Towards the direct measurement of bulk temperature in shock-compressed matter using inelastic X-ray scattering at XFELs

4th DyCoMaX Workshop
Session VI: New instrumental opportunities

Adrien Descamps, a.descamps@qub.ac.uk

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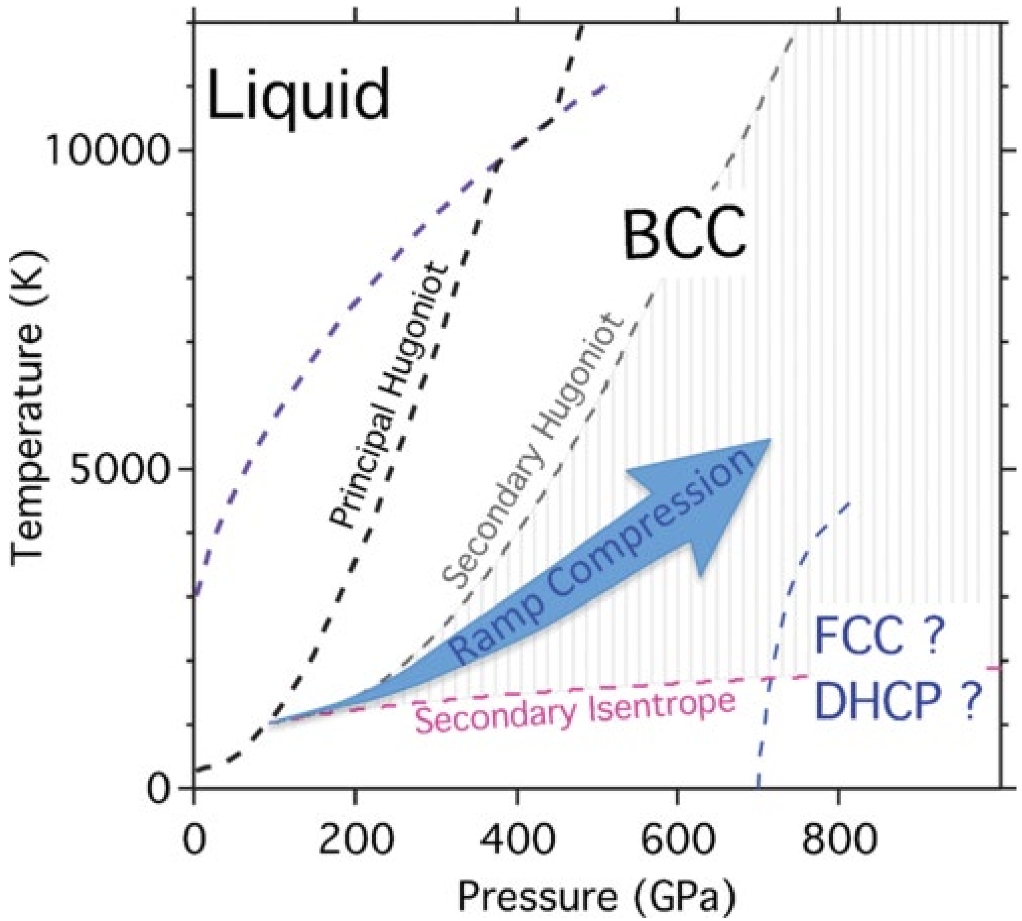
While pressure (density) is measured routinely, temperature remains challenging

Wang et al. Phys. Rev. B **94**, 104102 (2016)

