Versatile end station for ultrafast diffraction to understand reactions, phase transitions and lattice dynamics using hard or ultra-hard x-rays

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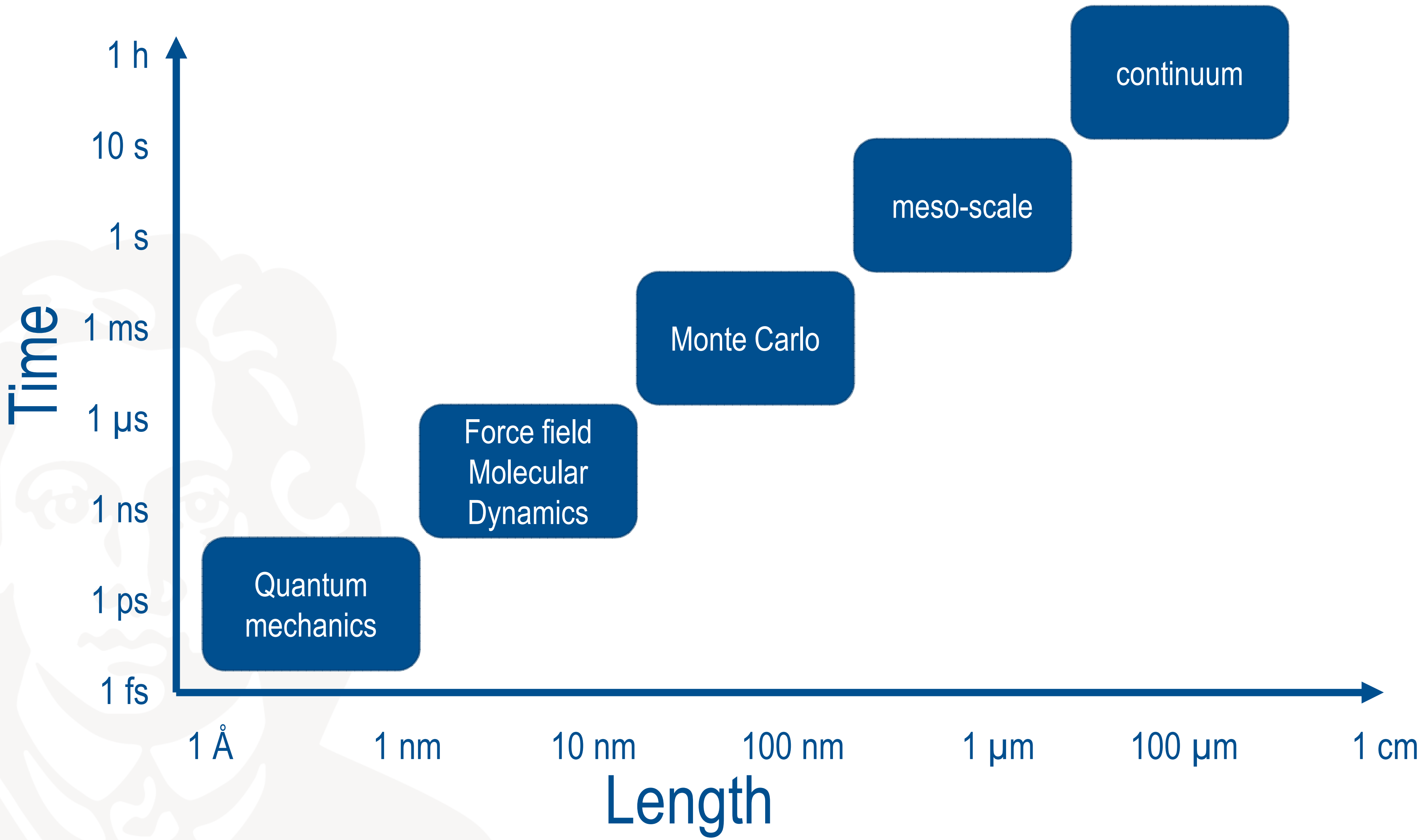
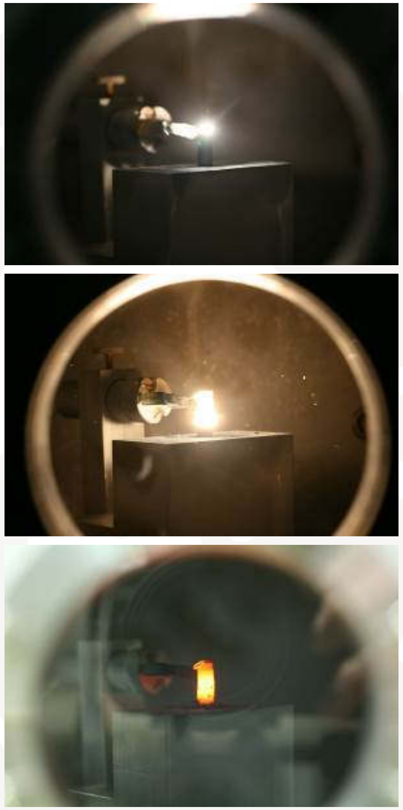
Accessible time and length scales

