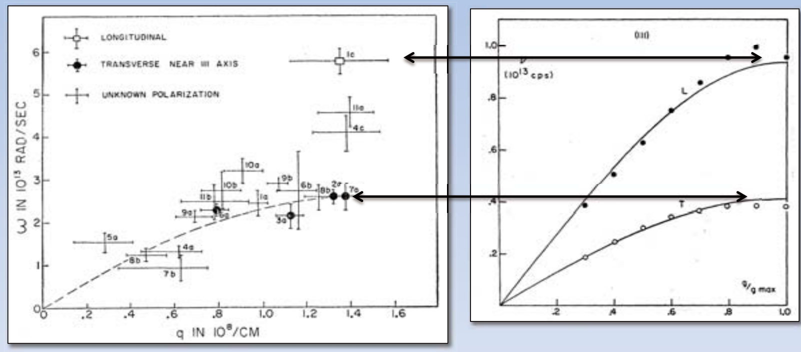
From x-rays to neutrons



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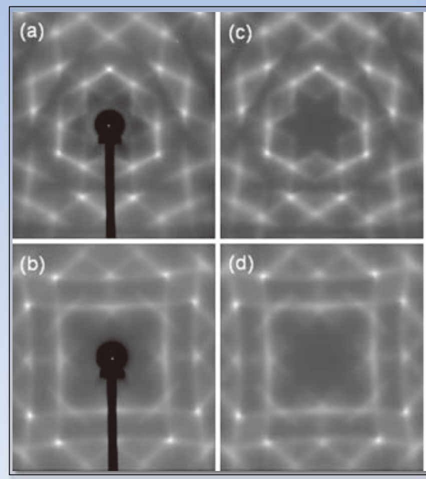
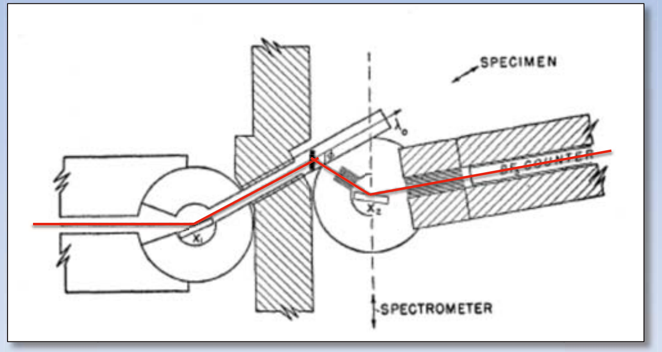
C. B. Walker "X-Ray Study of Lattice Vibrations in Aluminum", Phys. Rev., **103**, 547 (1956)

From to Neutrons back to SR X-rays



Ruqing Xul and Tai C. Chiang, "Determination of phonon dispersion relations by X-ray thermal diffuse scattering", Z. Kristallogr. **220,** 1009 (2005)

High Resolution X-Ray Scattering



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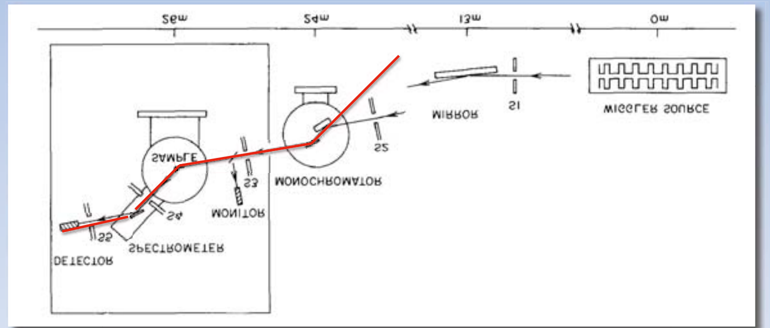
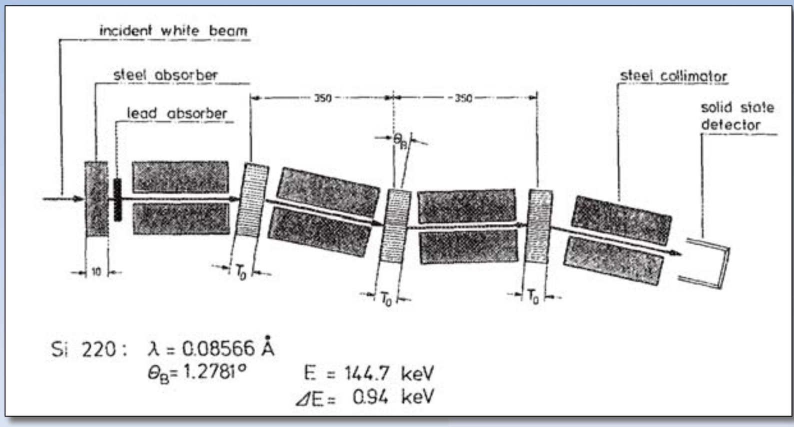
High Resolution X-Ray Scattering (1)



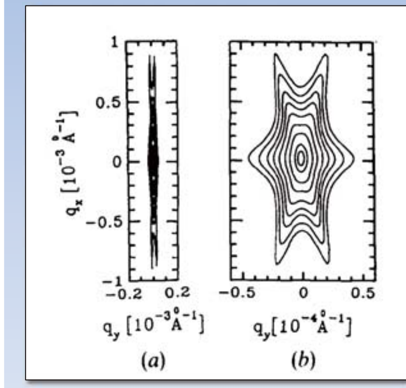
D.E. Moncton and G.S. Brown, "High-Resolution X-Ray Scattering", NIM, **208** 579-586 (1983)

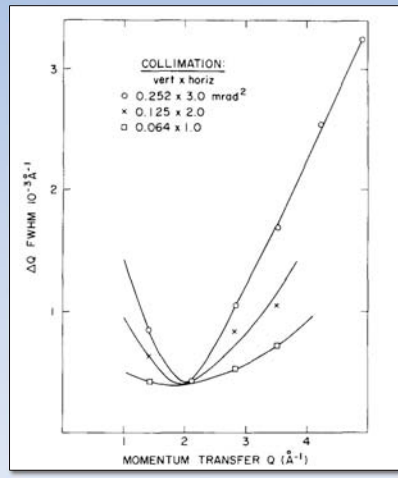
High Resolution X-Ray Scattering (2)



J.B. Hastings, D. P. Siddons, L. E. Berman, and J.R. Schneider "Three-crystal spectrometer for 150-keV synchrotron radiation", Rev. Sci. Instrum. **60,** 2398 (1989)

High Resolution X-Ray Scattering (3)

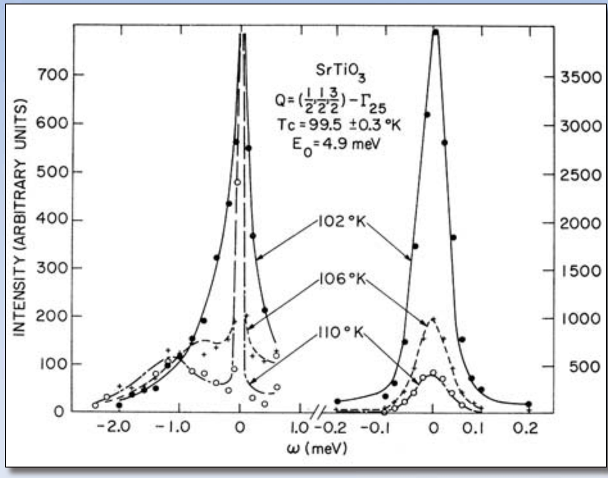




80 keV

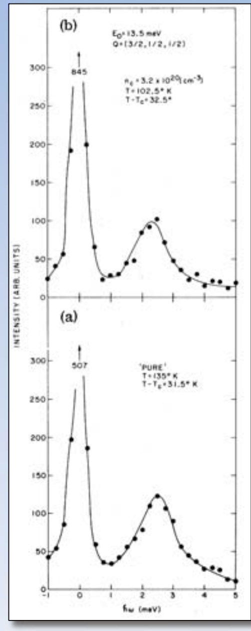
8 keV

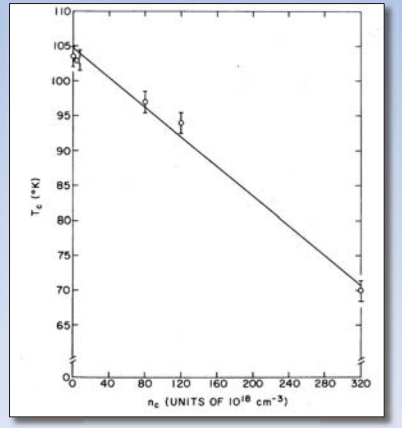
Central Peak in $SrTiO_3$: Two Length Scales



S. M. Shapiro, J. D. Axe, G. Shirane and T. Riste, "Critical Neutron Scattering in SrTi03 and KMnF3", Phys. Rev., **B6**, 4332 (1972)

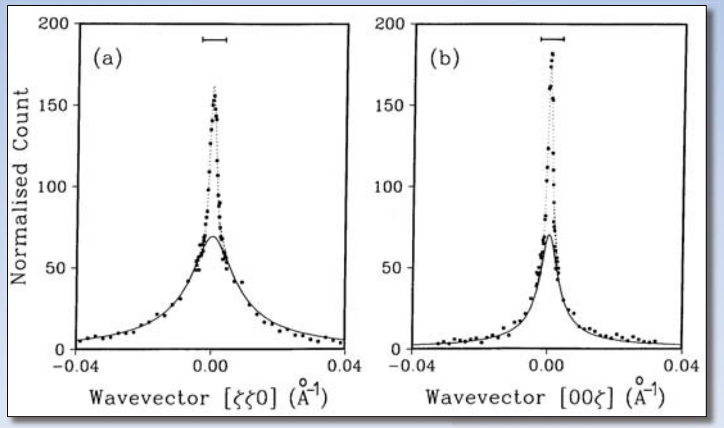
Central Peak in $SrTiO_3$: Two Length Scales and the Role of Defects





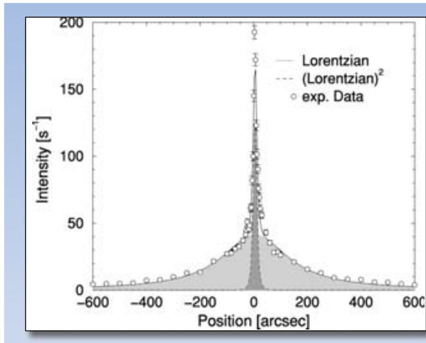
J. B. Hastings, S. M. Shapiro, and B. C. Frazer, "Central-Peak Enhancement in Hydrogen-Reduced SrTi03", Phys. Rev. Lett, 40, 237 (1978)

