Can there be just one ideal x-ray source? A personal view (With x-rays everything is imaging)

J. B. Hastings
SLAC National Accelerator Laboratory

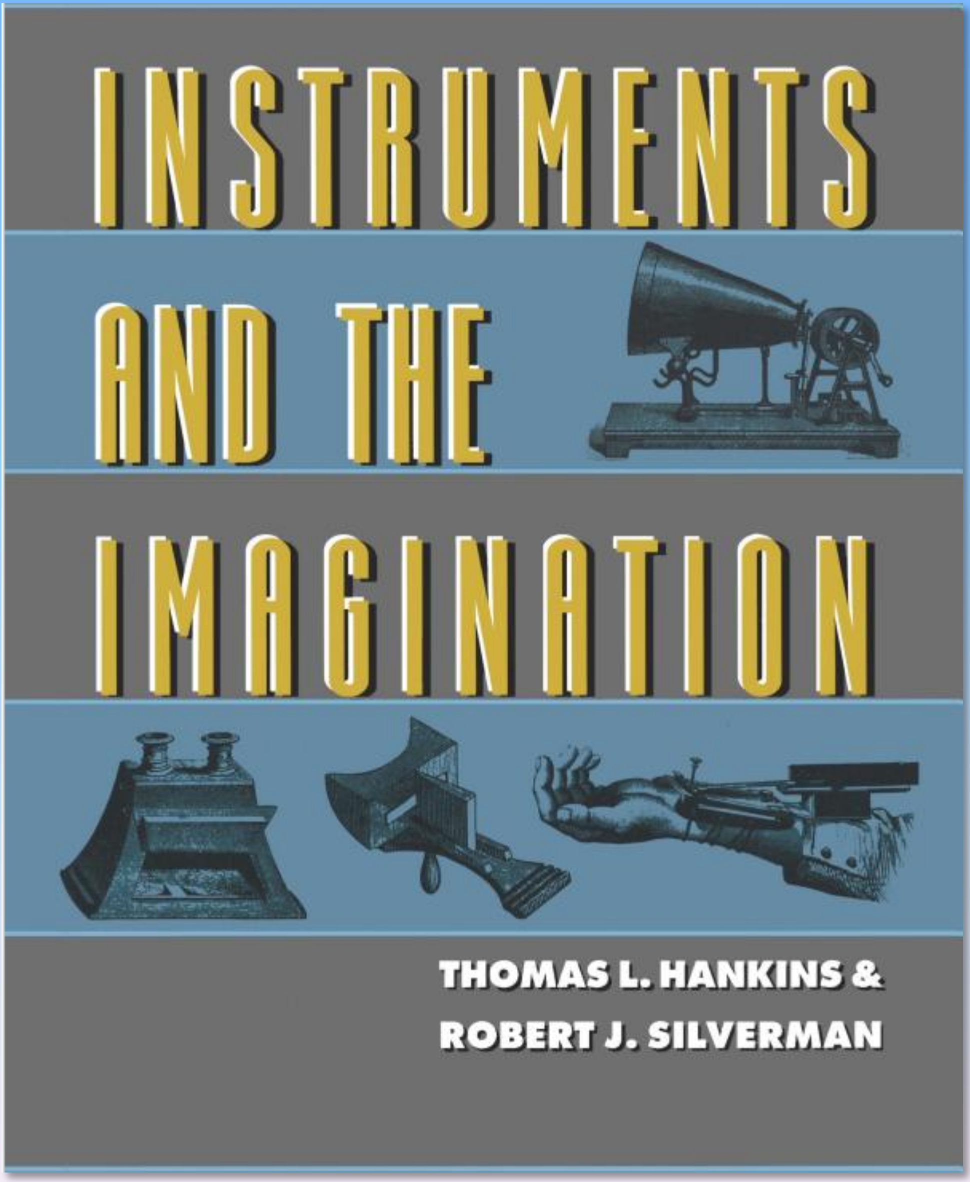
September 19, 2017

No!

Outline

- ***Introduction***
- Imaging in reciprocal space
  - Static structure
  - Dynamics-lattice vibrations
- Imaging in real space
  - Elemental mapping
  - Tomography
- Summary

Science and Scientific Instruments



"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 challenge:
Maximize the number of photons/electron/unit time

The solution:
Free Electron Lasers

The LCLS Proposal… 1992

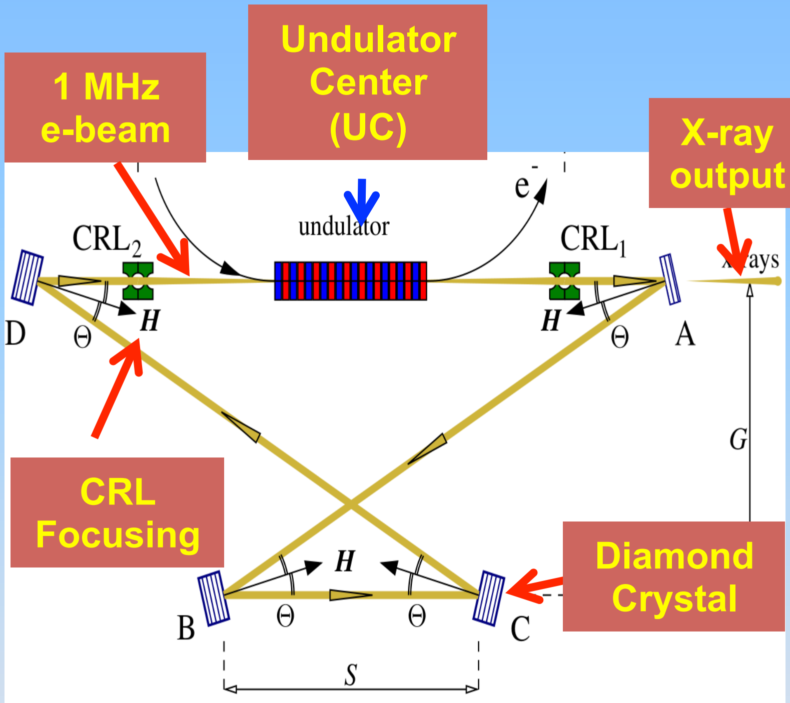
C. Pellegrini, *"A 4 to 0.1 nm FEL based on the SLAC linac"*, in Workshop on 4th Generation Light Sources, M. Cornacchia and H. Winick, (Eds), pp. 364-375, 1992. SSRL-Report-92/02.

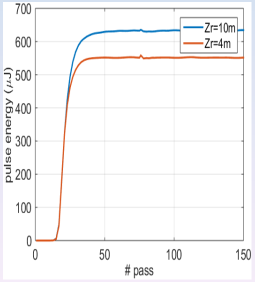
"…one is forced to have high gain, *i.e.* to use electron beams with large peak current, and at the same time small emittance and energy spread. The road to an X-ray FEL requires the development of electron beams with unprecedented characteristics."