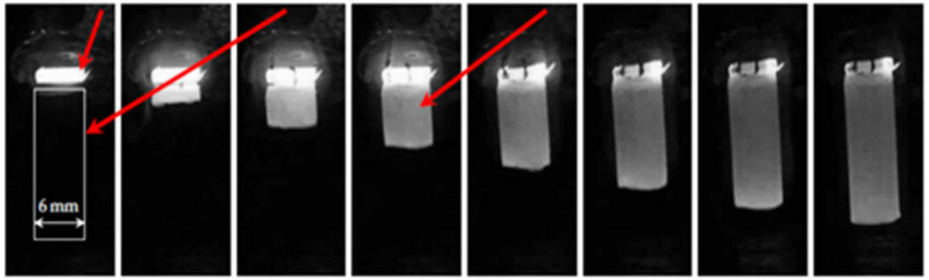


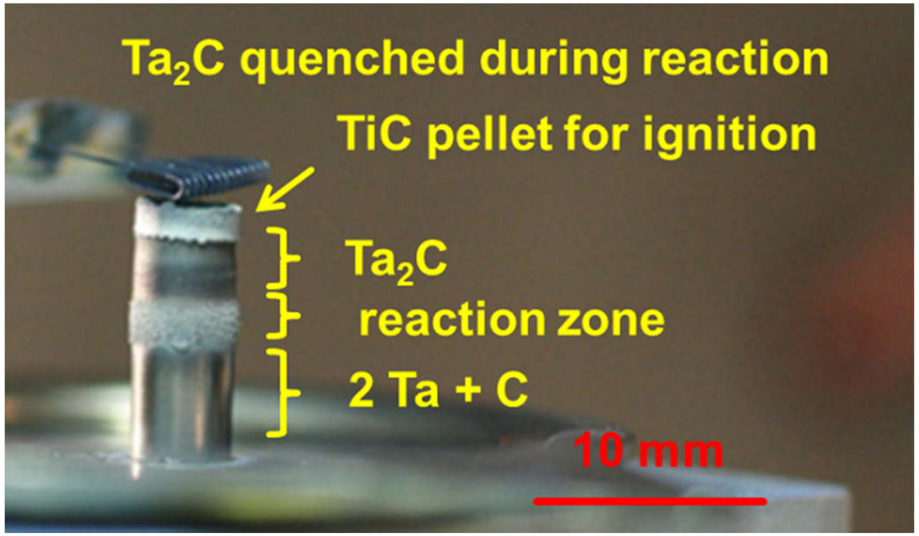
Scientific question

What happens DURING reactions and phase transitions?

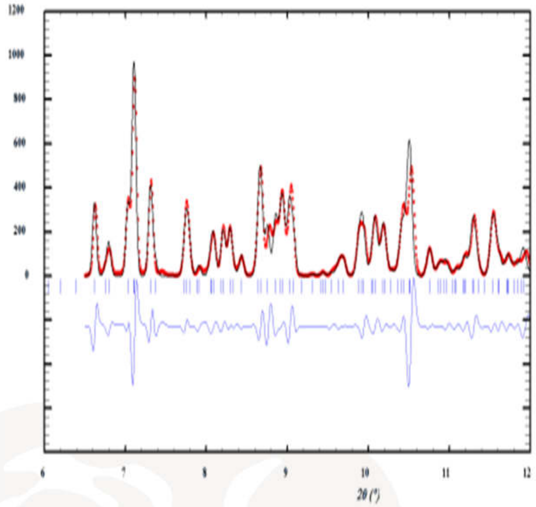
- solid flame and related reaction (e.g. thermite)
- crystallisation of supercooled melts
- shape memory alloys
- thermosalient crystals