Phase diagram of Molybdenum



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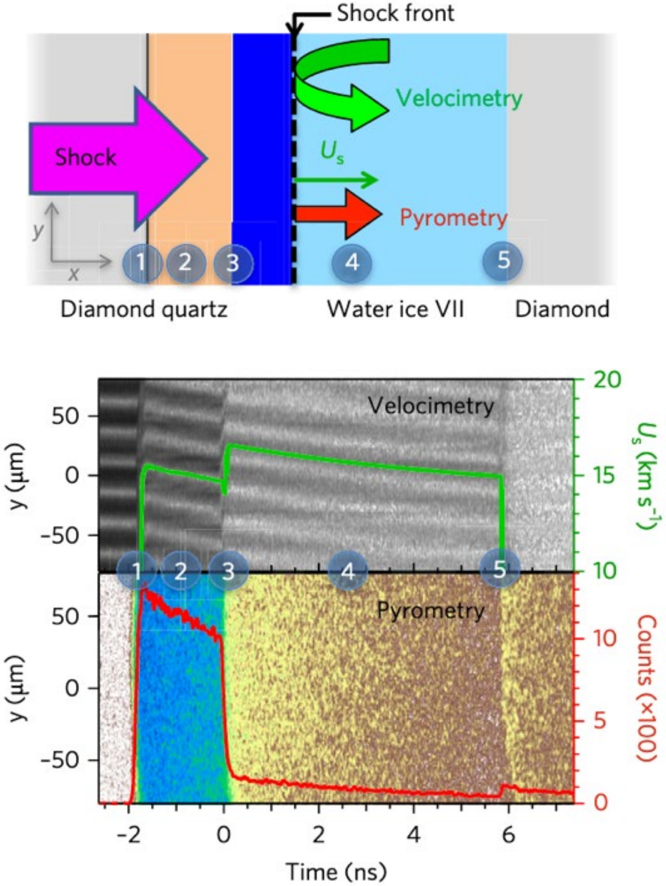
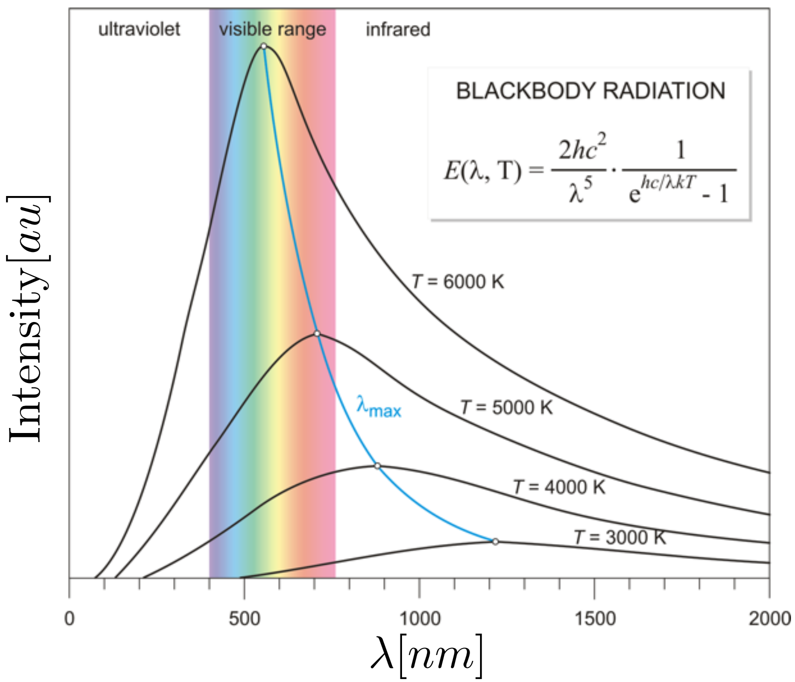
Commonly used techniques do not directly measure bulk temperature

Millot et al. Nature Physics **14**, pages 297–302 (2018)



Streaked optical pyrometry (SOP)



One approach would be to use ultra-bright, ultra-short X-ray sources for high resolution X-ray spectroscopy.