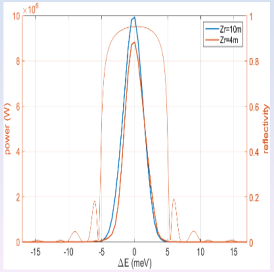
Let's use the X-Ray Free Electron Laser Oscillator (XFELO) as a test case

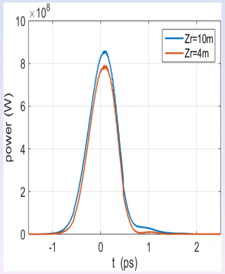
XFELO: Bragg refection for X-ray cavity

(R. Colella & A. Luccio,1983: K. Je-Kim, Y. Shvyd'ko, S. Reiche, 2007
Harmonic lasing, H.X. Deng, 2012)



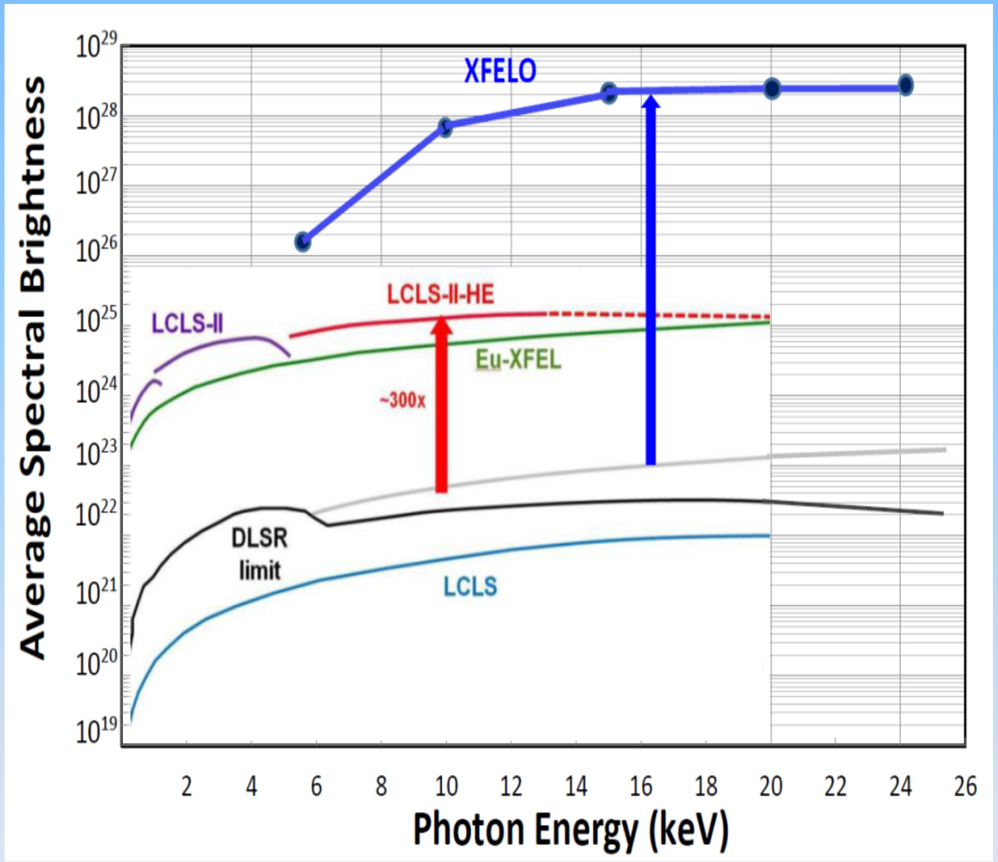






- Works best where Bragg scattering has high reflectivity and large bandwidth--- 5-25 keV
  - High energy, CW accelerator-- SCRF
- ~ 8 GeV SCRF linac with optimized injector (W. Qin)
  - LCLS-II-HE, Shanghai, EuroXFEL conversion
- For 14.4 keV λ_U=2 cm, K=1.49 → SC NbTi : Kmax=3.1→ 5.2 keV

XFELO with 8 GeV linac: B_{av}~ 10^{28} for ε_γ >10 keV



- ~10^{10} photons/pulse
  - ~ 10^{-2} × SASE
- $\Delta\omega/\omega$ ~ 10^{-7}
  - ~ 10^{-4} × SASE
- B~photons/$\Delta\omega/\omega$
  - B (XFELO/SASE) ~100
- For ε_γ >13 keV, XFELO >10^5 ×DLSR
- For 10 keV <ε_γ <13 keV, XFELO >10^3 ×SASE

Brightness units [photons/ (s mm^2 mrad^2 0.1% BW)]

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Observation of X-ray scattering from a crystal (1)

Interferenz-Erscheinungen bei Röntgenstrahlen.

Von **W. Friedrich, P. Knipping** und **M. Laue.**

Vorgelegt von A. Sommerfeld in der Sitzung am 8. Juni 1912.

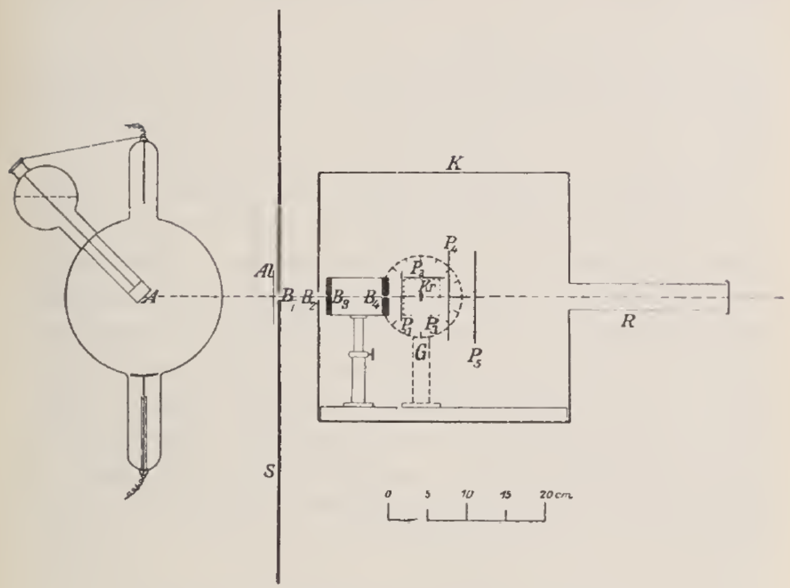
Theoretischer Teil

von **M. Laue.**

Experimenteller Teil

von **W. Friedrich** und **P. Knipping.**

Fig. 1.



Abstand	Antikathode-Kristall	350 mm
„	Kristall-P_1 resp. P_2 resp. P_3 .	25 „
„	Kristall-P_4	35 „
„	Kristall-P_5	70 „

Fig. 9

Observation of X-ray scattering from a crystal (2)

The Reflection of X-rays by Crystals.

By W. H. Bragg, M.A., F.R.S., Cavendish Professor of Physics in the University of Leeds; and W. L. Bragg, B.A., Trinity College, Cambridge.

(Received April 7,—Read April 17, 1913.)

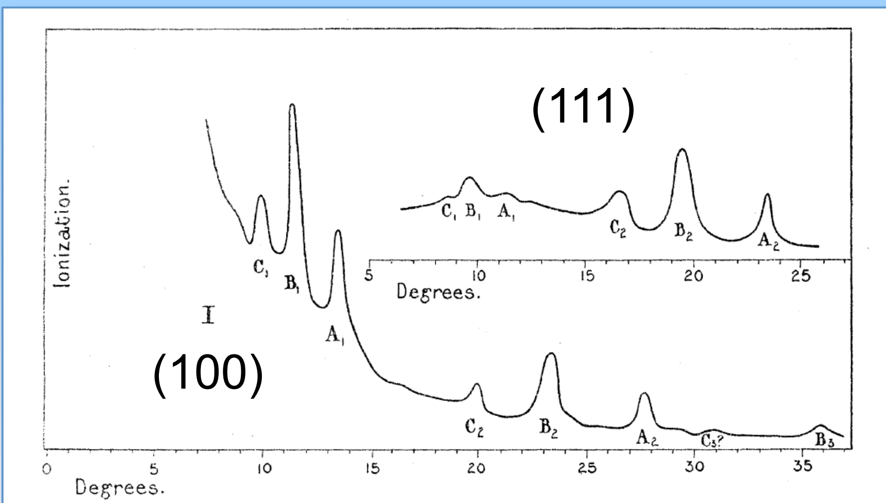


Fig. 3.—Reflection (I) from face (100) and (II) from face (111) of rock-salt. The curves show the variation of strength of reflected beam with angle of incidence.