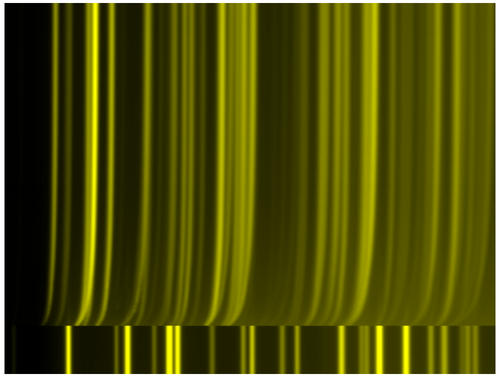


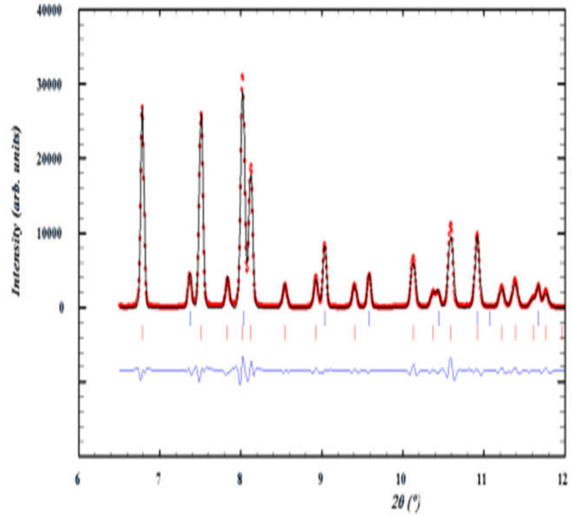




State-of-the-art

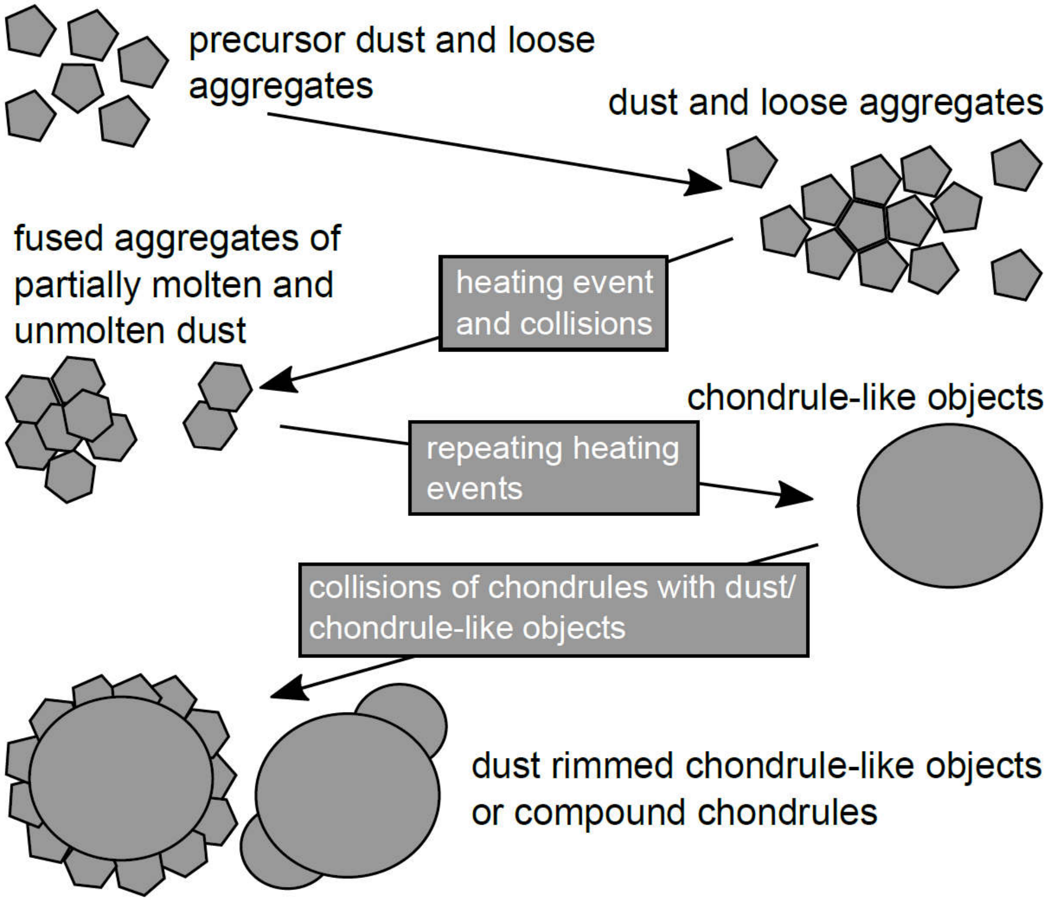


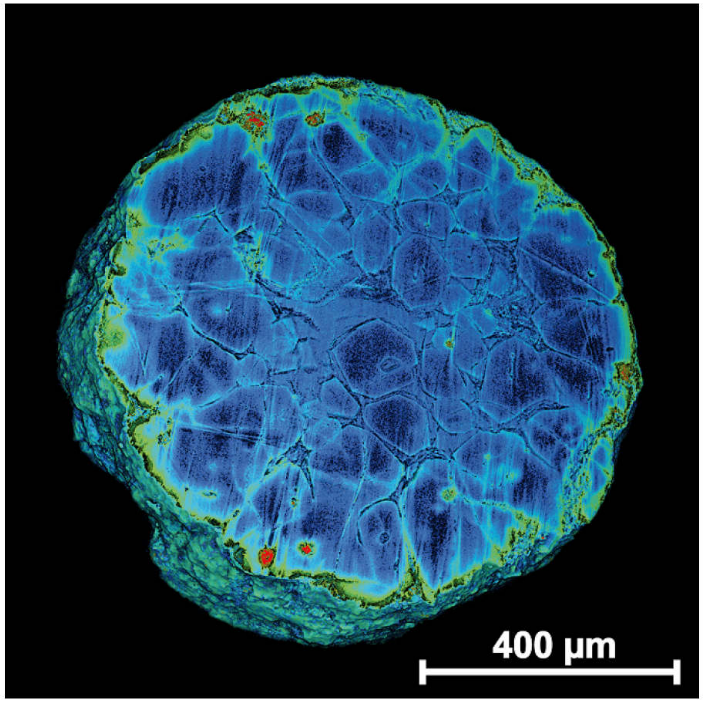




P07@PETRA III , 10 Hz frame rate, E = 71 keV

fs diffraction to understand planet formation



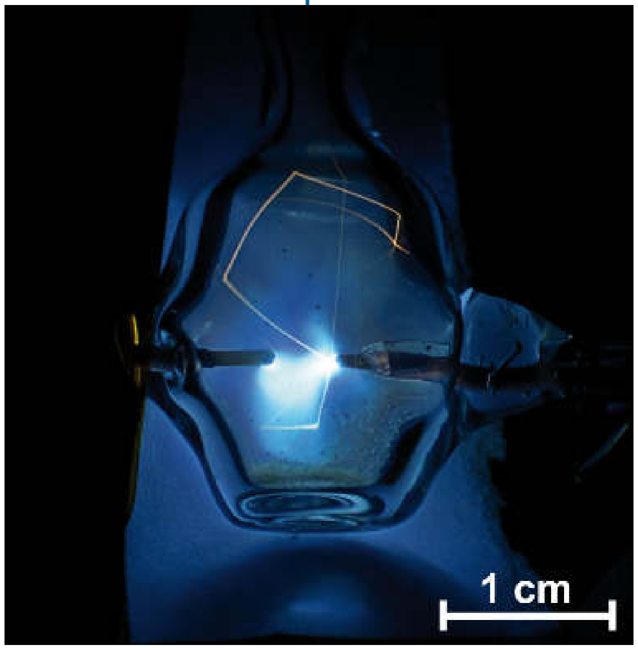


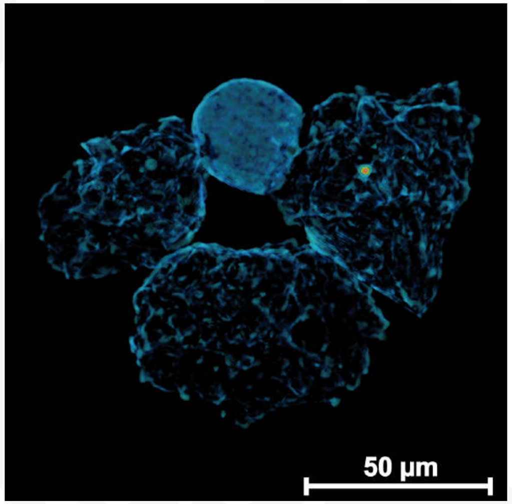
fs diffraction to understand planet formation

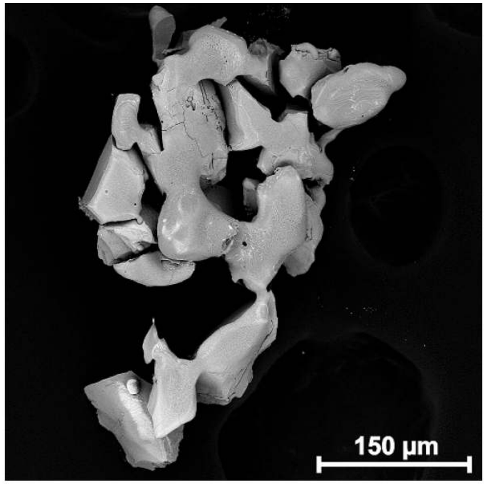
Chondrule formation by nebular lightning mimicked by arc discharges