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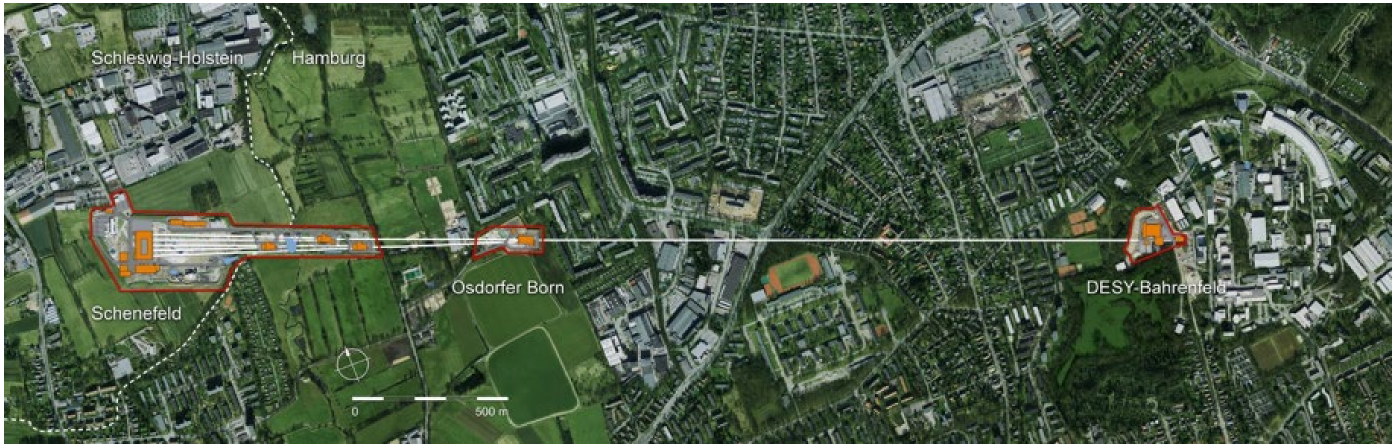
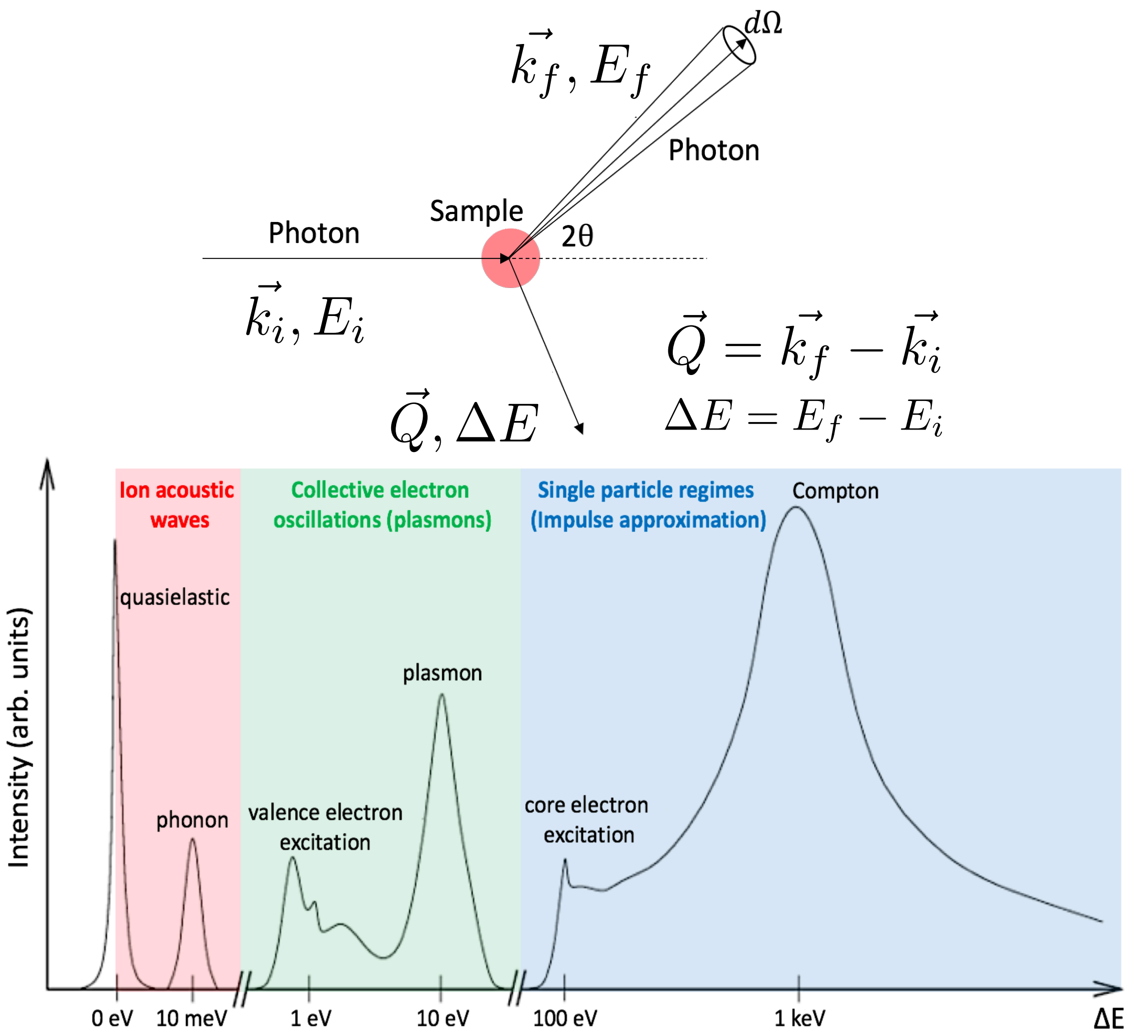
X-ray Free Electron Lasers provide ultrashort, ultrabright X-ray pulses