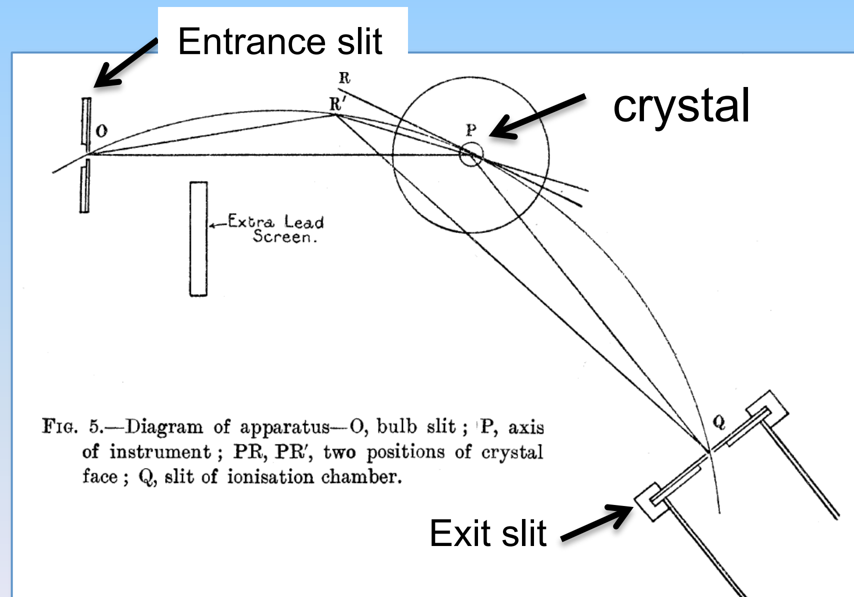


Fig. 5.—Diagram of apparatus—O, bulb slit; P, axis of instrument; PR, PR′, two positions of crystal face; Q, slit of ionisation chamber.

Cleaved NaCl: Faces labeled

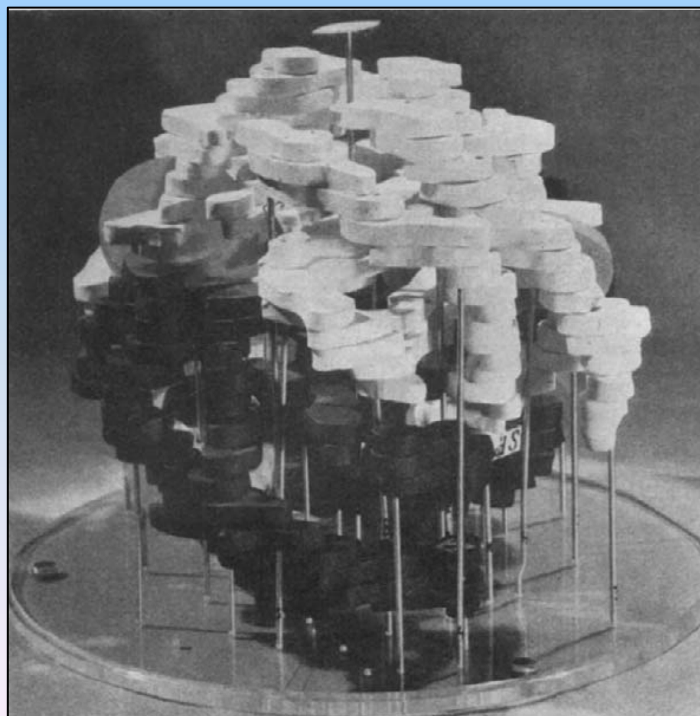
Structural biology: Reciprocal space imaging of macro molecules

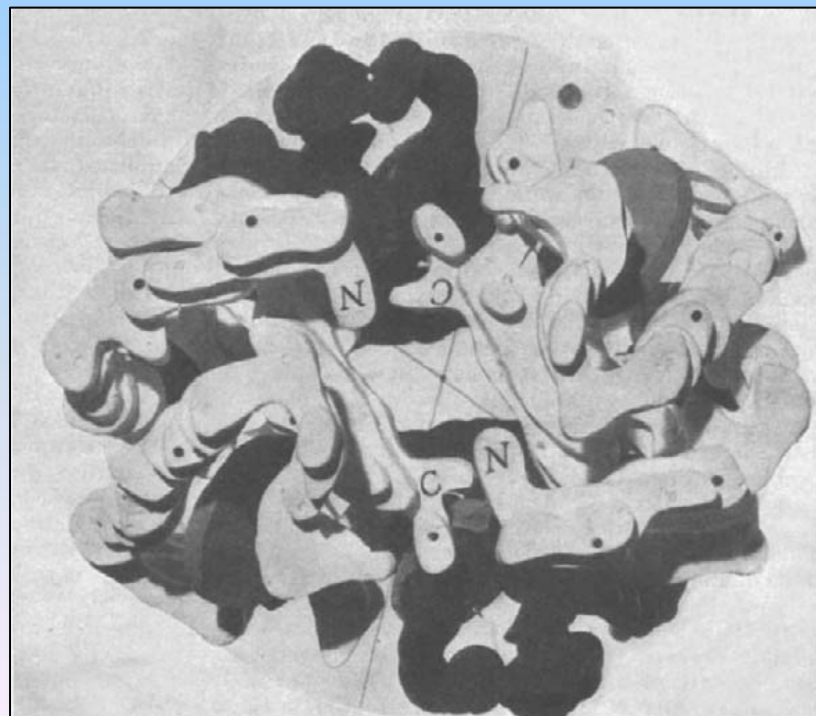
- Perutz et al. Hemoglobin
- SR-parasitic
- MAD phasing
- Serial Femtosecond Crystallography
- Single particle imaging
- Serial crystallography at SR

STRUCTURE OF HÆMOGLOBIN

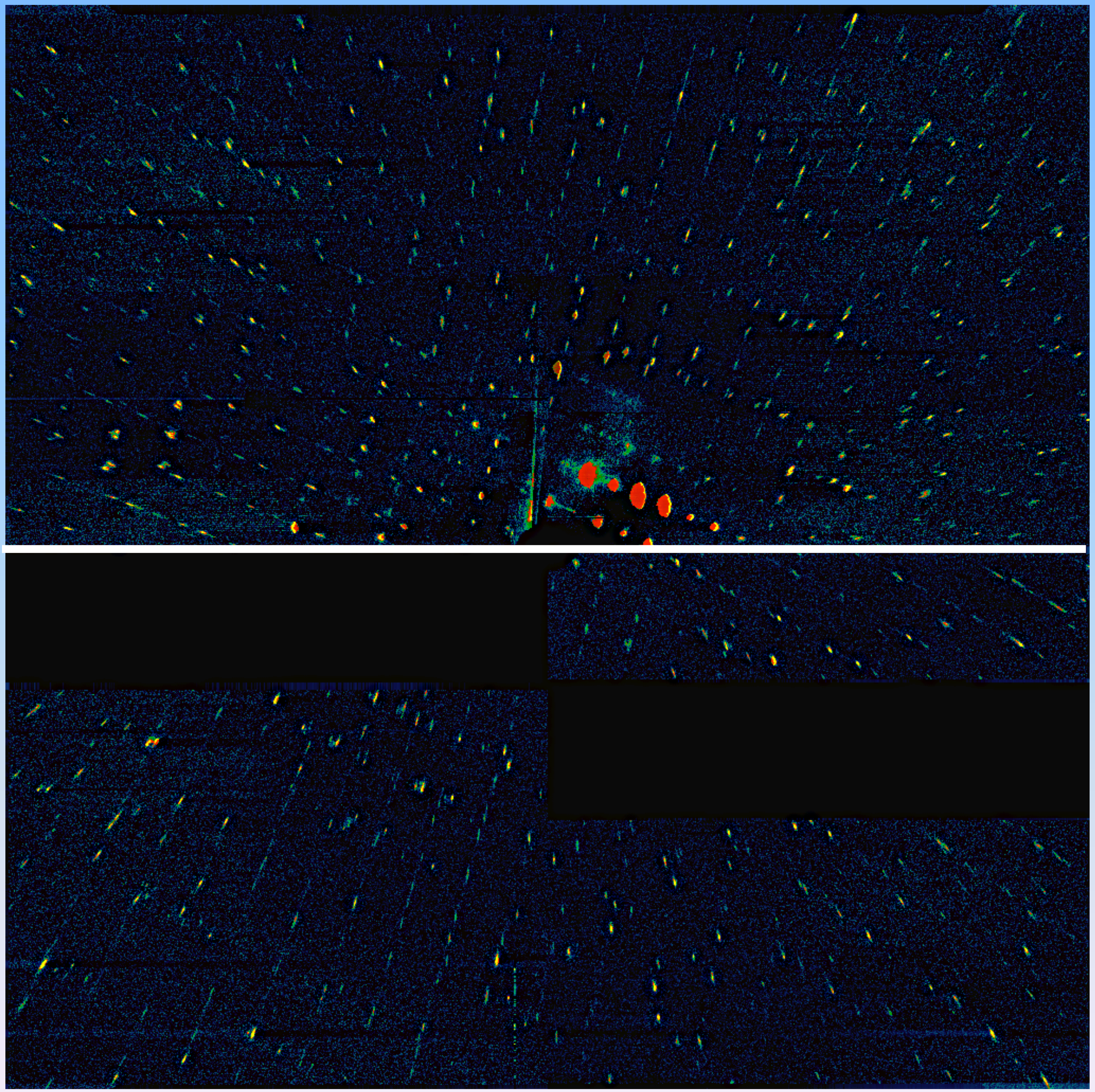
A THREE-DIMENSIONAL FOURIER SYNTHESIS AT 5·5-Å. RESOLUTION, OBTAINED BY X-RAY ANALYSIS