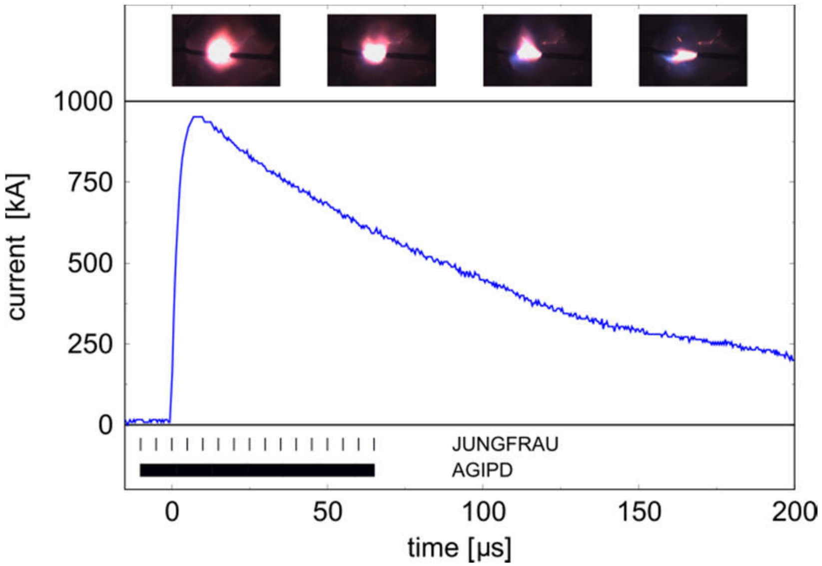
EXCISS experiment @ISS

Detailed observation by fs-diffraction and imaging

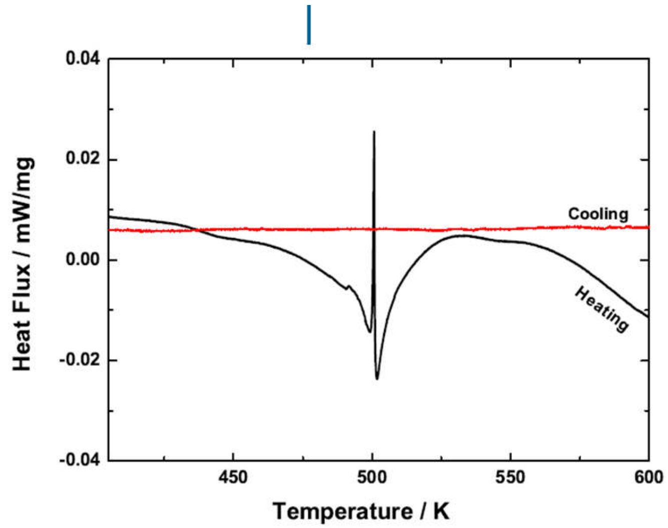






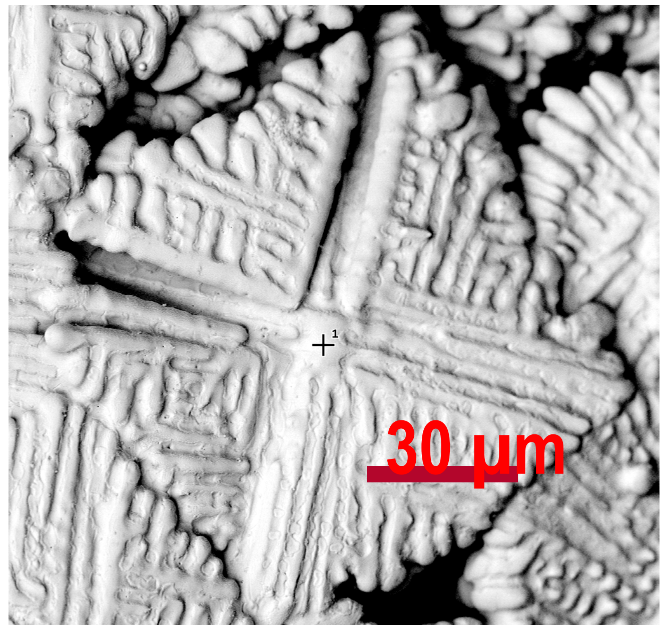


fs diffraction to understand phase formation and microstructures in arc melting and 3d laser printing



Observe the formation of nuclei and of changes in the melt structure by total scattering/pair distribution function analysis and small angle diffraction

Follow the evolution of crystal formation by wide angle diffraction



Synthetic Pt_3Cu_2Sn obtained by arc melting.

fs diffraction to understand lattice dynamics using TDS

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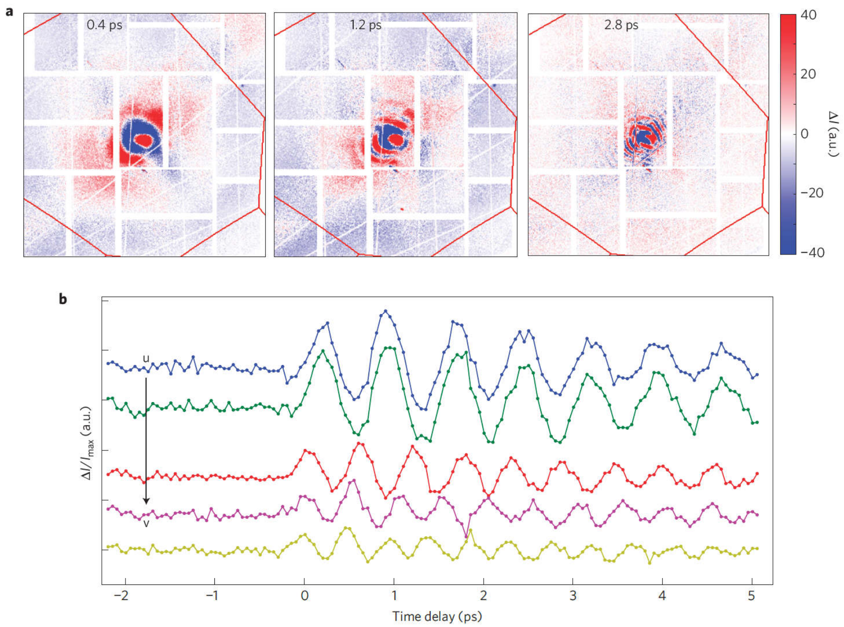
LETTERS
PUBLISHED ONLINE: 27 OCTOBER 2013 | DOI: 10.1038/NPHYS2788
nature physics

Fourier-transform inelastic X-ray scattering from time- and momentum-dependent phonon–phonon correlations