Central Peak in $SrTiO_3$: Two Length Scales 11.2 keV x-rays

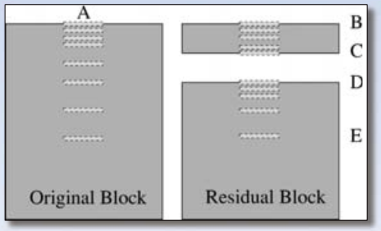


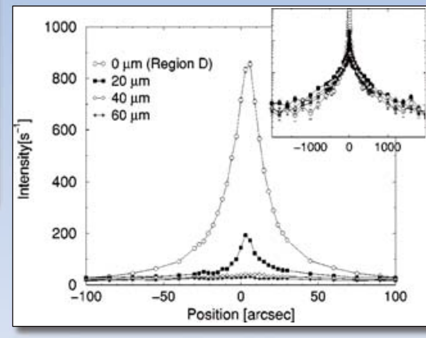
D.F. McMorrow, N. Hamaya, S. Shimomura, Y. Fujii, S. Kishimoto and H. Iwasaki, "On the Length Scales of the Critical Fluctuations in $SrTiO_3$", Solid State Commun. **76**, 443 (1990)

Central Peak in $SrTiO_3$: Two Length Scales 100 and 120 keV x-rays



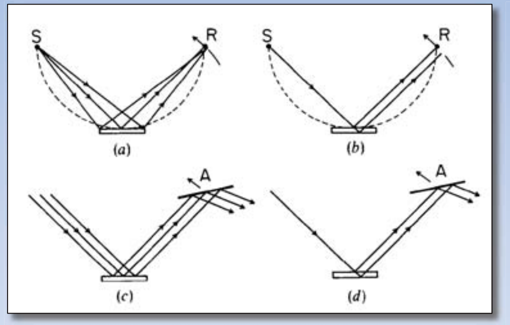
20 μm from surface 0.5 K above T_c

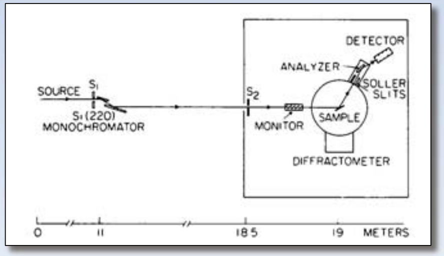




H. Hünnefeld, T. Niemöller, J. R. Schneider, U. Rütt, S. Rodewald, J. Fleig, and G. Shirane Phys. Rev. B **66**, 014113 (2002)

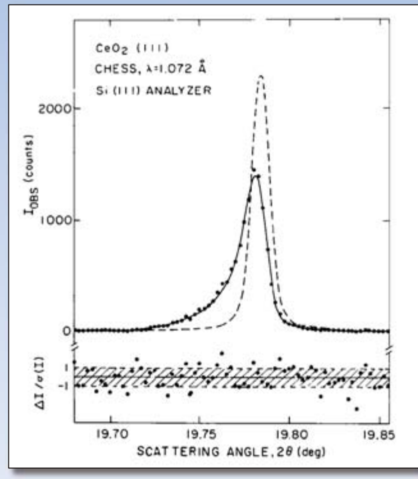
High Resolution Powder Diffraction

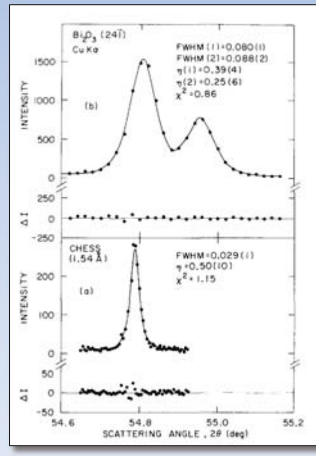




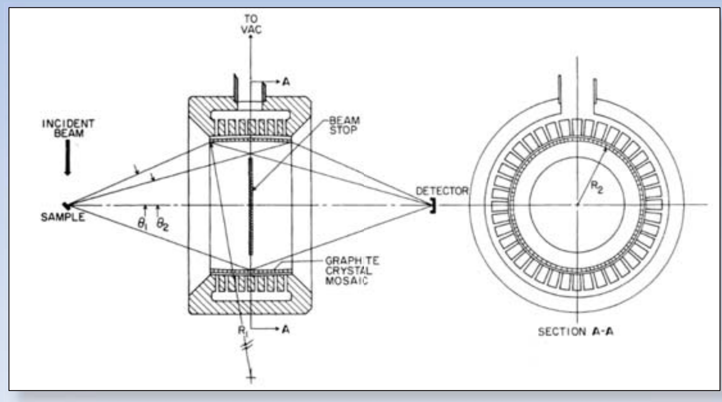
J. B. Hastings, W. Thomlinson and D. E. Cox, "Synchrotron X-ray Powder Diffraction", J. Appl. Cryst. (1984). 17, 85-95

High Resolution Powder Diffraction





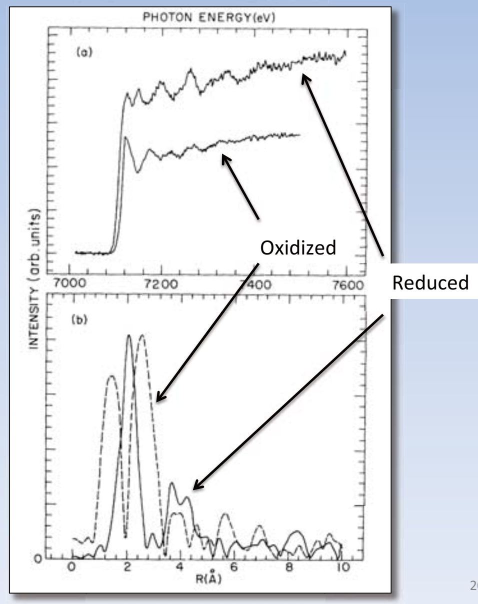
A detour: X-ray spectroscopy



J. B. Hastings, P. Eisenberger, B. Lengler, M. L. Perlman, "Local structure Determination at High Dilution: Internal Oxidation of 75-ppm Fe in Cu", Phys. Rev. Lett., **43**,1807 (1979)

A detour: X-ray spectroscopy (2)

The observed spectra for the oxidized state indicate that none of the proposed constituents, FeO, Fe_3O_4 and $CuFe_2O_4$, of the fully oxidized state are present. Fe atoms appear to be clustered with Fe and have Cu and 0 near neighbors as well.



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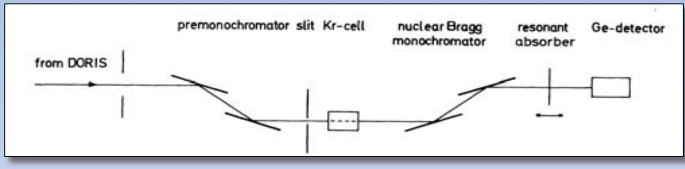
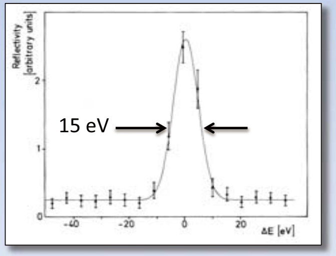
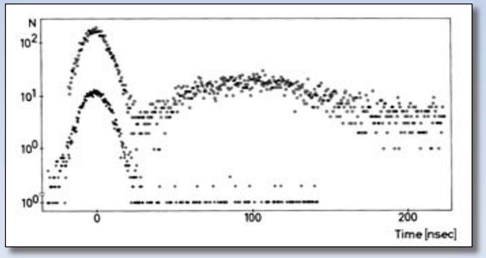
Nuclear Resonant Scattering

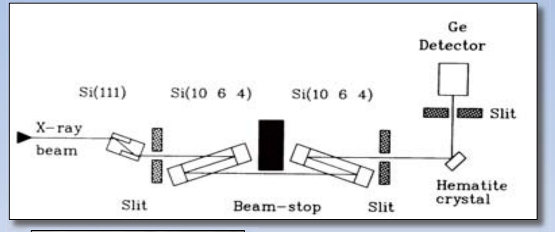


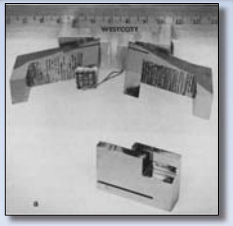


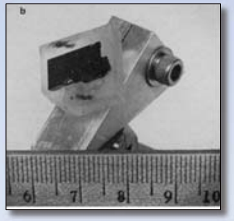


E. Gerdau, R. Rüffer, H. Winkler, W. Tolksdorf. C. P. Klages, J. P. Hannon, "Nuclear Bragg Diffraction of Synchrotron Radiation in Yttrium Iron Garnet", Phys. Rev. Lett., **54,**835 (1985)

Nuclear Resonant Scattering (1)

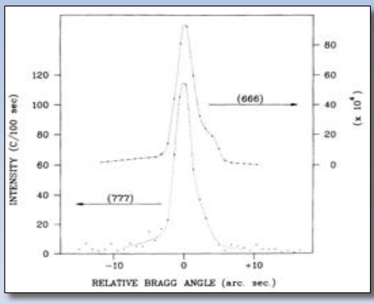


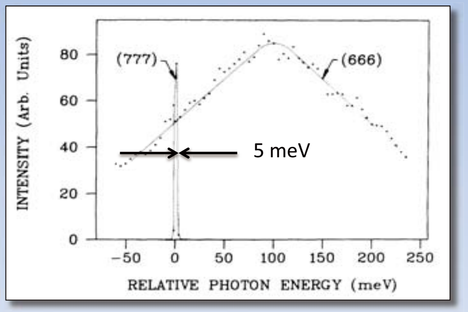




G. Faigel, D. P. Siddons, J. B. Hastings, P. E. Haustein, and J. R. Grover, J. P. Remeik, and A. S. Cooper, "New Approach to the Study of Nuclear Bragg Scattering of Synchrotron Radiation", Phys. Rev. Lett., **58,** 2699 (1987)

Nuclear Resonant Scattering (2)