LCLS, MEC



European XFEL, HED

Inelastic X-ray scattering and the principle of detailed balance can be measured to measure the bulk temperature

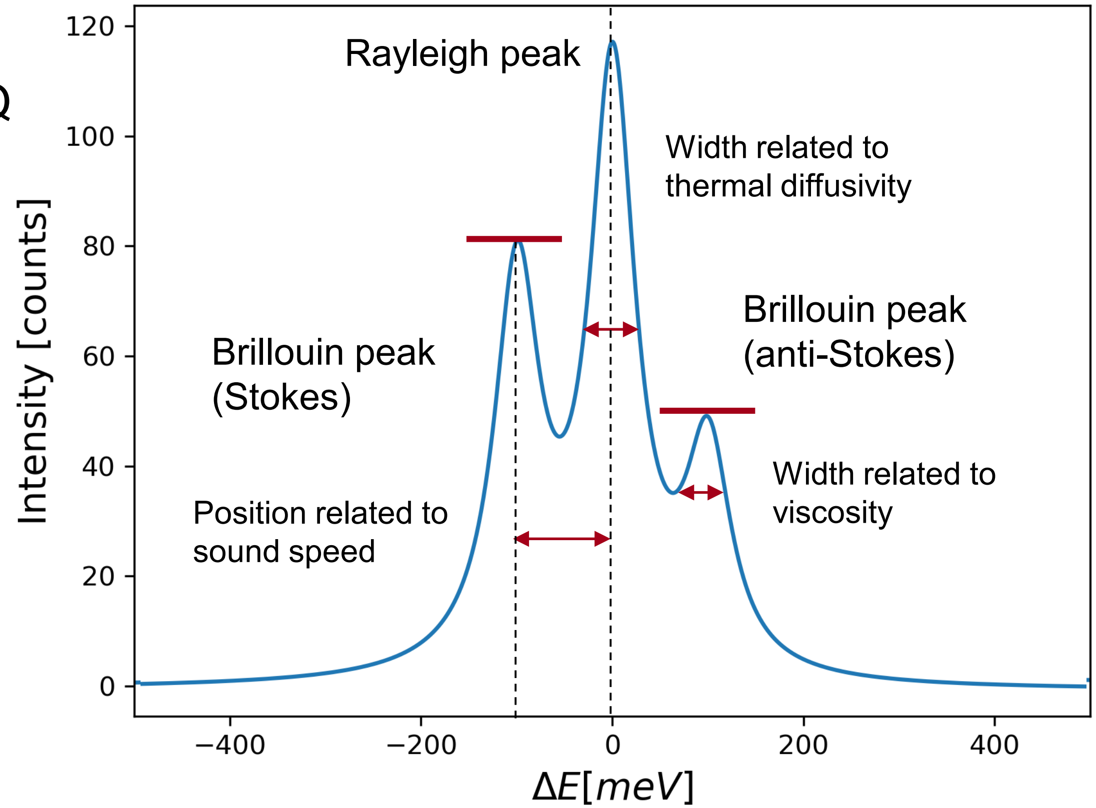


The principle of detailed balance causes a temperature dependent asymmetry of the recorded spectra