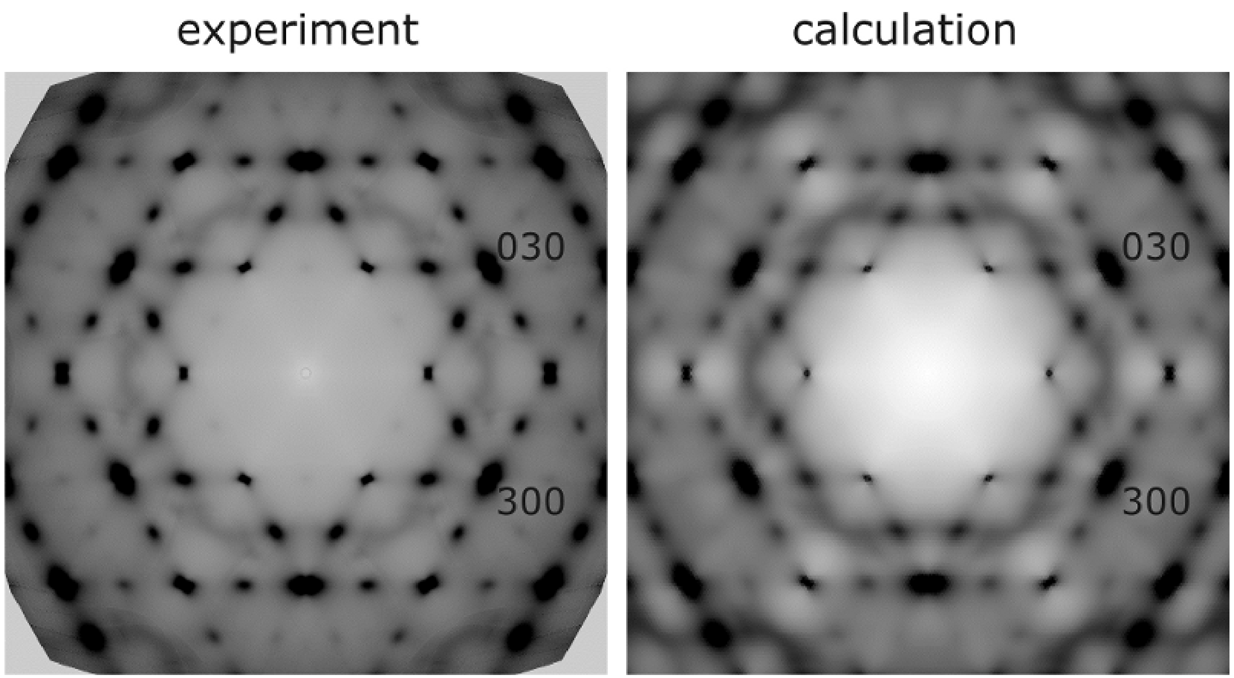
M. Trigo[1,2]*, M. Fuchs[1,2], J. Chen[1,2], M. P. Jiang[1,2], M. Cammarata[3], S. Fahy[4], D. M. Fritz[3], K. Gaffney[2], S. Ghimire[2], A. Higginbotham[5], S. L. Johnson[6], M. E. Kozina[2], J. Larsson[7], H. Lemke[3], A. M. Lindenberg[1,2,8], G. Ndabashimiye[2], F. Quirin[9], K. Sokolowski-Tinten[9], C. Uher[10], G. Wang[10], J. S. Wark[5], D. Zhu[3] and D. A. Reis[1,2,11]*



Inelastic X-ray scattering from phonons

$$I_1(Q) = \frac{\hbar N I_{\mathrm{inc}}}{2} \sum_{\nu} \Omega_{q,\nu} \left| \sum_{s} \frac{f_s(Q)}{\sqrt{m_s}} e^{-W_{s,Q}} (Q e_{Q,\nu,s}) e^{-iQ\tau_s} \right|^2$$

$$\Omega_{q,\nu} = \frac{1}{\omega_{q,\nu}} \coth\left(\frac{\hbar\omega_{q,\nu}}{2k_B T}\right)$$



In-between Bragg reflections: thermal diffuse scattering and vibrational spectroscopy with x-rays

A Bosak[1], D Chernyshov[2], B Wehinger[3,4], B Winkler[5], M Le Tacon[6] and M Krisch[1]

J. Phys. D: Appl. Phys. **48** (2015) 504003

Side station @ ID28

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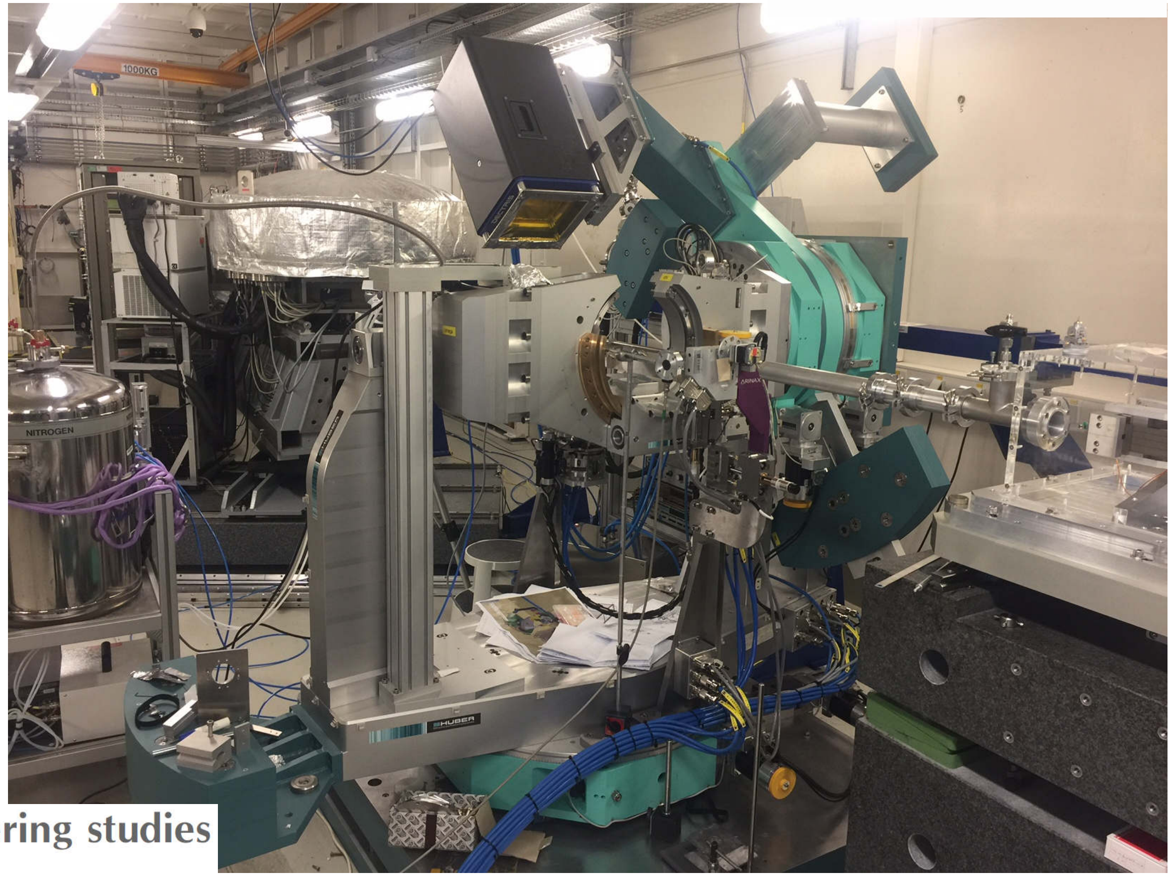
Federal Ministry
of Education
and Research