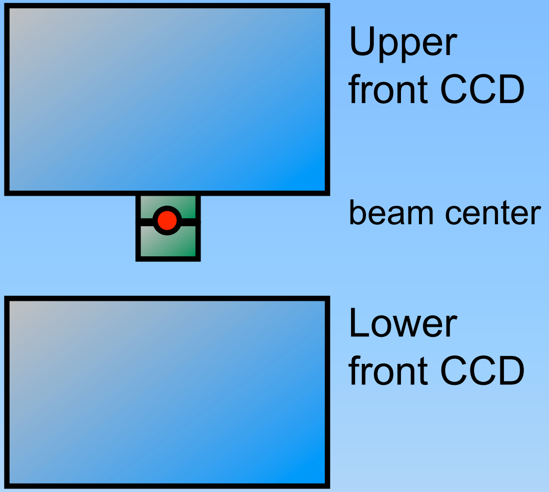
By Dr. M. F. PERUTZ, F.R.S., Dr. M. G. ROSSMANN, ANN F. CULLIS, HILARY MUIRHEAD and Dr. GEORG WILL
Medical Research Council Unit for Molecular Biology, Cavendish Laboratory, University of Cambridge
AND
Dr. A. C. T. NORTH
Medical Research Council External Staff, Davy Faraday Research Laboratory, Royal Institution, London, W.1





Single shot X-ray scattering from a crystal of Photosystem I





Resolution at corner = 8.6Å

Single shot at LCLS
E = 1.8 keV
80 fs pulse
2 mJ pulse energy

H.N. Chapman et al., Nature **470,** 73 (2011)

Lattice dynamics

- Diffuse scattering
- IXS – SR based history
- Time domain

Determination of phonon dispersion in Al: A diffuse x-ray scattering study

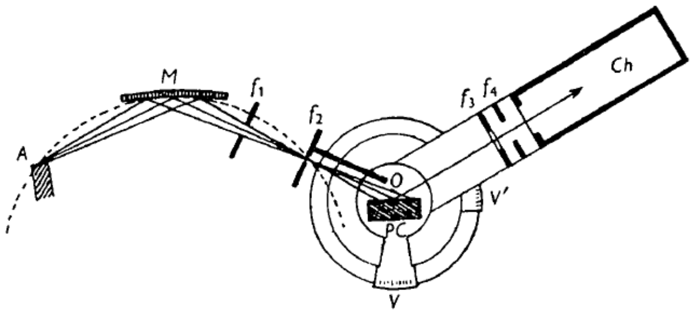
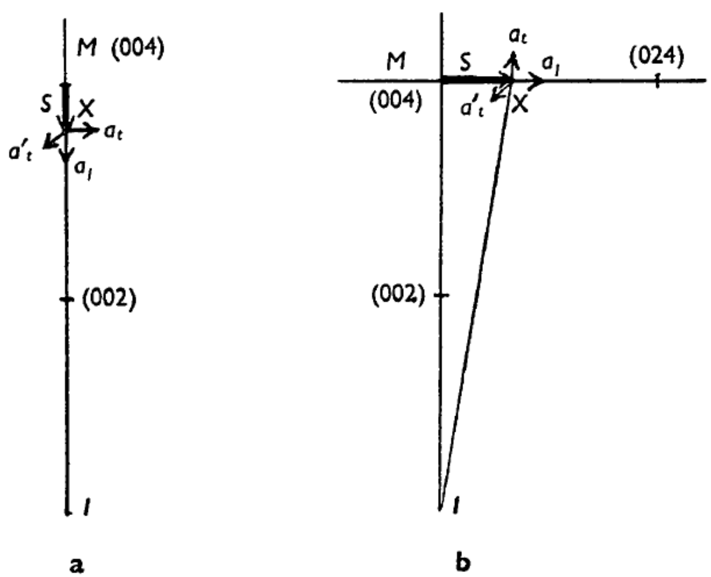


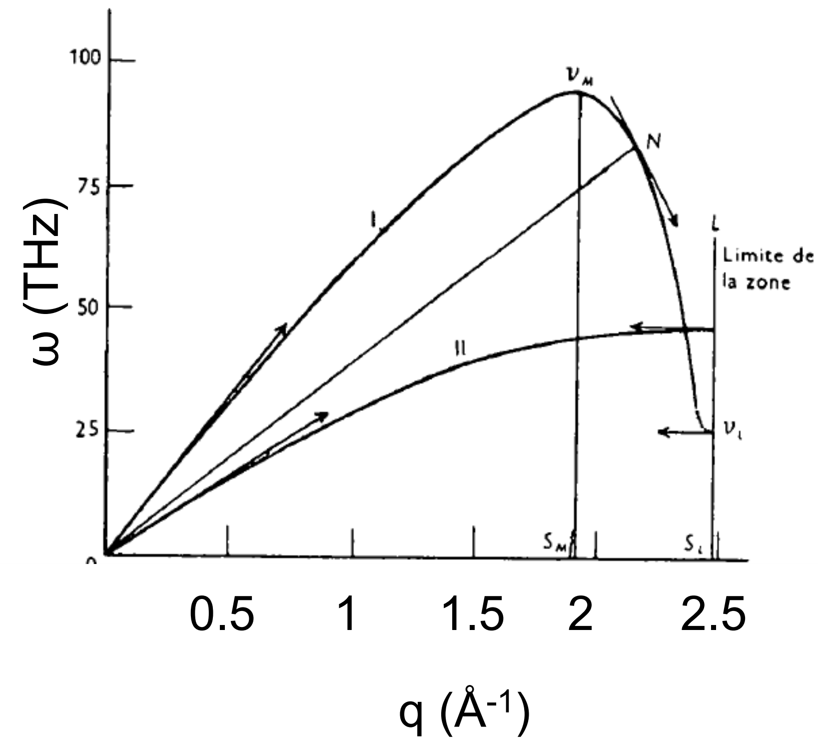
Fig. 1. Schéma général de l'appareillage: *A*, anticathode; *M*, monochromateur; f_1, f_2, f_3, f_4, fentes; *PC*, porte-cristal; *O*, axe du spectromètre; *Ch*, chambre d'ionisation; *V*, *V'*, verniers de lecture.