Hydrodynamic region:
small momentum transfer Q

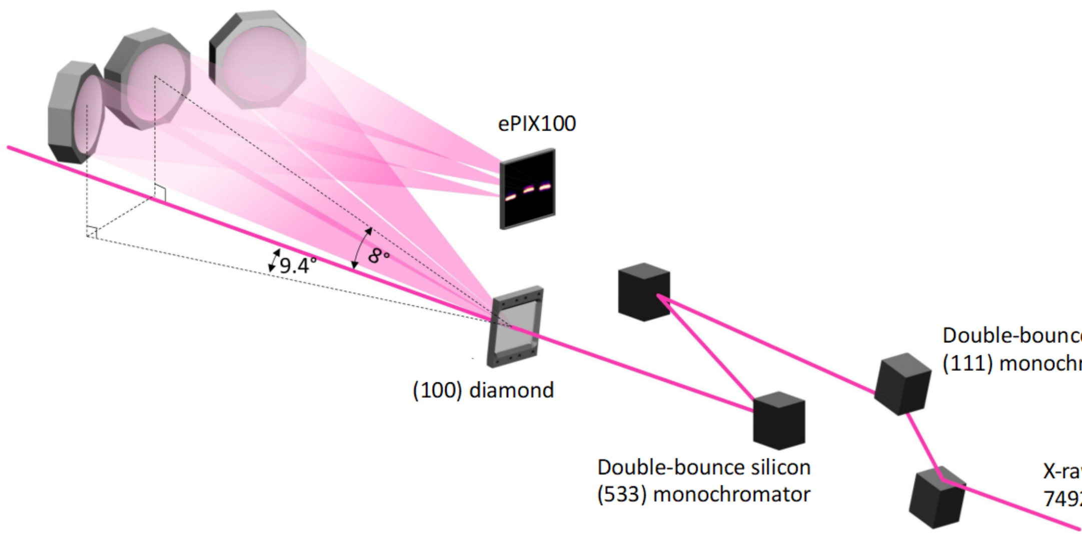
$$25\ \mathrm{meV} \sim 290\ \mathrm{K}$$

$$1\ \mathrm{eV} \sim 11600\ \mathrm{K}$$

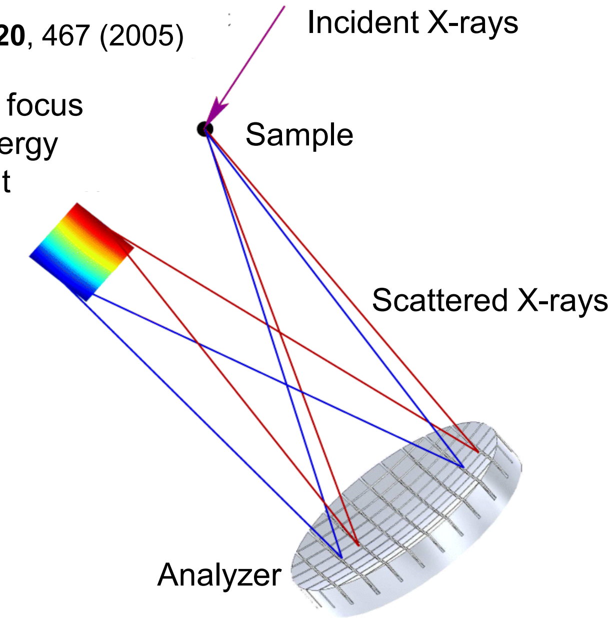


$$\frac{\mathrm{S}(-\hbar\omega, -\mathrm{Q})}{\mathrm{S}(\hbar\omega, \mathrm{Q})} = \mathrm{e}^{\hbar\omega/\mathrm{k_B T}}$$