C(311)[splitter]-Si(422)
monochromator

0.52-0.98 Å

flux ~10^{12} ph/s @ 17.8 keV

focal spot down to 20x40 μm

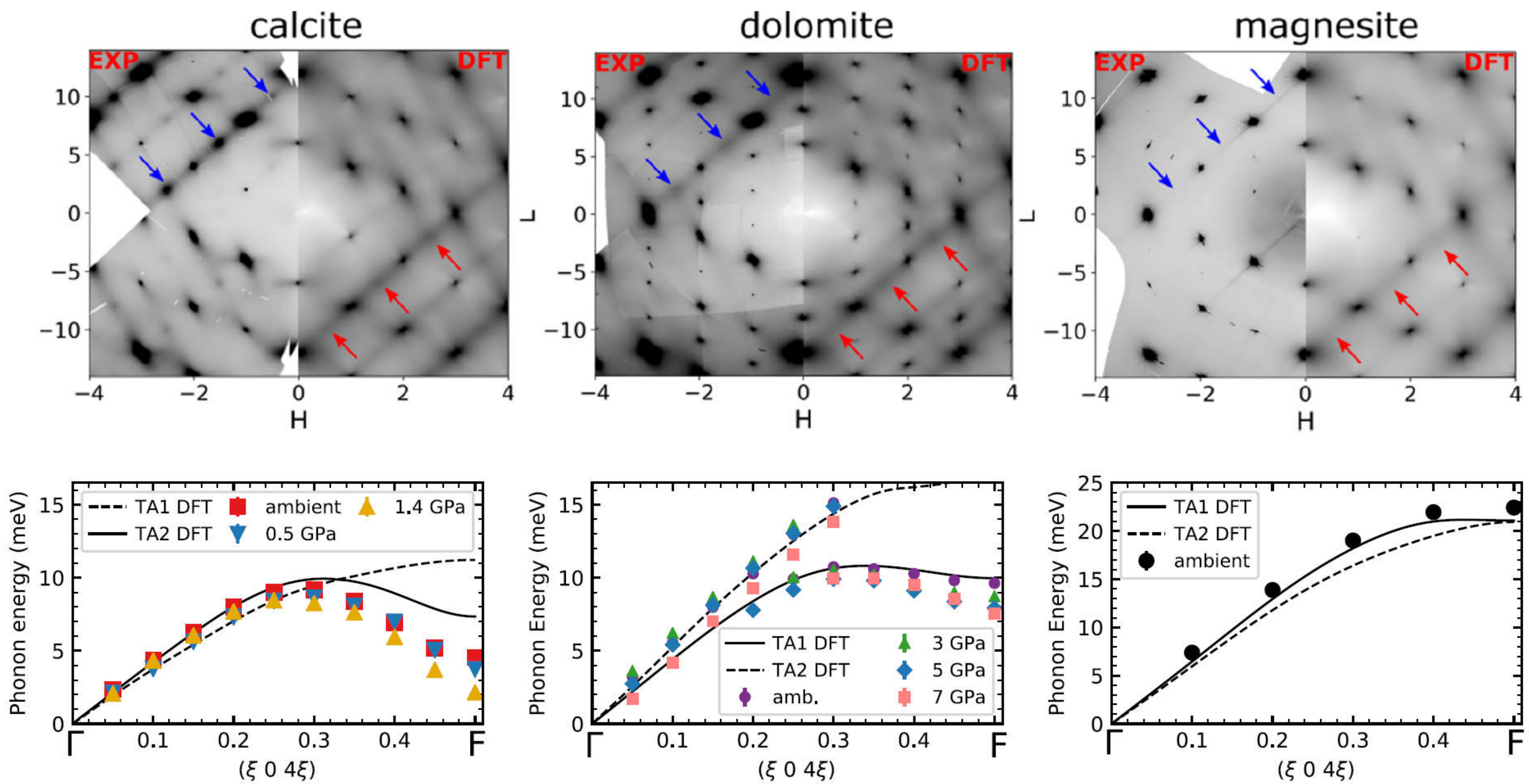


A new diffractometer for diffuse scattering studies on the ID28 beamline at the ESRF
A. Girard,[a]* T. Nguyen-Thanh,[b] S. M. Souliou,[b] M. Stekiel,[a] W. Morgenroth,[a]
L. Paolasini,[b] A. Minelli,[b] D. Gambetti,[b] B. Winkler[a] and A. Bosak[b]*
J. Synchrotron Rad. (2019). **26**

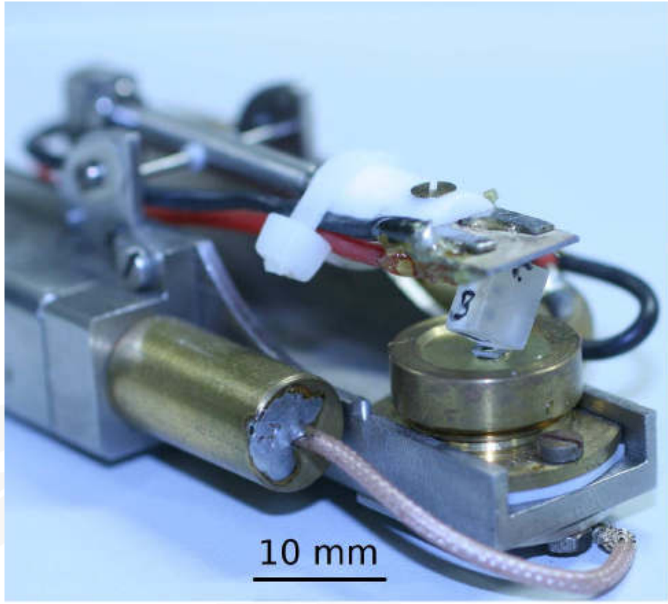
PHYSICAL REVIEW B **99**, 054101 (2019)