Acta Cryst. (1948). **1**, 57

Dispersion des Vitesses des Ondes Acoustiques dans l'Aluminium

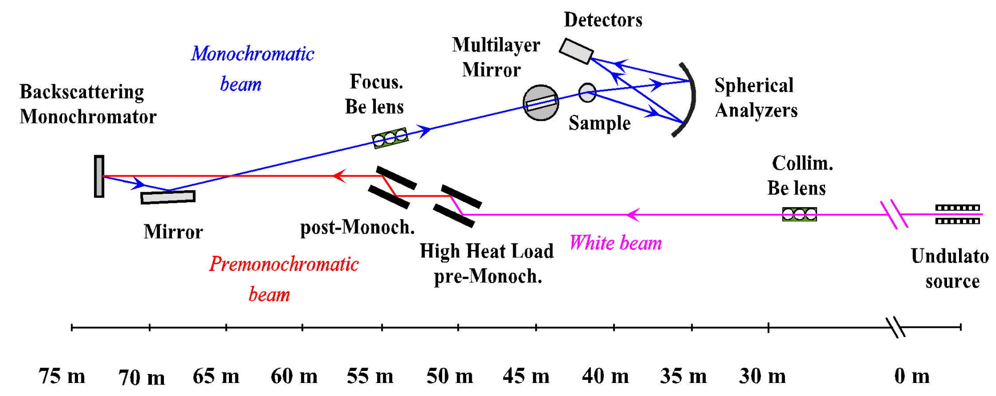
Par Ph. Olmer
Laboratoire de Minéralogie à la Sorbonne, Paris V, France

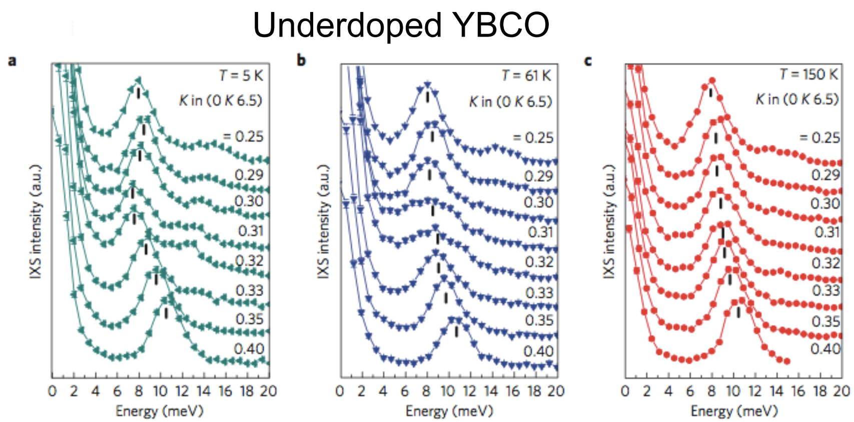




Inelastic X-ray Scattering:

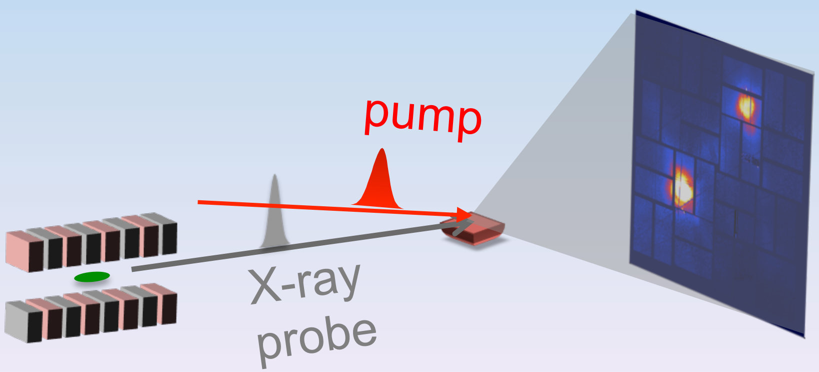
$$S(\vec{Q},\omega) \propto \sum_j \int \mathrm{d}t e^{i\omega t} \langle u_{j,\vec{Q}}(0) u_{j,-\vec{Q}}(t) \rangle$$





M. Le Tacon et. al, Nat. Phys. 10,52 (2014)

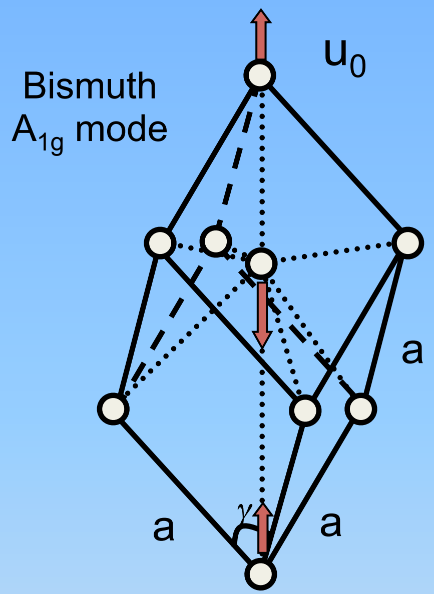
Time and momentum-domain x-ray scattering:

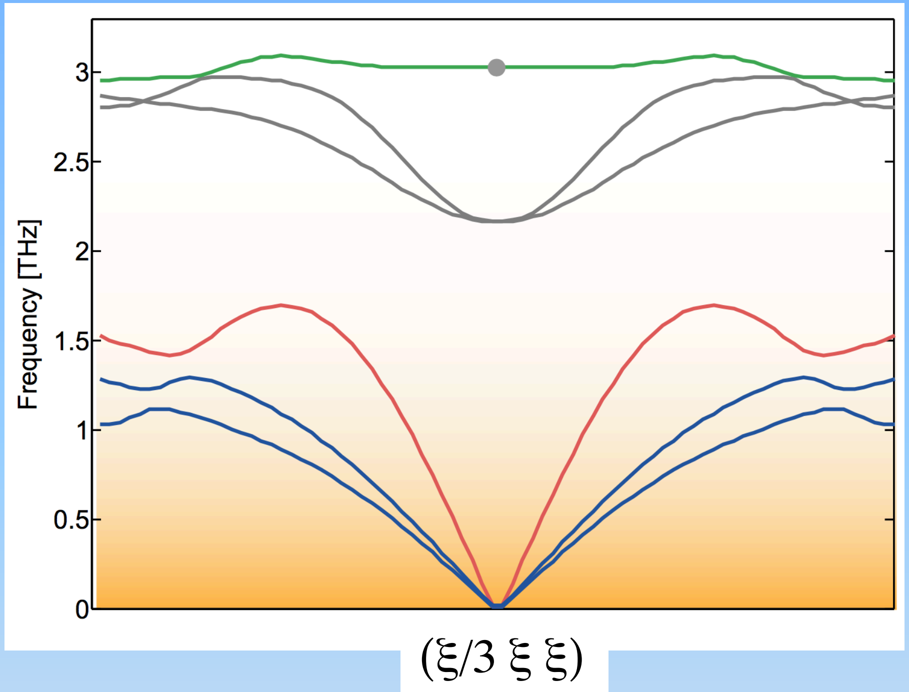


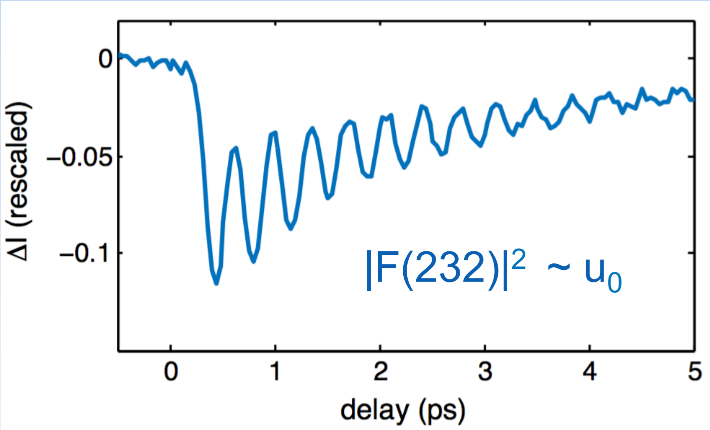
$$S(\vec{Q};\tau) \propto \sum_{j,j'} \langle u_{j,\vec{Q}}(\tau) u_{j',-\vec{Q}}(\tau) \rangle$$