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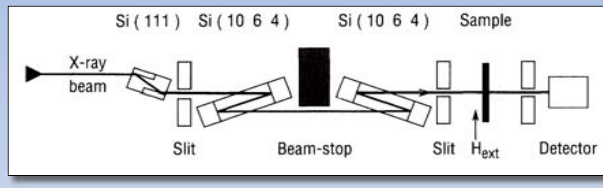
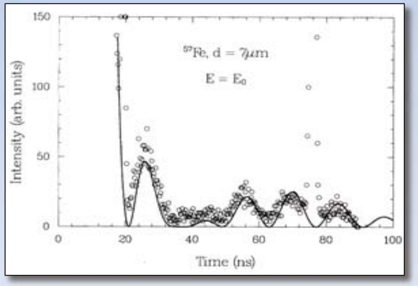
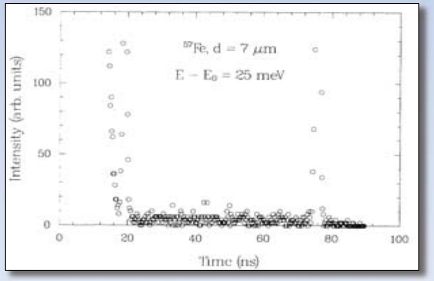


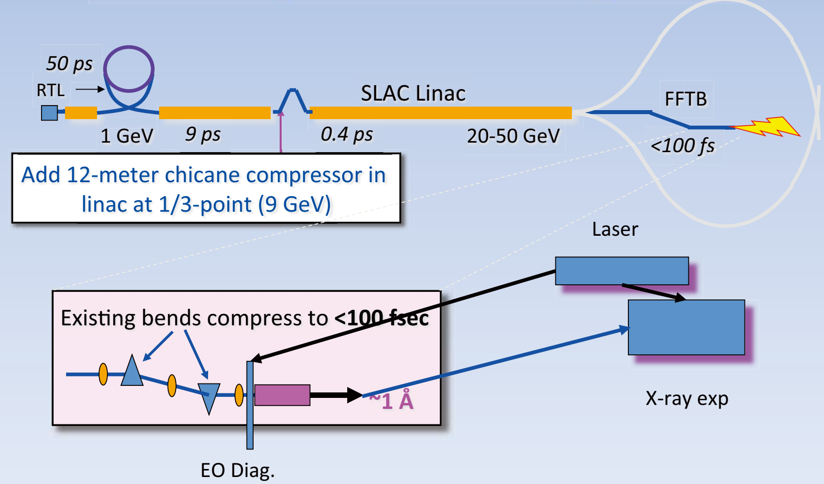




J. B. Hastings, D. P. Siddons, U. van Bürck, R. Hollatz, and U. Bergmann, "Mössbauer Spectroscopy Using Synchrotron Radiation", Phys. Rev. Lett., **66,** 770 (1991)

The Sub-Picosecond Pulsed Source (SPPS)

Bunch Length/Arrival Time Diagnostics



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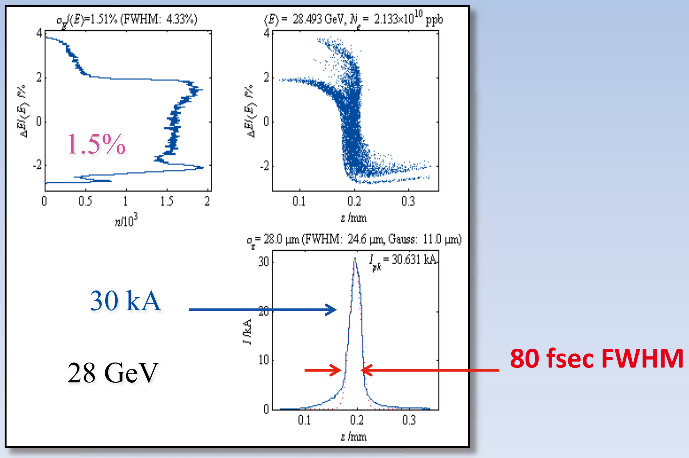
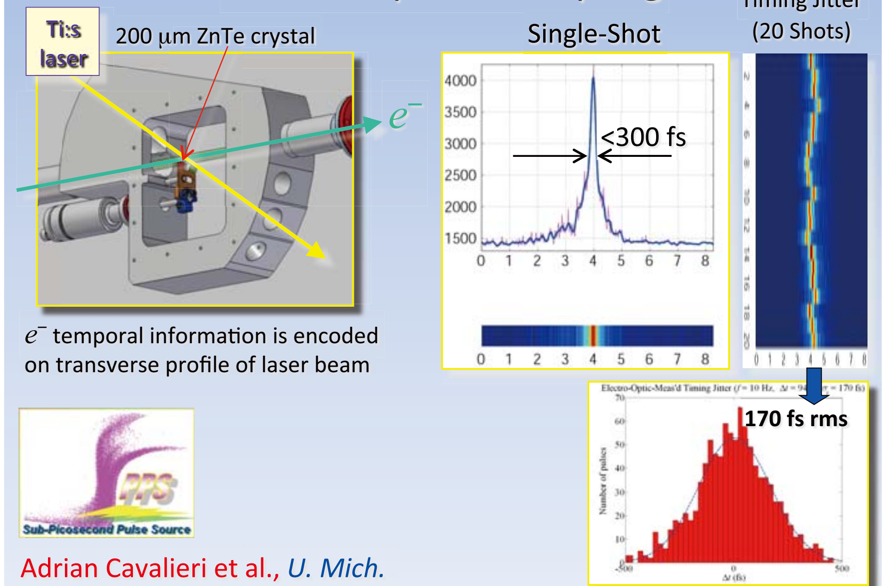


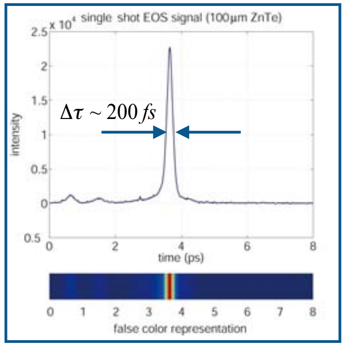
Electro-Optical Sampling

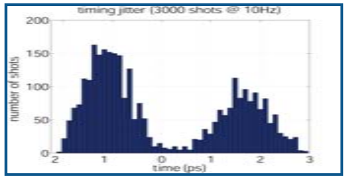


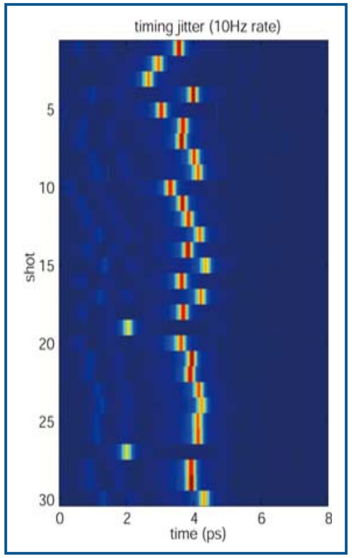
e^- temporal information is encoded on transverse profile of laser beam

Adrian Cavalieri et al., *U. Mich.*

(Typical)Single-Shot EOS Data at SPPS (100µm ZnTe)

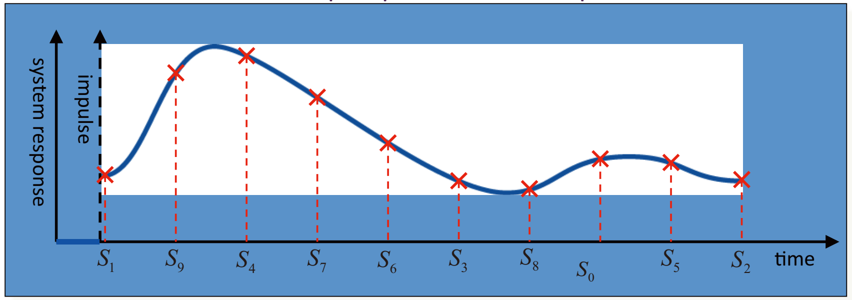






EOS and "Pump-Probe"

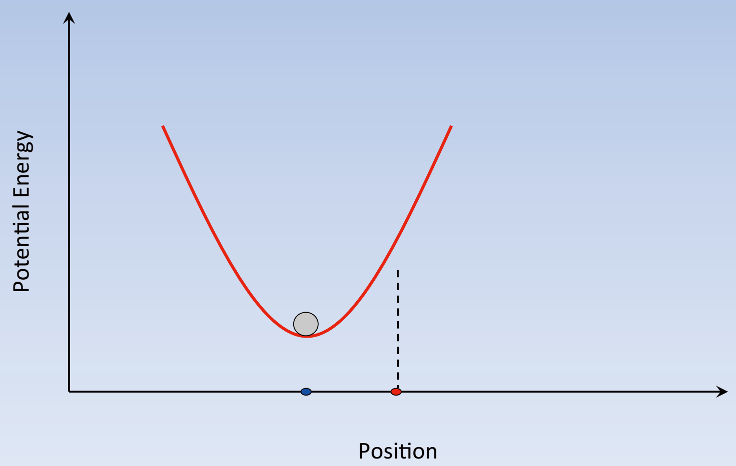
Typical time resolved experiment utilizes intrinsic synchronization between pump excitation and probe



Electro-Optic Sampling (EOS) delivers arrival time to users

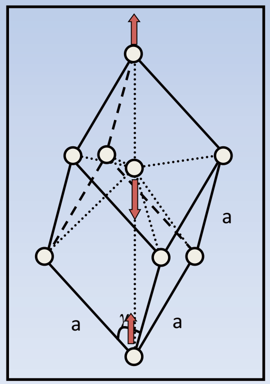
- Pump-Probe experiments now possible at XFELs
- Machine jitter exploited to sample time-dependent phenomena

Displacive Excitation



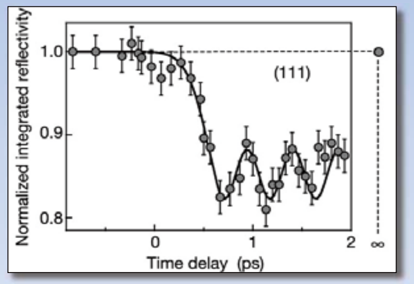
Dynamics of high amplitude coherent optical phonons