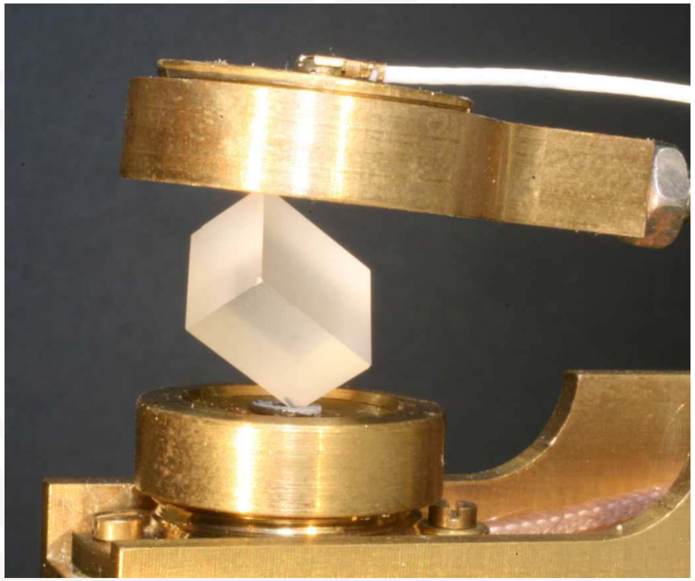
Phonon-driven phase transitions in calcite, dolomite, and magnesite

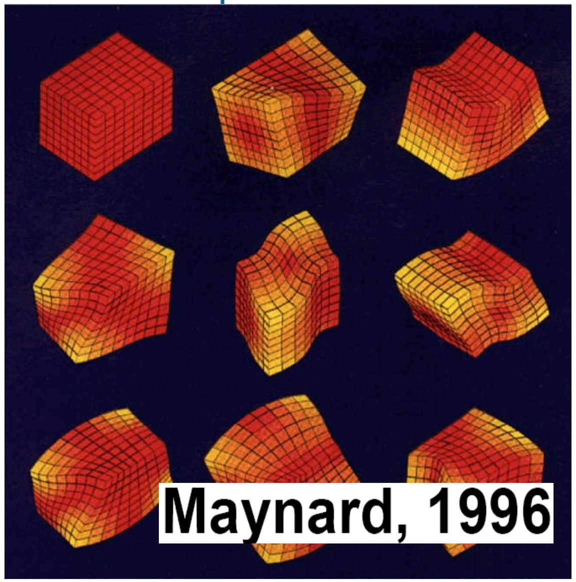
Michal Stekiel,[1,*] Adrien Girard,[1] Tra Nguyen-Thanh,[2] Alexei Bosak,[2] Victor Milman,[3] and Bjoern Winkler