Trigo et al. Nature Physics. 9, 790, 2013

Parametric phonon resonance

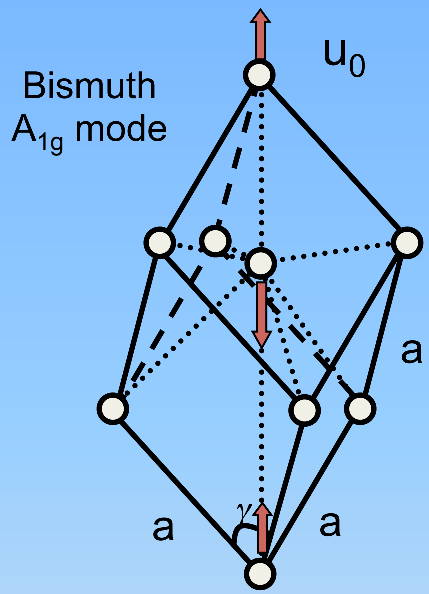


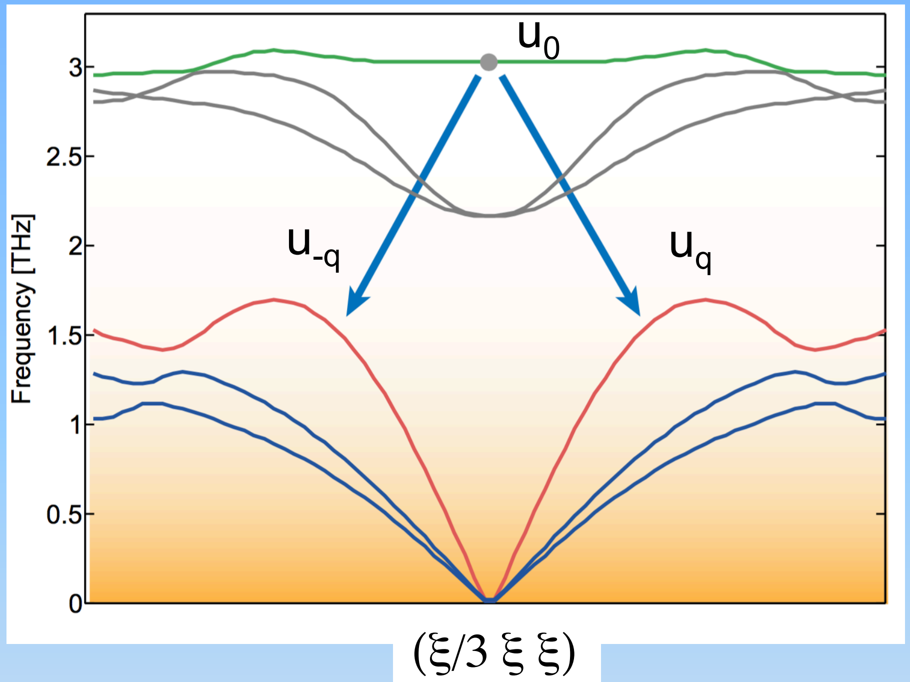


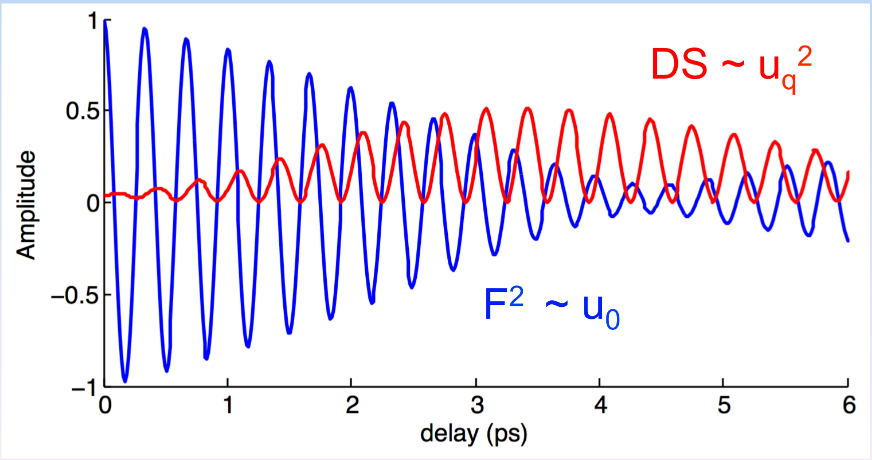


M. Trigo et al.

Parametric phonon resonance





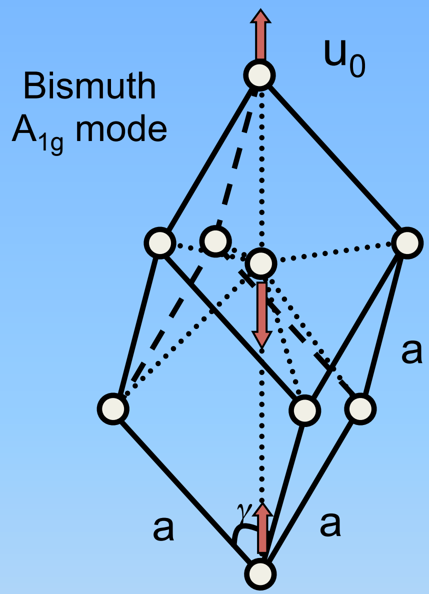


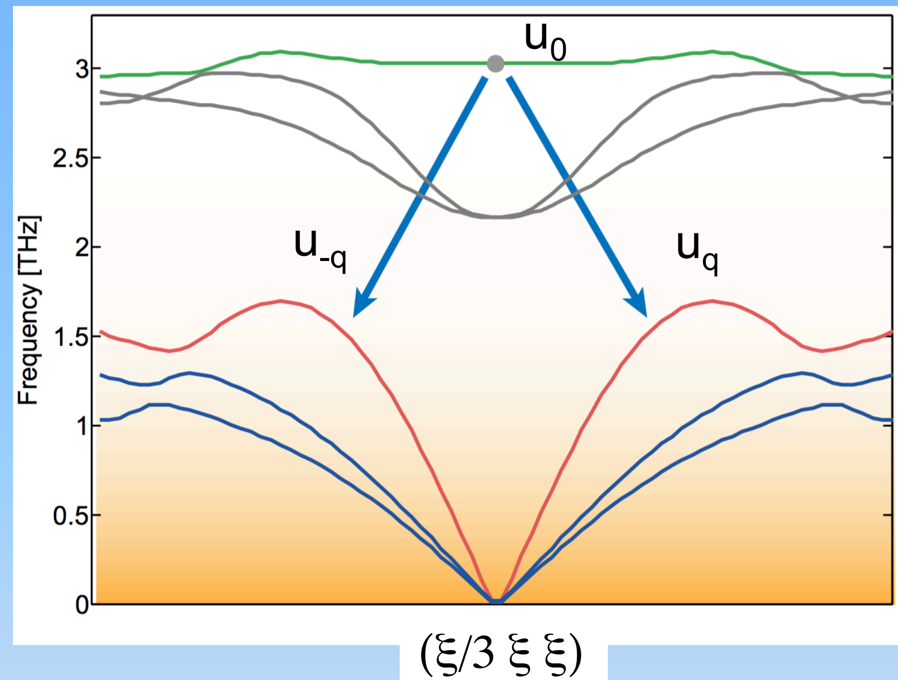
$$\ddot{u}_0 + \Gamma_0 \dot{u}_0 + \omega_1^2 u_0 + g\, u_q^2 = 0$$

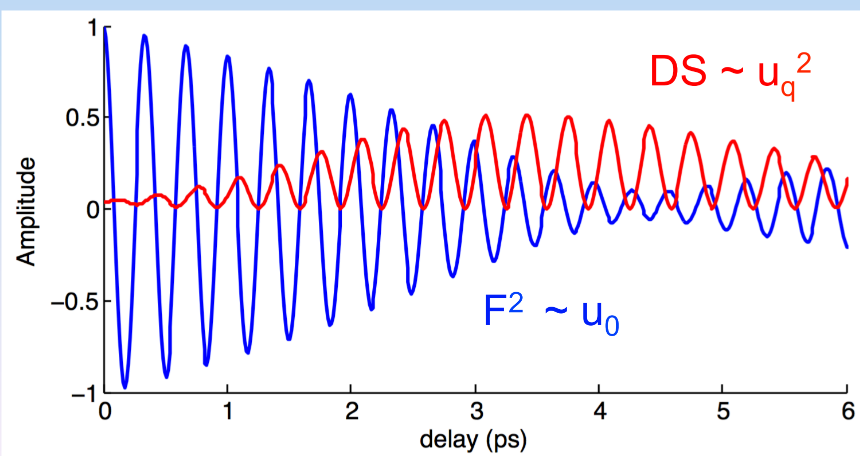
$$\ddot{u}_q + \Gamma_0 \dot{u}_q + (\omega_q^2 + 2g\, u_0) u_q = 0$$