Bi structure

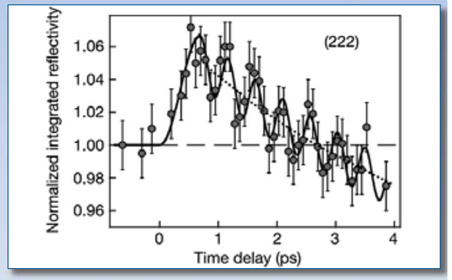


X-rays diffraction – direct probe of atomic motion

111 forbidden in simple cubic

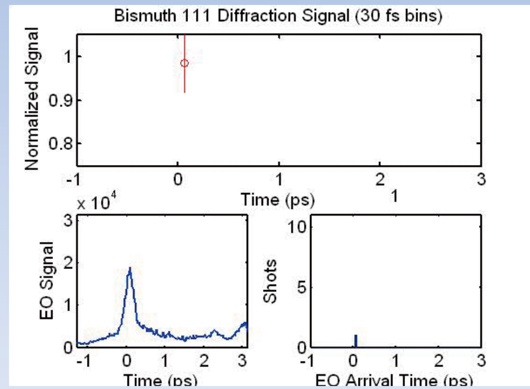


222 “perfect” in simple cubic



Sokolowski-Tinten *et al.*, Nature, 422 (2003)

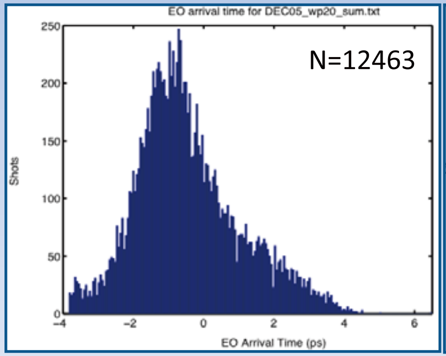
Using the jitter at SPPS for Random Sampling



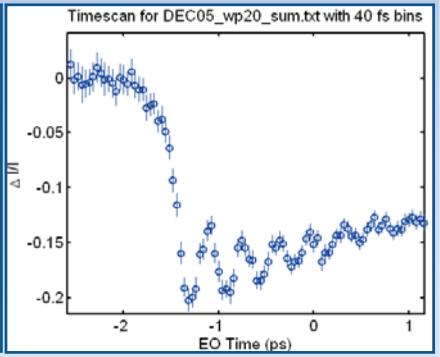
Ultrafast Bond Softening in Bismuth: Mapping a Solid's Interatomic Potential with X-rays D. M. Fritz *et al.* *Science* **315**, 633 (2007)

Using the jitter at SPPS for Random Sampling

1.74 mJ/cm^2 (absorbed), <n>~1% f =2.5 THz* A = 0.92 pm <Δx> = 5pm



Arrival time distribution

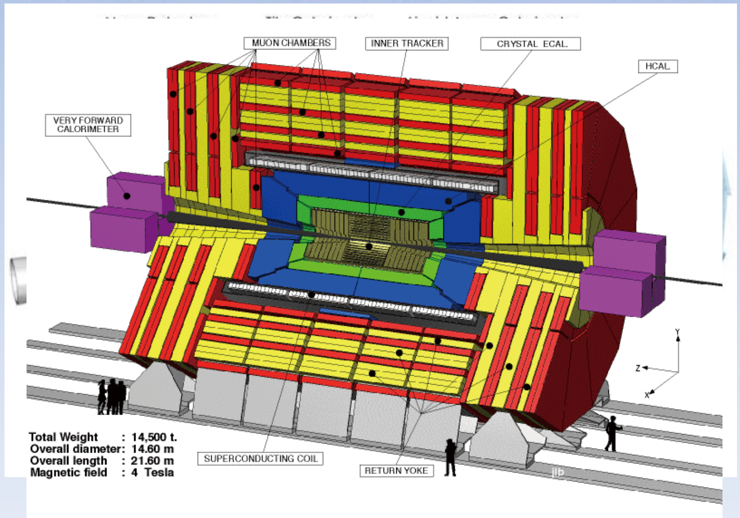


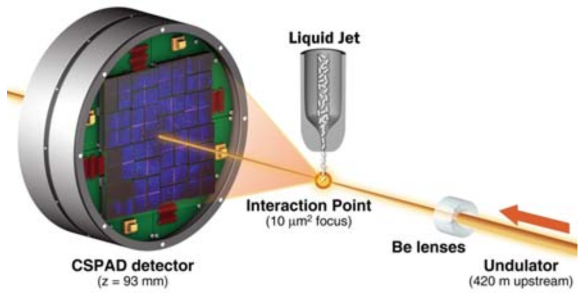
Sorted normalized data

Ultrafast Bond Softening in Bismuth: Mapping a Solid's Interatomic Potential with X-rays D. M. Fritz *et al.* *Science* **315**, 633 (2007)

Free Electron Lasers: What’s so special?

The challenge:
Fit these detectors into an LCLS Hutch





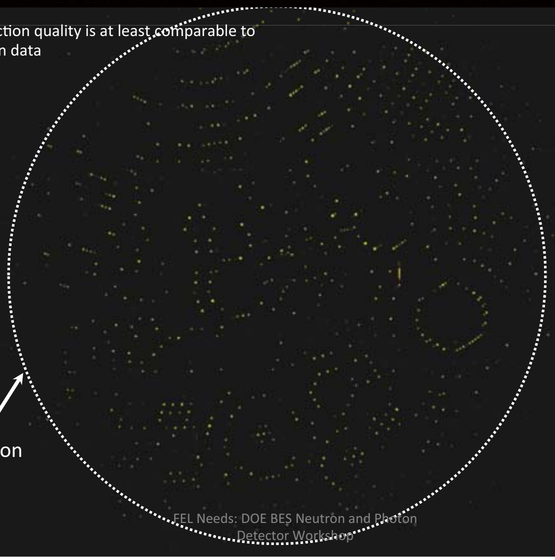
Photosystem I Single Nanocrystal at CXI

Nanocrystal diffraction quality is at least comparable to that of synchrotron data

9.3 keV

40 fs

Single shot

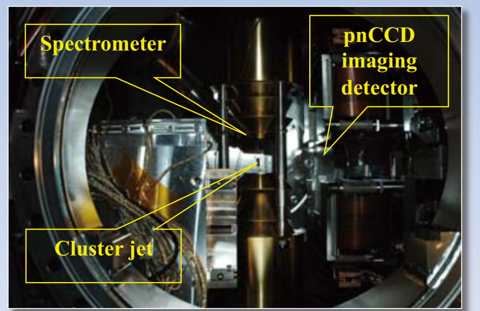


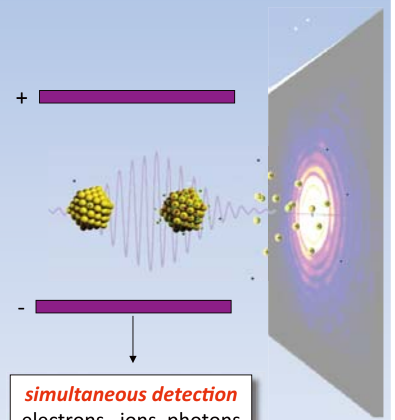
3.5 Å resolution

S. Boutet SLAC

FEL Needs: DOE BES Neutron and Photon Detector Workshop

CAMP Chamber





simultaneous detection
electrons, ions, photons
Single shot recording

L. Strüder et al. Nucl. Instr. Meth. A 610, 483 (2010)

LCLS Dynamics in Clusters

LCLS / SLAC
Christoph Bostedt (PI), John Bozek, et al.

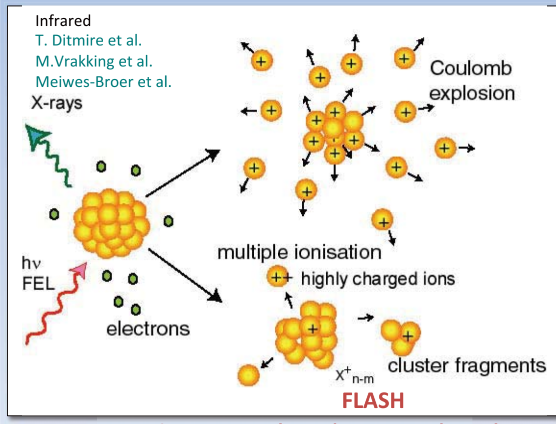
TU-Berlin
Marcus Adolph,
Daniela Rupp,
Sebastian Schorb,
Tais Gorkover,
Thomas Möller

Max-Planck ASG
Sascha Epp,
Lutz Foucar,
Robert Hartmann,
Daniel Rolles,
Artem Rudenko, et al.,

Project leaders: I. Schlichting, L. Strüder, J. Ullrich

FEL SCIENCE

Non-linear cluster ionization



Clusters as „nanolab":
- bulk density
- no energy dissipation
- intra- vs. interatomic effects

Driving questions:
- mechanism of absorption and ionisation
- are non-linear / multi-photo processes observed?
- time scale of electron emission and of ion motion

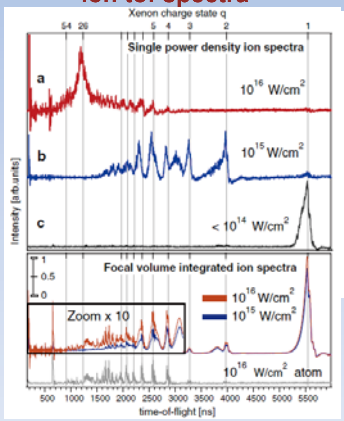
LCLS

λ= 100nm (2002) 13 nm (2005) now 0.7 nm

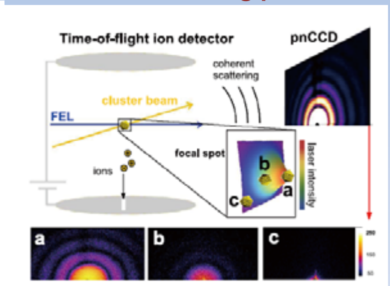
Cluster physics yields insight into fundamental questions of the light – matter interaction