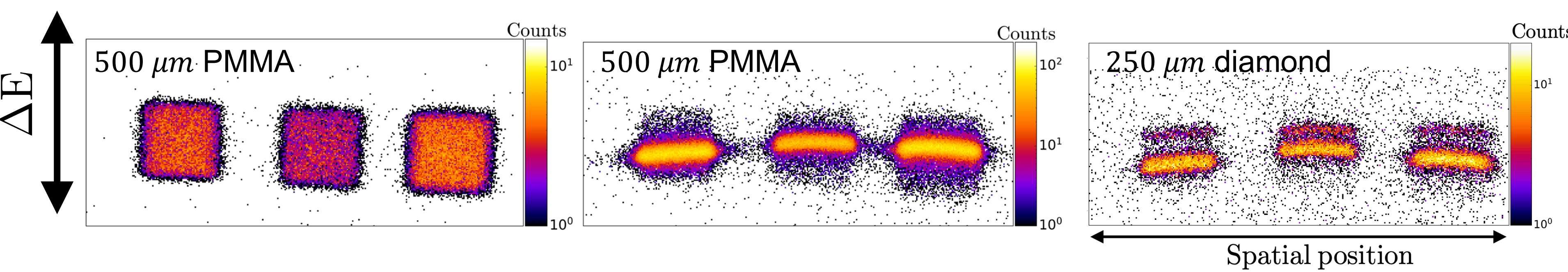
Experimental platform to measure high resolution inelastic X-ray scattering



Huotari et al., *J. Synch. Rad.* **20**, 467 (2005)



Without monochromator | **With monochromator**



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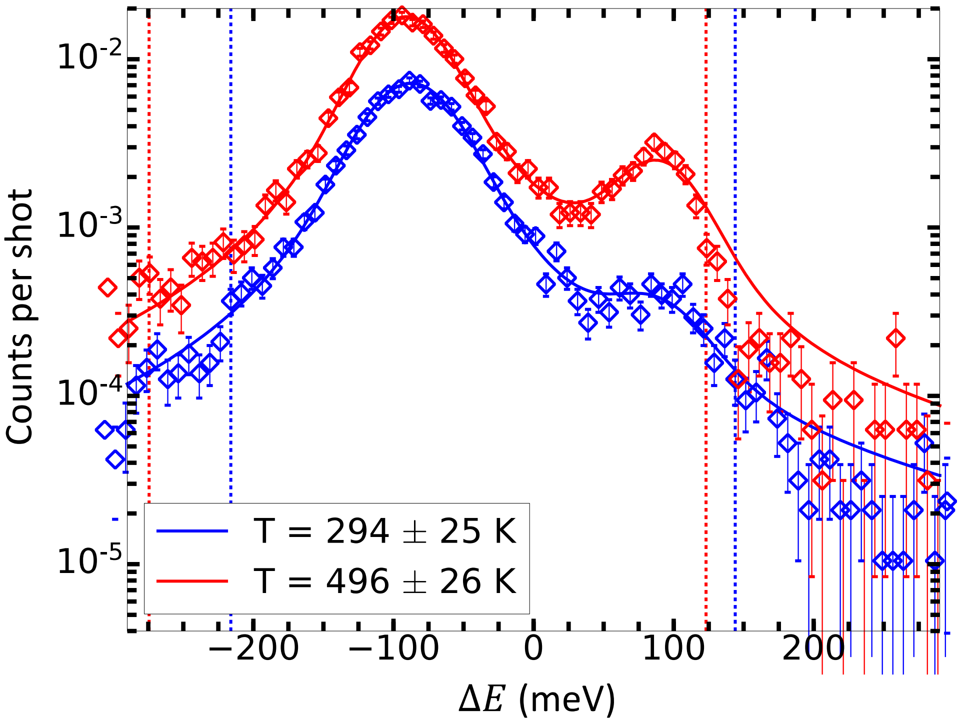
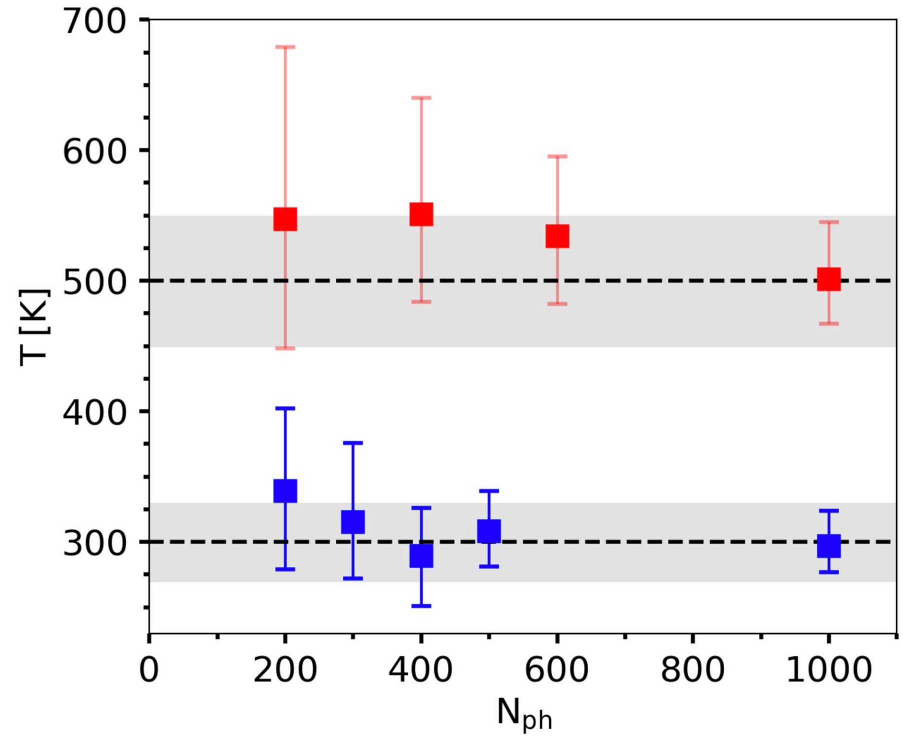
Accurate temperature measurement was demonstrated on single crystal diamond at the HED endstation at EuXFEL