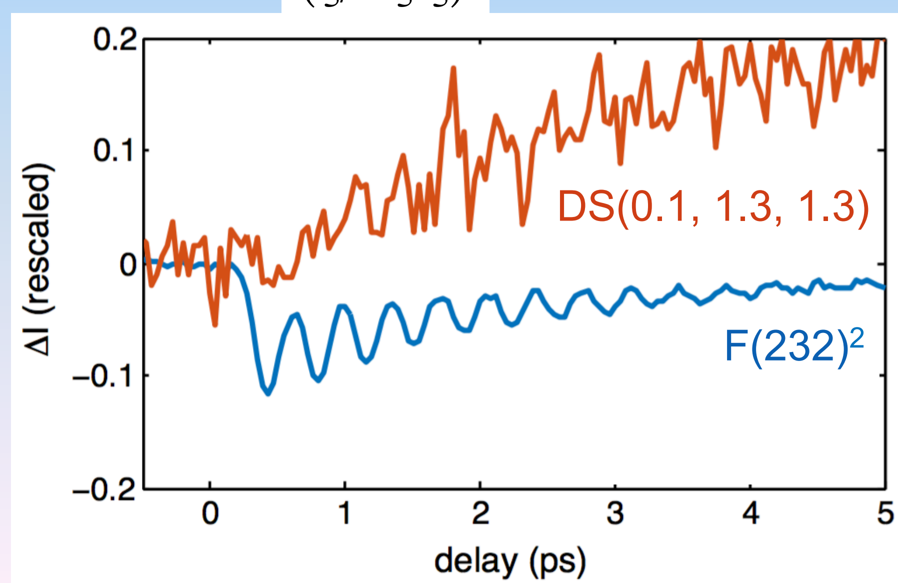
$$H_{\text{anharm}} = g u_0 u_q^2$$

Parametric phonon resonance

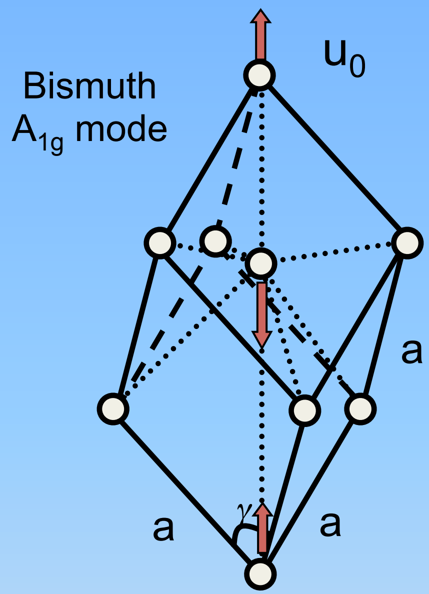


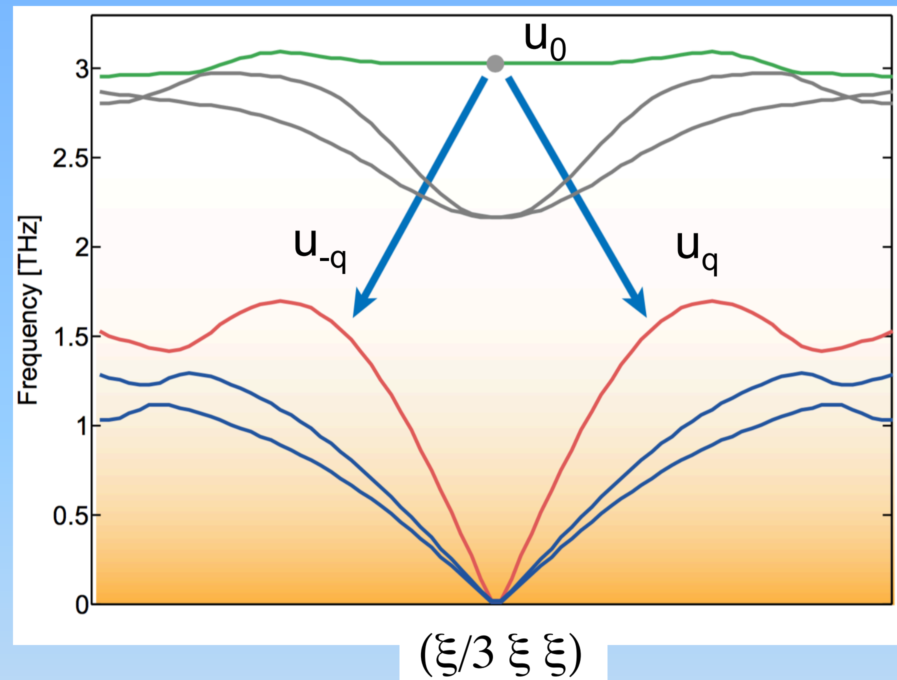


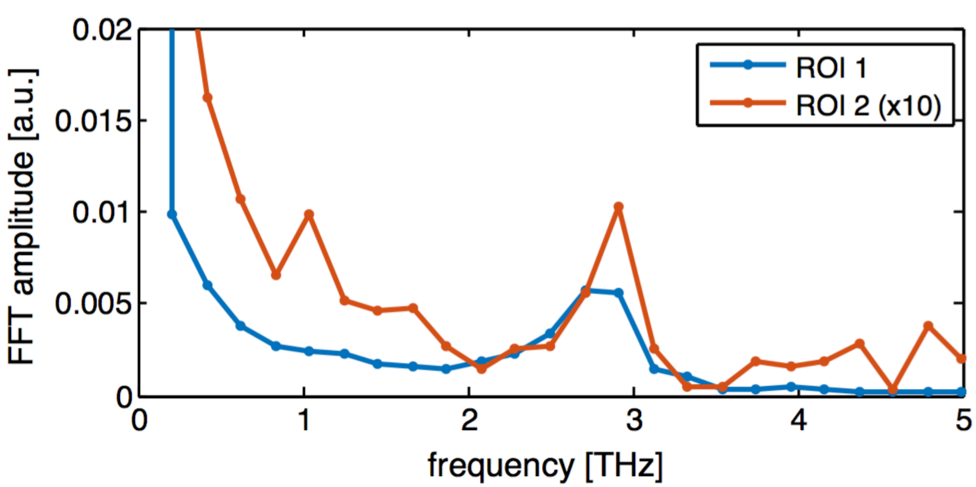


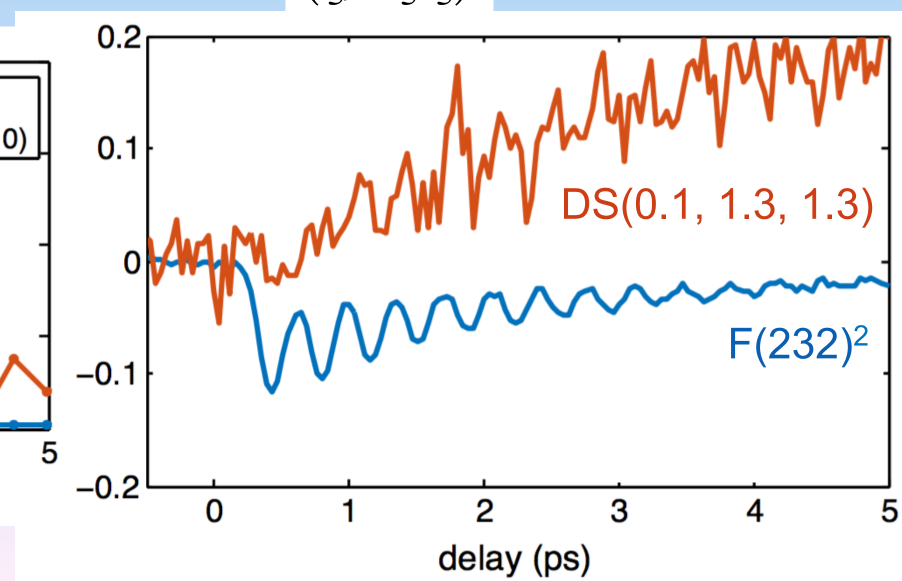


Parametric phonon resonance









How does the XFELO do?