Many vs. single cluster ionization

ion tof spectra



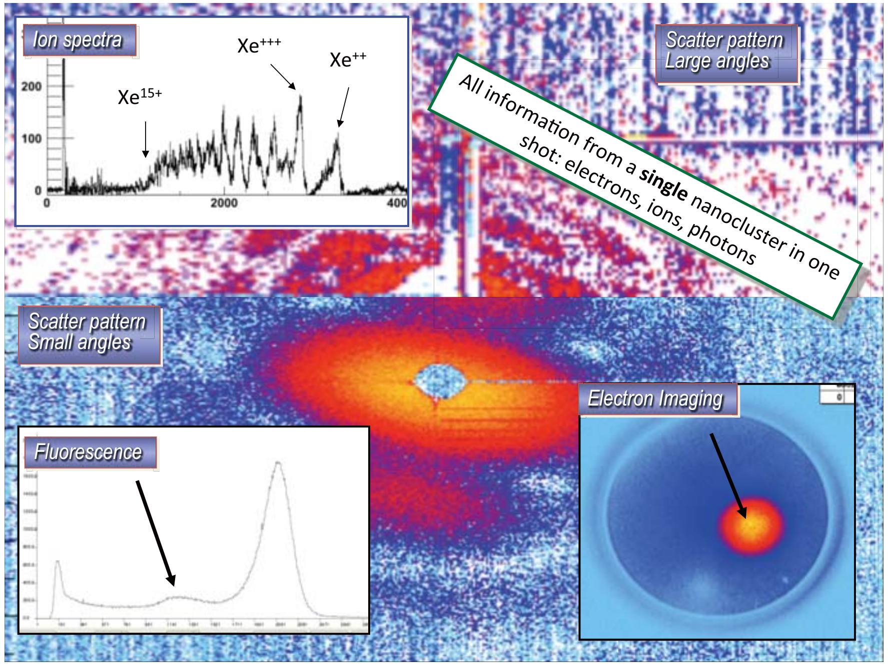
scattering pattern



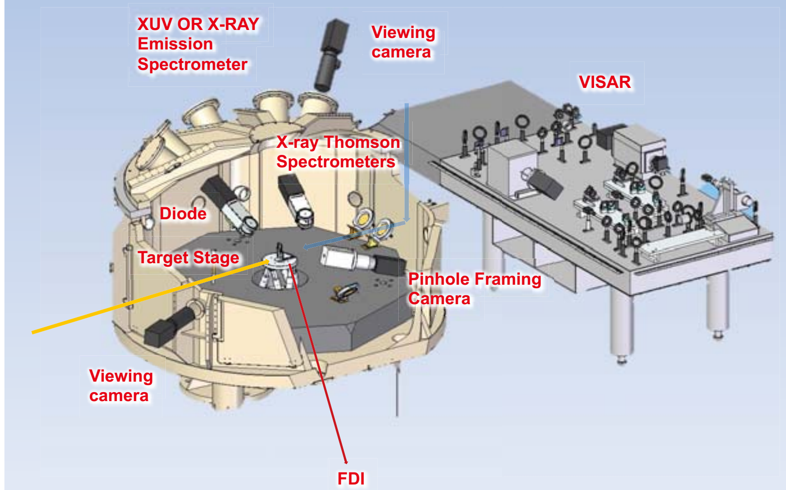
Coincident spectroscopy and imaging allows deconvolution of focal volume and size distribution

Nanoplasma dynamics are very sensitive to power density: for highest density recombination suppressed

Gorkhover et al., Phys. Rev. Lett. 108, 245005 (2012).



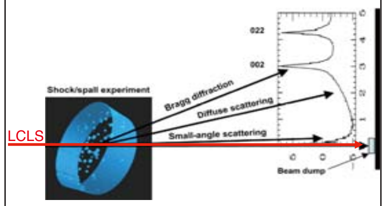
MEC Instrument: Target Chamber and Diagnostics



SAX, WAX simultaneously

Future:

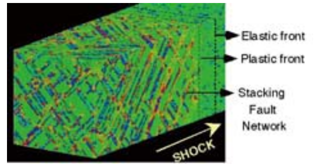
Same measurements during shock



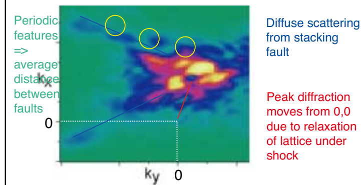
- LCLS will provide unprecedented fidelity to measure dynamics of the microstate with sub-picosecond resolution

Current Status

Elastic Scattering

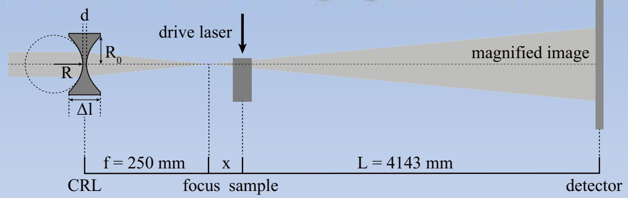


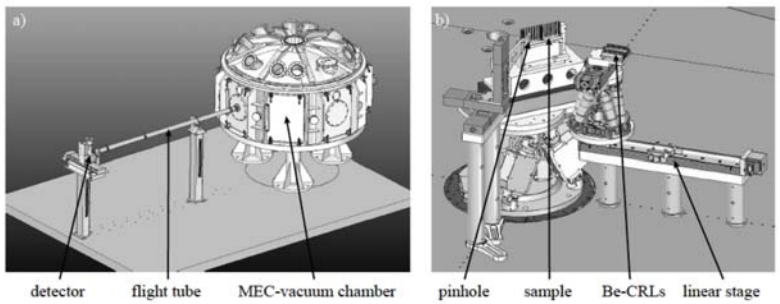
- MD simulation of FCC Cu taking 400,000 CPU hours



- X-ray diffraction image using LCLS probe of the (002) shows *in situ* stacking fault information

Phase contrast imaging of shock waves





Phase Contrast Imaging of shock waves: A. Schropp et al., unpublished

Phase contrast imaging of shock waves

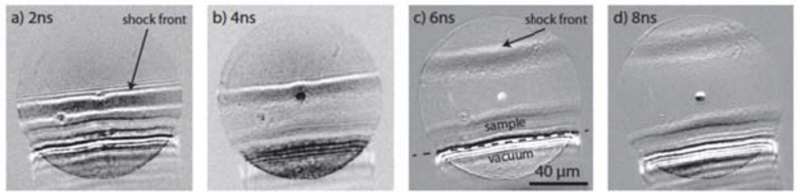


Figure 1: Shock wave in glass for different time delays. Specific values are indicated in each image.

Phase Contrast Imaging of shock waves: A. Schropp et al., unpublished

X-ray/optical SFG experiment: The idea

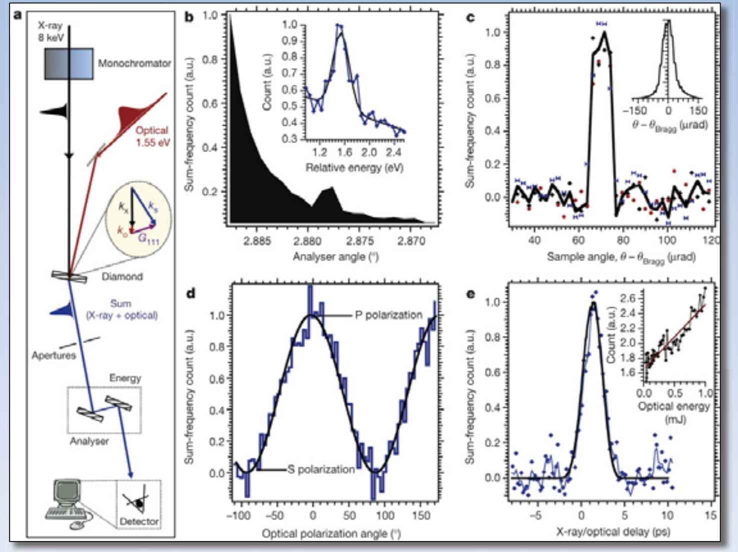
PHYSICAL REVIEW A VOLUME 3, NUMBER 3 MARCH 1971

Mixing of X-Ray and Optical Photons

P. M. Eisenberger and S. L. McCall
Bell Telephone Laboratories, Murray Hill, New Jersey 07974
(Received 26 August 1970)

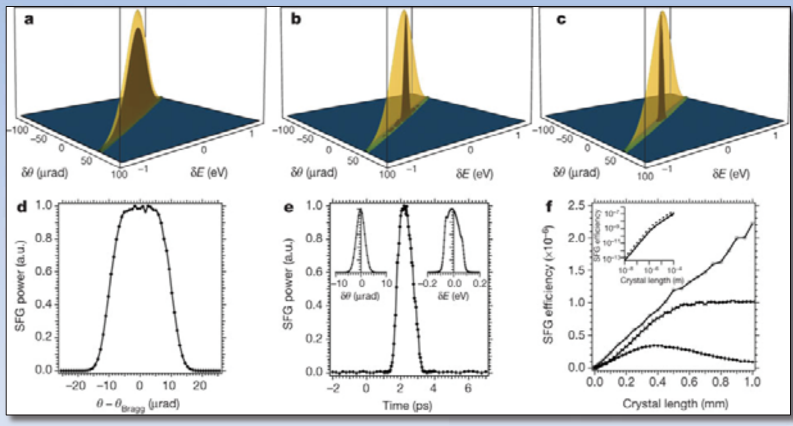
Nonlinear effects involving x-ray and optical photons are described with particular emphasis on the generation of sum and difference frequencies. Efficiencies for sum and difference frequency generation are calculated and found to be large enough to be observable. The expected advent of x-ray lasers should enhance the usefulness of such mixing techniques in the measurement of excited-state wave functions. Under favorable circumstances, the mixing technique may provide a means of efficiently tuning x-ray laser outputs.

X-ray/optical SFG experiment.



TE Glover et al. Nature **488**, 603-608 (2012)

Wave equation simulations.

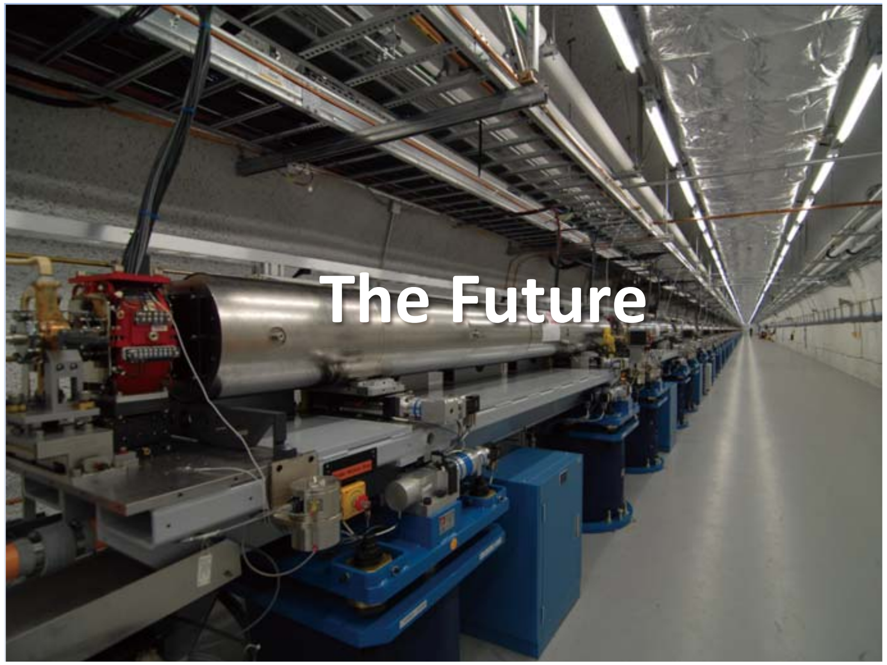


T=1μm
3.7μrad, 970 meV

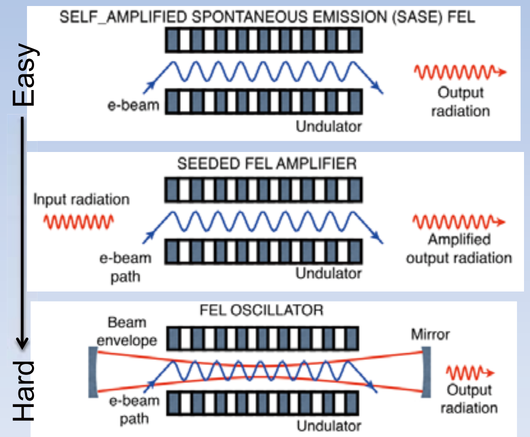
T=10μm
3.7μrad, 210 meV

T=500μm
3.7μrad140meV

TE Glover et al. Nature **488**, 603-608 (2012)