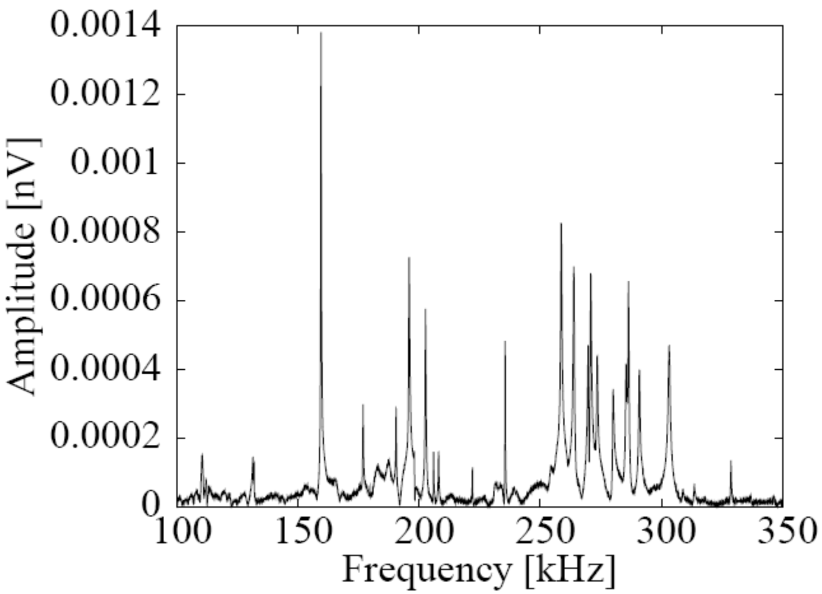


Resonant ultrasound spectroscopy



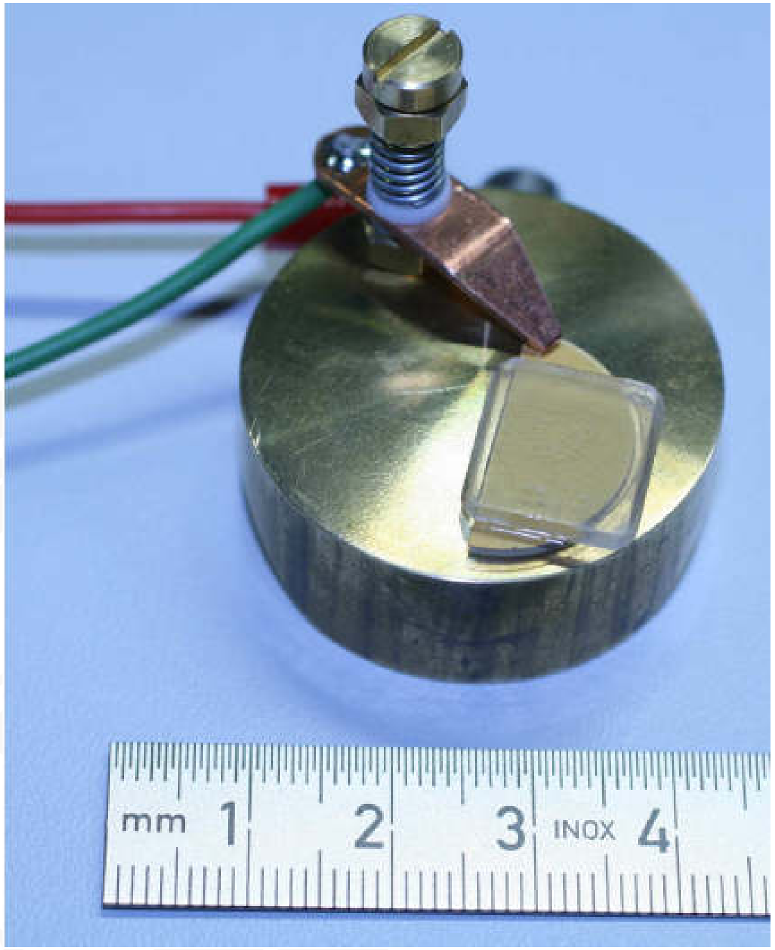


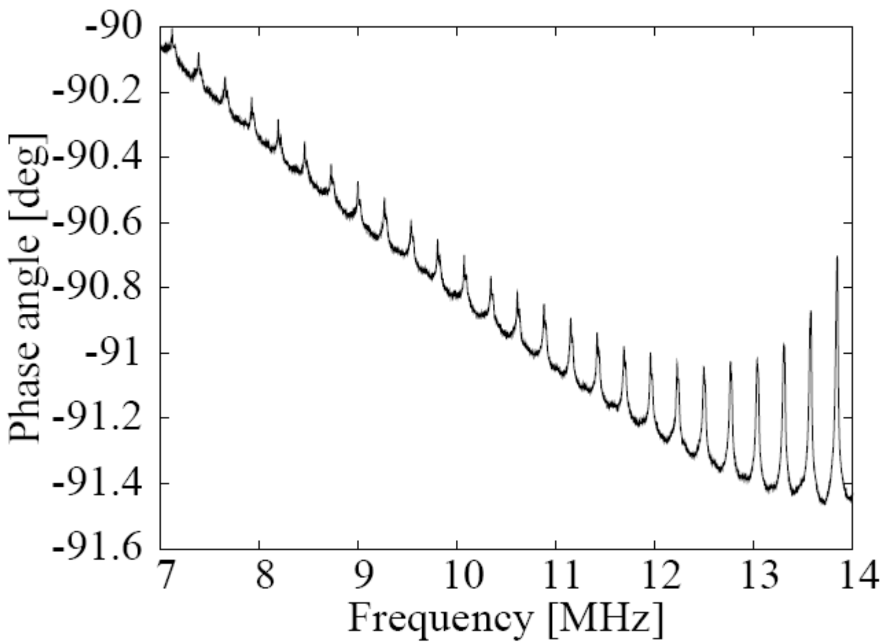




E. Haussühl, J. Schreuer, S. Haussühl, B. Winkler, L. Bayarjargal, V. Milman (2012) Structure-property relations and thermodynamic properties of monoclinic petalite, $LiAlSi_4O_{10}$. J. Phys.: Condens. Matter **24**, 345402

Parallel plate / plane wave ultrasound spectrocopy





Piezoelastic properties of retgersite determined by ultrasonic measurements

D. Arbeck, E. Haussühl, L. Bayarjagal, B. Winkler, N. Paulsen, S. Haussühl and V. Milman

Eur. Phys. J. B **73**, 167–175 (2010)

Requirements

Why fs time resolution ?

processes occur on µs - ps time scale – so to understand changes, ns - fs diffraction is required

Reaction fronts travel with up to 1.5 m/s

Heating rates up to 10^6 K/s, cooling rates up to 10^5 K/s

lattice dynamics are on ps time scale

Why hard x-rays ?

To establish stable reaction fronts, macroscopic samples need to be studied

- need > 50 keV to penetrate 4 mm cylinder with high Z elements

Need > 50 keV to have large enough Q-range in pair distribution function experiments

Need > 30 keV to penetrate RUS samples

Why versatile "large" (e.g. 100 x 100 µm^2) beam ?

- Reactions require macroscopic samples, i.e. you cannot get a reaction front in a micron-sized sample
- RUS samples have to be large (mm edges) as otherwise you cannot excite resonances
- electrodes in plasma-based experiments are spaced a few mm apart

Will it work ?

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P02.2: 10^9 photons / 44 ps / 4 µm^2 @ 25 keV

XFEL: 10^{10} photons / 10 fs / 10.000 µm^2 @ 50 keV
(for SHS: 4000 x 50 = 20.000 µm^2)

Photo absorption coefficient decreases by ~1 order of magnitude for high Z elements when going from 25 keV (0.4949 A) to 50 keV (0.2479 A)

< 0.4 µJ / µm^2 , less than damage threshold in Si (Koyama et al., 2013)

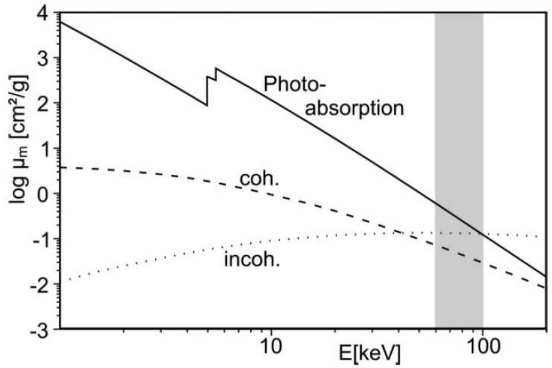

Figure 2
Partial interaction coefficients for coherent scattering, incoherent scattering and photoabsorption of $Ti_{0.6}V_{0.4}$ as a function of photon energy. The shaded area marks the high-energy regime, where the ratio between coherent scattering and other interaction channels is most favorable.

High-energy X-ray diffuse scattering

I. B. Ramsteiner,[a*] A. Schöps,[a] H. Reichert,[a] H. Dosch,[a] V. Honkimäki,[b] Z. Zhong and J. B. Hastings[d]

Acta Cryst. (2009). A**42**, 392–400

Can we measure a diffraction pattern ?

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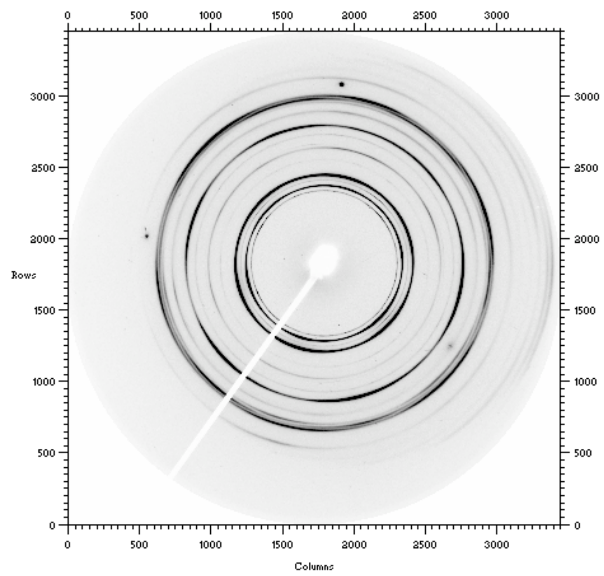

10^{10} photons / 10 fs

< 10^9 photons are diffracted

< 10^8 photons per Laue cone

< 5 x 10^4 photon/pixel for 200 x 200 μm^2 pixel at 300 mm distance

Summary

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A versatile diffractometer with a large, fast area detector for hard x-ray fs diffraction would

- allow to study a large range of phenomena and provide understanding of reactions, phase transformations and lattice dynamics a relevant time scale

- would require a minimum of sample environment, as the sample environments would typically be portable and would be provided by the user groups

- hence would be attractive for a large user community

A more even distribution of photon pulses would simplify most of these experiments