- ***Static imaging in reciprocal space***
  - Serial crystallography – FELs, SR, DLSR, XFELO
  - SFX-need short pulses-diffract before destroy - FELs
  - MAD phasing – SR, DLSR, FELs, XFELO
  - Single Particle Imaging - SASE FELs
- ***Dynamics in reciprocal space***
  - Energy domain – average spectral brightness - XFELO
  - Time domain – FELs, XFELO

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  - Elemental mapping
  - Tomography
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Elemental mapping

- ***Focal spot size – photons/unit area***
  - Maia detector
  - Minimum detectable limit

Tomography

- Focal spot size – photons/unit area
- Spatial resolution
- Object size – beam size
- Photon energy

X-Ray Microtomography

ARTICLE

doi:10.1038/nature23456

New infant cranium from the African Miocene sheds light on ape evolution

Isaiah Nengo[1,2], Paul Tafforeau[3], Christopher C. Gilbert[4,5,6], John G. Fleagle[7], Ellen R. Miller[8], Craig Feibel[9,10], David L. Fox[11], Josh Feinberg[11], Kelsey D. Pugh[5,6], Camille Berruyer[3], Sara Mana[12], Zachary Engle[10] & Fred Spoor[13,14]

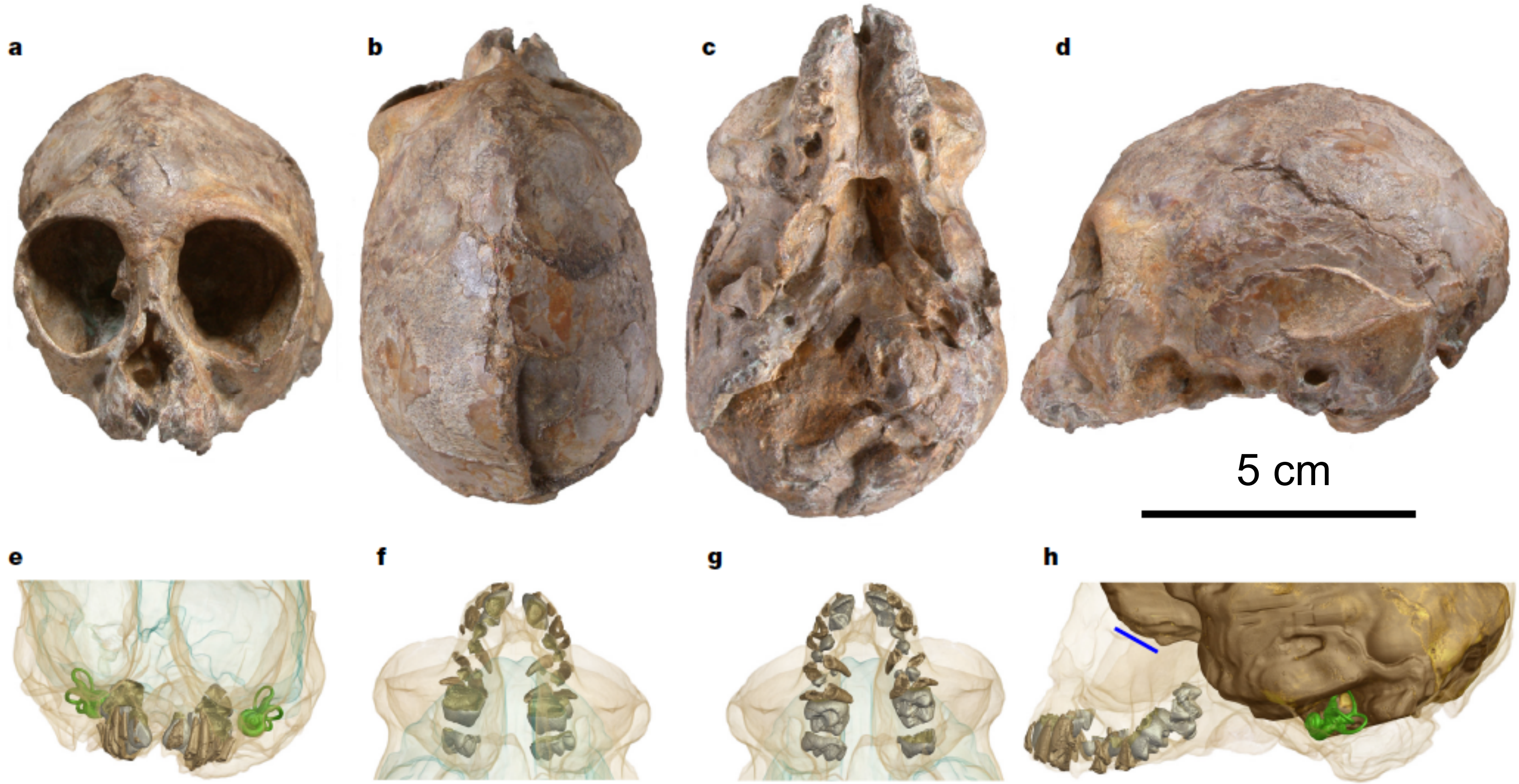

Figure 1 | KNM-NP 59050. a–d, Specimen as preserved in anterior view (**a**), superior view (**b**), inferior view (**c**), and left lateral view (**d**). **e–h**, Three-dimensional visualizations based on X-ray microtomography, in views matching **a–d**, and with the bone rendered transparent to show the deciduous dental roots (beige), the unerupted permanent tooth crowns (grey), the bony labyrinths (green), and the endocast (blue transparent in **e–g** and beige in **h**; the olfactory fossa marked by the blue line placed directly underneath). Scale bar, 5 cm.

X-Ray Microtomography

X-ray microtomography. KNM-NP 59050 was scanned using propagation phase-contrast X-ray synchrotron microtomography at beamline ID19 of the European Synchrotron Radiation Facility in Grenoble, France. The purpose was to visualize the specimen from a full overview down to virtual histology for the study of dental development. Four configurations were therefore used, providing voxel sizes of 28.06, 12.86, 3.44, and 0.74 µm. All acquisition parameters are summarized in Supplementary Table 3. Extant hominoid crania were scanned for comparative purposes using beamline BM05 of the European Synchrotron Radiation Facility in polychromatic mode (average energy between 100 and 130 keV), the GE phoenix v|tome|x s240 at the American Museum of Natural History, New York, and the BIR ACTIS 225/300 of the Max Planck Institute for Evolutionary Anthropology, Leipzig. Voxel sizes varied between 22.93 and 53.19 µm depending on the size of the specimens. VGStudioMax 3.0 (Volume Graphics), Avizo 7.1 (FEI), and Amira 5.6 (FEI) were used for two- and three-dimensional visualization, segmentation, reconstruction, and measurements.

X-Ray Microtomography

Supplementary Table 3 | Scanning parameters used for KNM-NP 59050. The fossil was scanned on beamline ID 19 of the European Synchrotron Radiation Facility (ESRF) in Grenoble, France. Four different voxel sizes were used, and the associated scanning parameters are given here.

	complete cranium	teeth, ear region	Long period lines in teeth	enamel microstructure
Voxel size	28.06 µm	12.86 µm	3.44 µm	0.72 µm
Average energy	126.2 keV	140.8 keV	100.8 keV	60.2 keV

How does the XFELO do?

- Elemental mapping – DLSR, XFELO
- Tomography – DLSR, XFELO

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Summary

- ***We need all the new sources***
  - ***Cost independent – XFELO gives the highest spectral brightness***
  - ***DLSR cover the broadest photon energy range and beam sizes to match the experimental needs***
  - ***SASE/seeded FELs provide the highest peak intensity (energy per pulse) for non-linear x-ray optics***

NOTE: This is very much a personal perspective