Options for X-Ray Free Electron Lasers



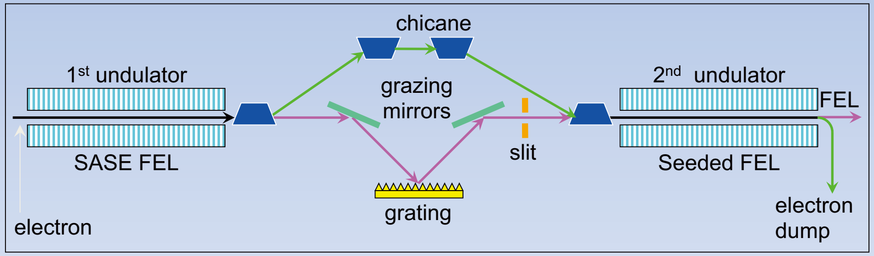
LCLS USA
SACLA Japan
FLASH Germany
XFEL Germany
SWISSFEL Switzerland
PAL FEL Korea

FERMI Italy
FLASH-II Germany
HXRSS LCLS

Proposal ANL USA

Introduction to the Physics of Free Electron Lasers
Kwang-Je Kim (ANL) and Zhirong Huang (SLAC)

Seeded FEL Concept

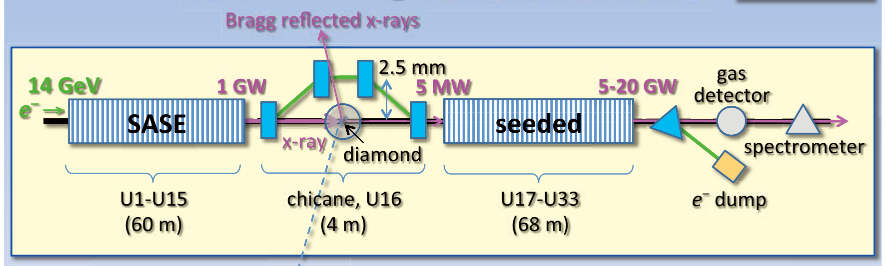


J. Feldhaus , E.L. Saldin, J.R. Schneider, E.A. Schneidmiller, M.V. Yurkov , "Seeded FEL concept possible application of X-ray optical elements for reducing the spectral bandwidth of an X-ray SASE FEL" Opt. Comm. **140**, 341 (1997)

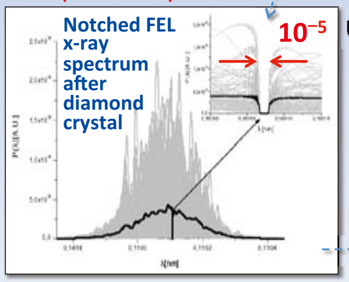
LCLS Hard X-ray Self Seeding Overview

- Great idea from ***DESY:***
  Geloni, Kocharyan, Saldin, *DESY 10-133*, Aug. 2010
- ***SLAC*** collaboration with ***ANL/APS*** & ***TISNCM*** (Moscow)
- Remove 16th undulator segment (of 33 total)
- Replace with 4-dipole chicane & diamond monochromator
- Transmitted (monochromatic) x-rays seed 2nd half of FEL
- Generates 5×10^{-5} BW (narrowed by 50) at 1.5 Å wavelength
- Switched **on** or **off** at any time allowing SASE mode
- Chicane also serves as phase shifter (for SASE)
- System installed Jan. 3-6 and commissioned Jan. 7-12, 2012

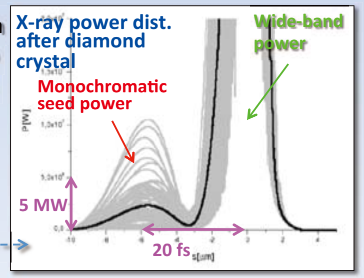
Self-Seeding Scheme @ *LCLS*



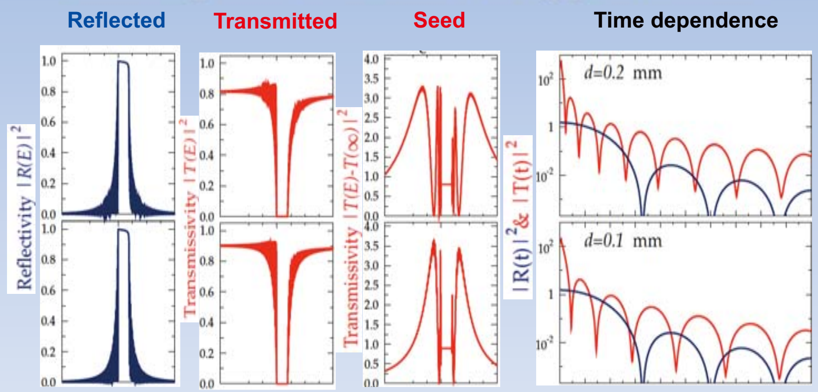
Geloni, Kocharyan, Saldin (*DESY 10-133*)

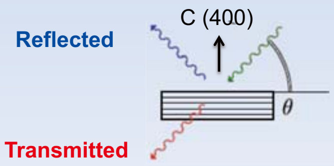


Use 10-fs bunch (low charge) to self-seed 1.5 Å (20-40 pC)



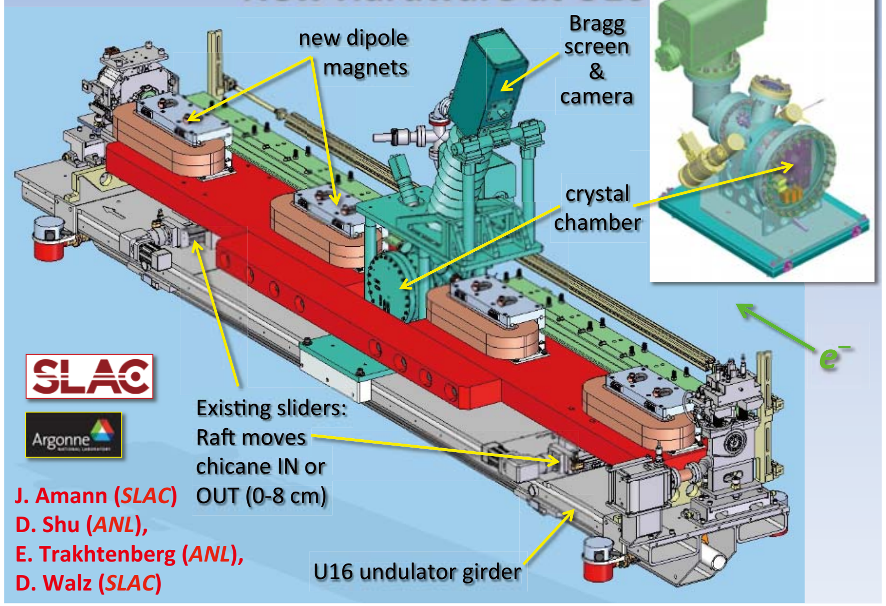
Seeding due to forward Bragg diffraction





R. Lindberg, Y. Shvyd'ko, PRSTAB 2012

New Hardware at U16



The Diamond Crystal and Positioning System

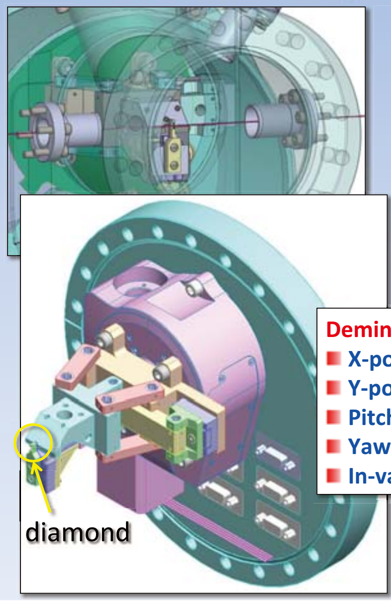
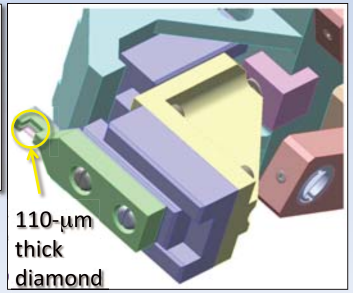


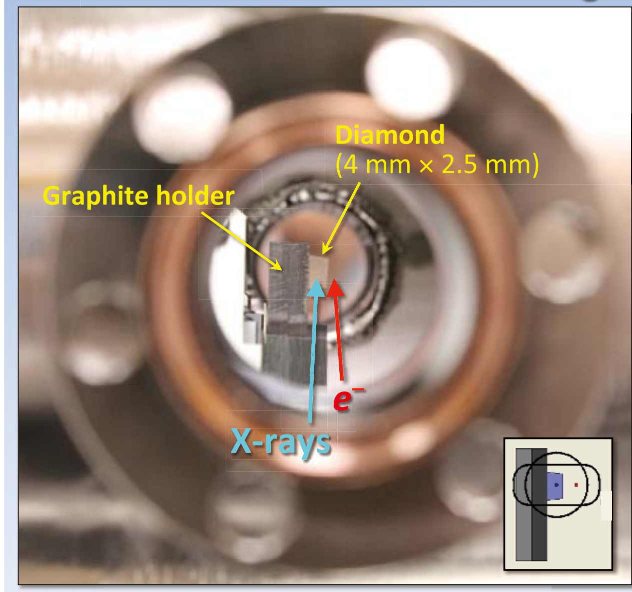
Table 6. Crystal chamber, YAG diagnostic, and crystal positioning parameters.

parameter	value	units
x and y position full control range	±2	mm
x and y position settability (rms)	<0.05	mm
crystal extraction range (approx).	0 - 10	mm
crystal pitch angle full control range	45 - 95	deg
pitch angle settability (rms)	<0.005	mrad
crystal yaw (optional) angle control range	±3	deg
crystal yaw (optional) angle settability (rms)	<0.010	mrad
crystal temperature stability	~1	degC
screen and camera position resolution	<0.02	mm
expected rms spot size on screen	30-50	µm
max. camera update rate	≥10	Hz

Deming Shu (*ANL*)
- **X-pos control**
- **Y-pos control**
- **Pitch angle ctrl**
- **Yaw angle ctrl**
- **In-vac. stages**



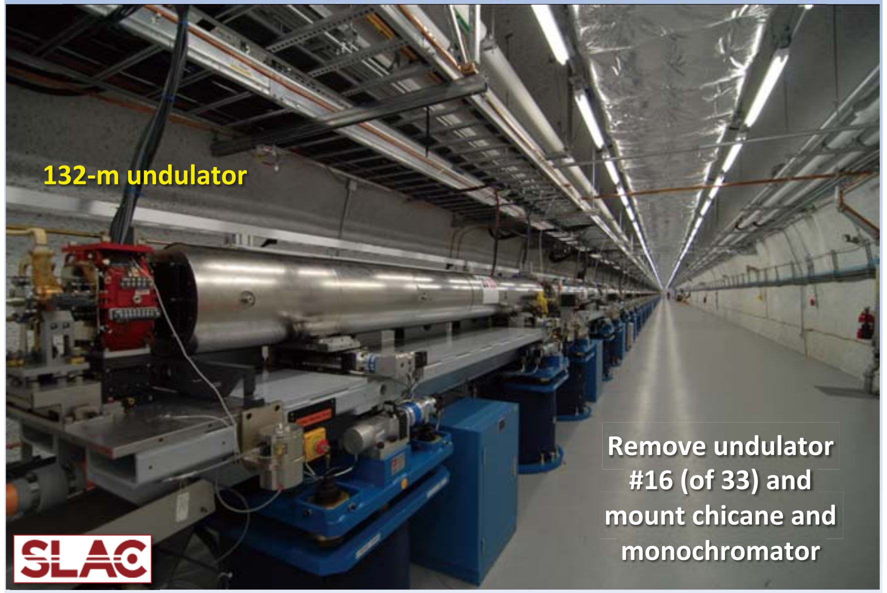
Diamond & Holder Seen Through Beam Pipe



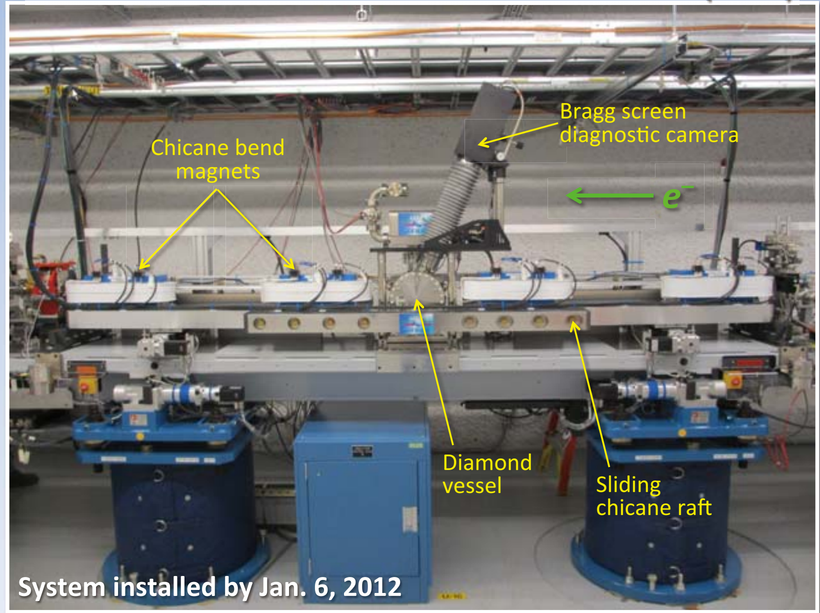
Crystal is high quality **110-µm thick** type-IIa diamond crystal plate with (004) lattice orientation.

Grown from high-purity (99.9995%) graphite at the *Technological Institute for Super-hard and Novel Carbon Materials* (**TISNCM**, Troitsk, Russia) using the temperature gradient method under high-pressure (5 GPa) and high-temperature (~1750 K) conditions.

LCLS Undulator (33 4-m segments, 132 m long)

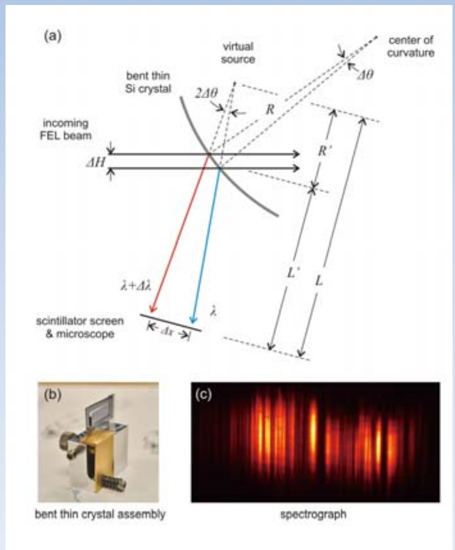


Chicane and Monochromator at Undulator #16 (of 33)



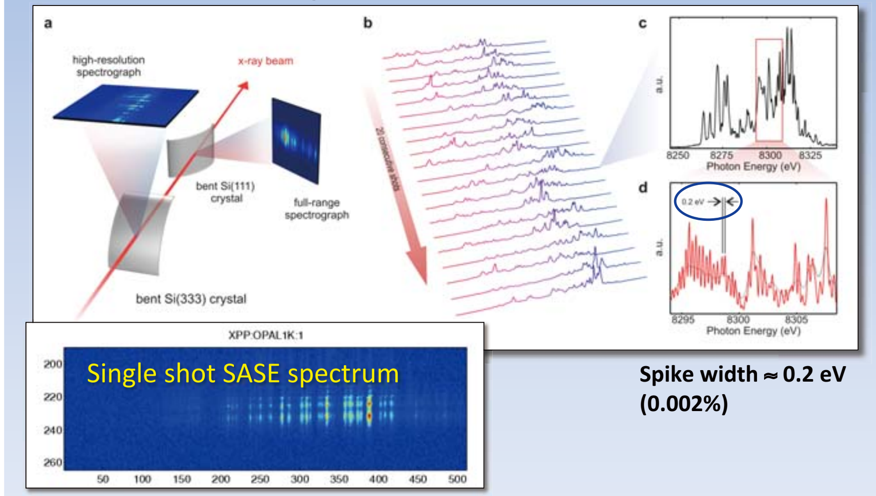
Hard X-ray Spectrometer

Single-shot and Transmissive



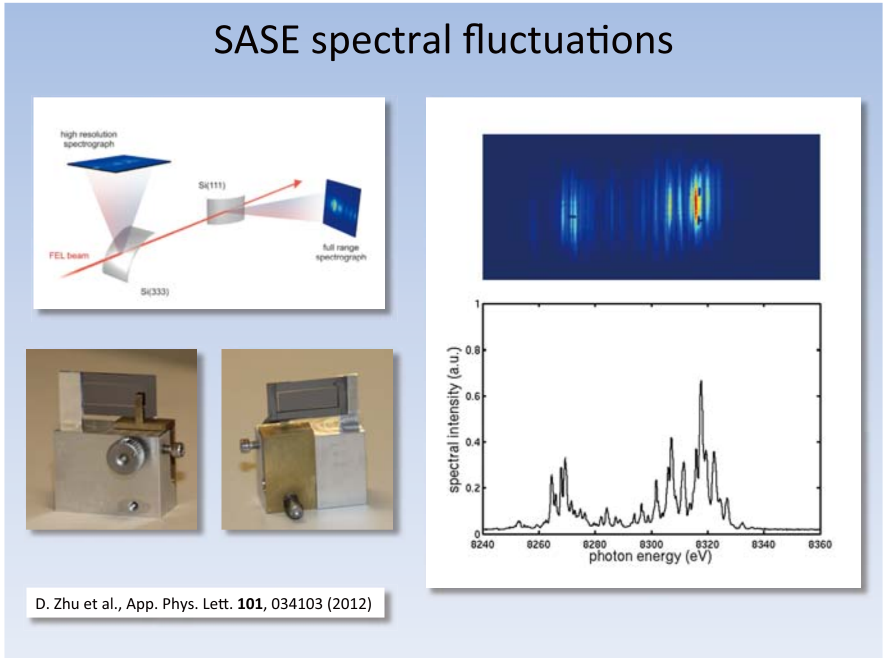
Hard X-ray Spectrometer

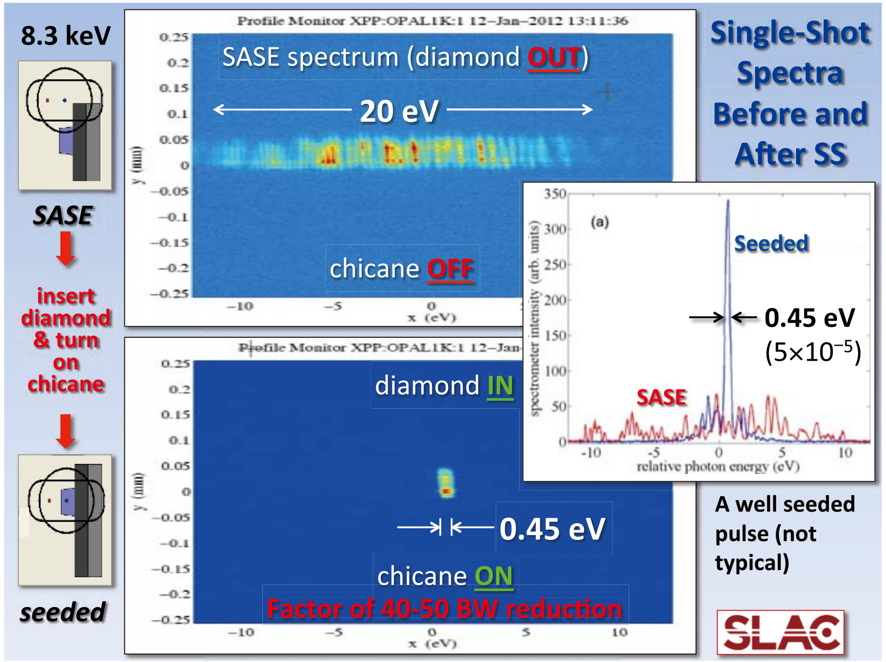
Single-shot and Transmissive

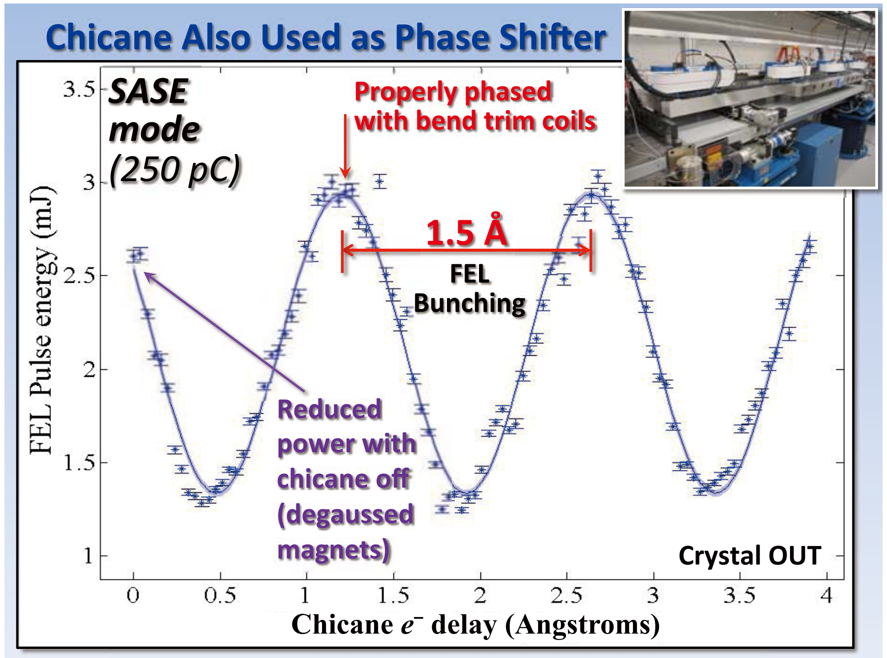


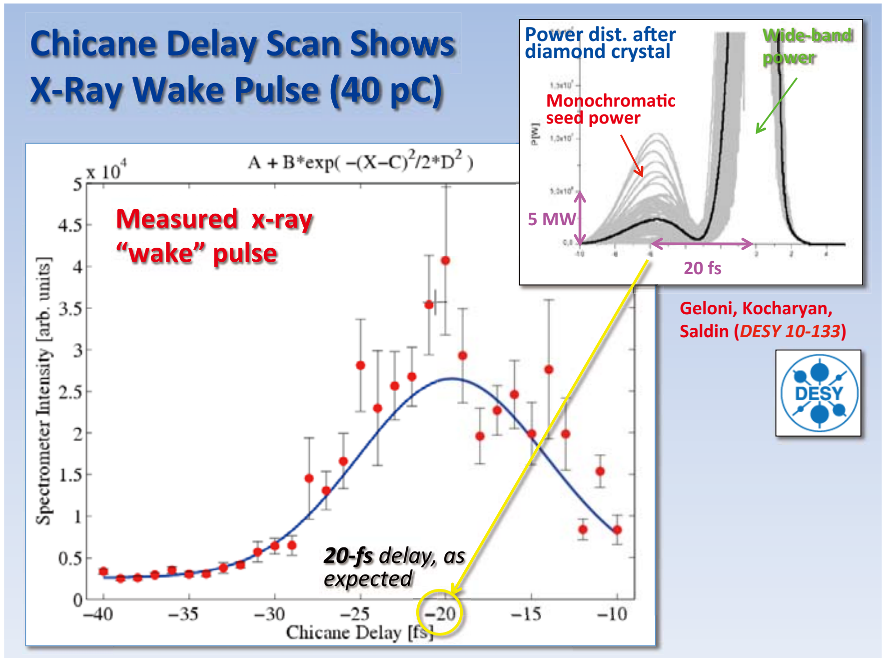
Spike width ≈ 0.2 eV (0.002%)

D. Zhu, M. Cammarata, J. Feldkamp, D. Fritz, J. Hastings, S. Lee, H. Lemke, A. Robert, J. Turner, and Y Feng*

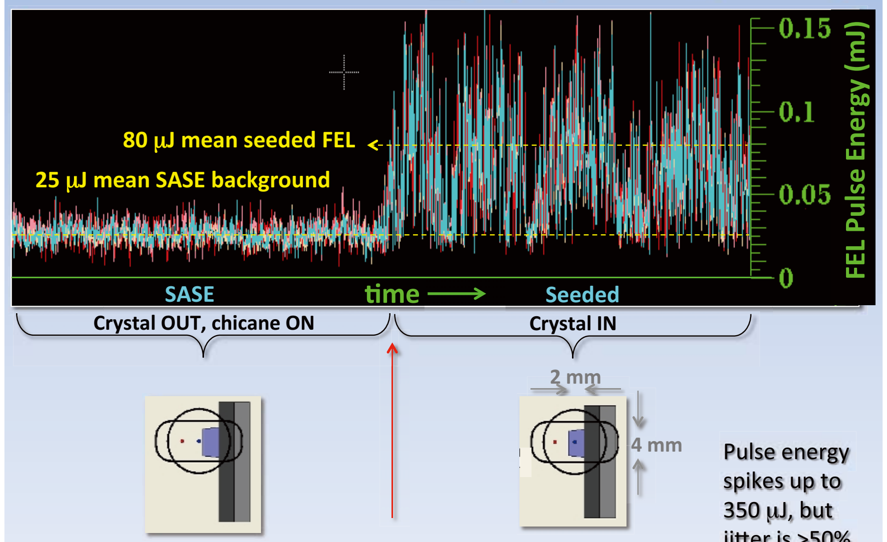

SASE spectral fluctuations
high resolution spectrograph
Si(111)
FEL beam
Si(333)
full range spectrograph
spectral intensity (a.u.)
photon energy (eV)
D. Zhu et al., App. Phys. Lett. 101, 034103 (2012)


8.3 keV
SASE
insert diamond & turn on chicane
seeded
SASE spectrum (diamond OUT)
20 eV
chicane OFF
diamond IN
0.45 eV
chicane ON
Factor of 40-50 BW reduction
Seeded
0.45 eV
(5×10⁻⁵)
SASE
relative photon energy (eV)
Single-Shot Spectra Before and After SS
A well seeded pulse (not typical)
SLAC


Chicane Also Used as Phase Shifter
SASE mode
(250 pC)
Properly phased with bend trim coils
1.5 Å
FEL Bunching
Reduced power with chicane off (degaussed magnets)
Crystal OUT
FEL Pulse energy (mJ)
Chicane e⁻ delay (Angstroms)


Chicane Delay Scan Shows X-Ray Wake Pulse (40 pC)
A + B*exp(−(X−C)²/2*D²)
Measured x-ray "wake" pulse
20-fs delay, as expected
Spectrometer Intensity [arb. units]
Chicane Delay [fs]
Power dist. after diamond crystal
Wide-band power
Monochromatic seed power
5 MW
20 fs
Geloni, Kocharyan, Saldin (DESY 10-133)
DESY

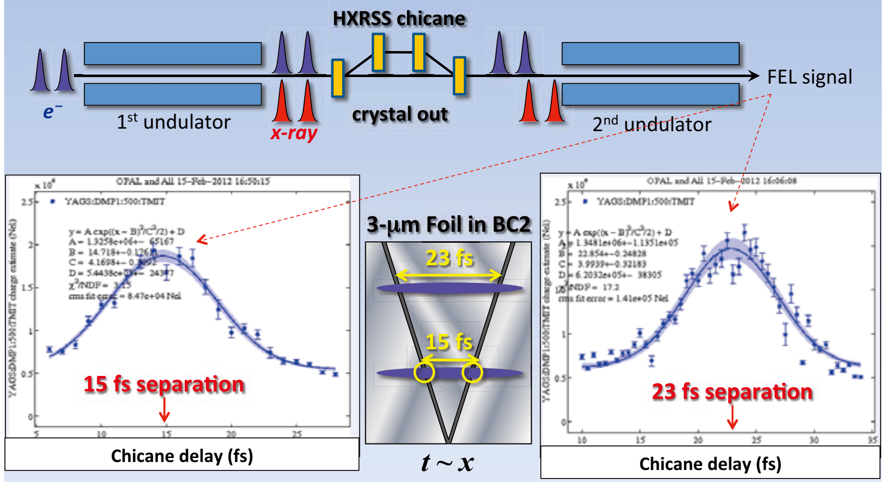
Seeded Power & SASE Power (40 pC, well tuned, U1 OUT)



Pulse energy spikes up to 350 μJ, but jitter is >50%

Crystal inserted here (1.5-mm position change)
[chicane is always ON in this plot]

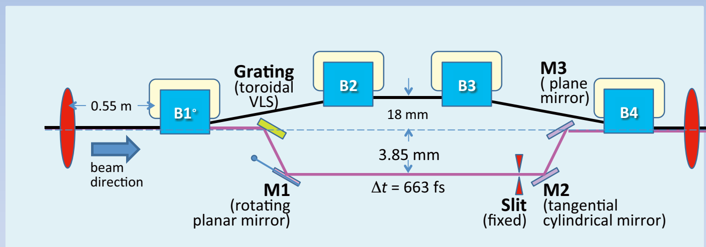
Diagnostic: Cross-correlation of e^- and x-ray pulses



Y. Ding

measured rms pulse duration is <4 fs

Soft X-ray Self Seeding



- Toroidal variable-line-spacing grating G
  - Tangential radius of curvature R_t
  - Sagittal radius of curvature R_s
- Plane post-mirror M1
- Slit
- Cylindrical focusing mirror M2
- Plane mirror M3 for steering

Summary

- Accelerator based x-ray sources are important tools for chemistry, materials science, structural biology and many other fields
- Development of new methods and instruments have been crucial in the development
- New accelerator based sources: the X-ray Free Electron Lasers, LCLS, SACLA and those to come, offer opportunities for future development of methods and instruments
- FELs are require a unique interplay between source and experiment
- ***The future is bright***

THANKS!