Descamps. A *et al. Sci Rep* **10,** 14564 (2020)

Inelastic X-ray scattering spectrum
250 μm diamond



Accuracy of the temperature measurement



The technique was demonstrated on a resistively heated sample as a proof of principle and was further expanded on laser compressed systems.

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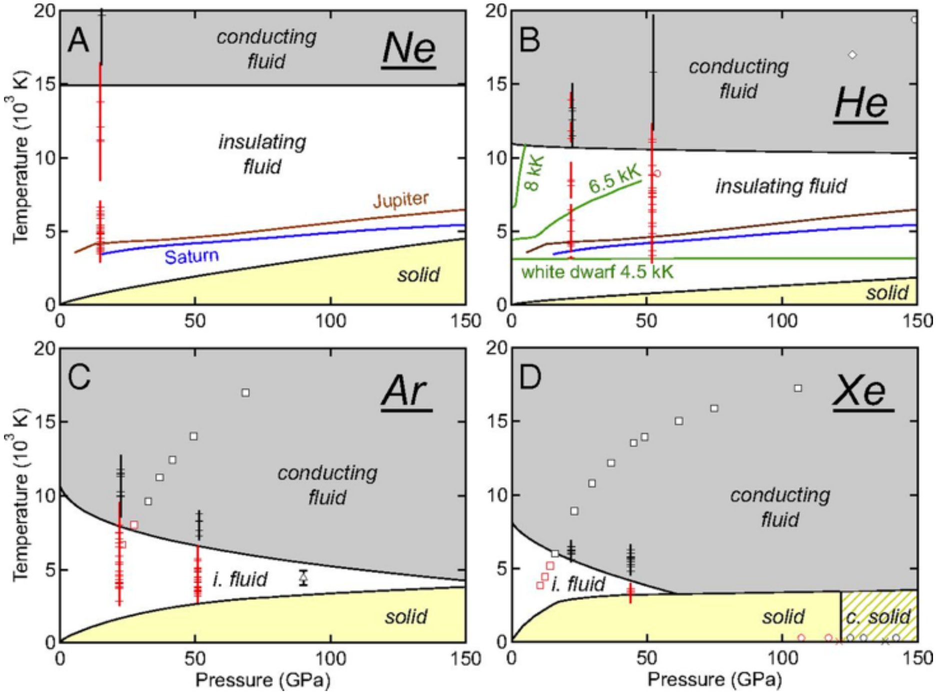
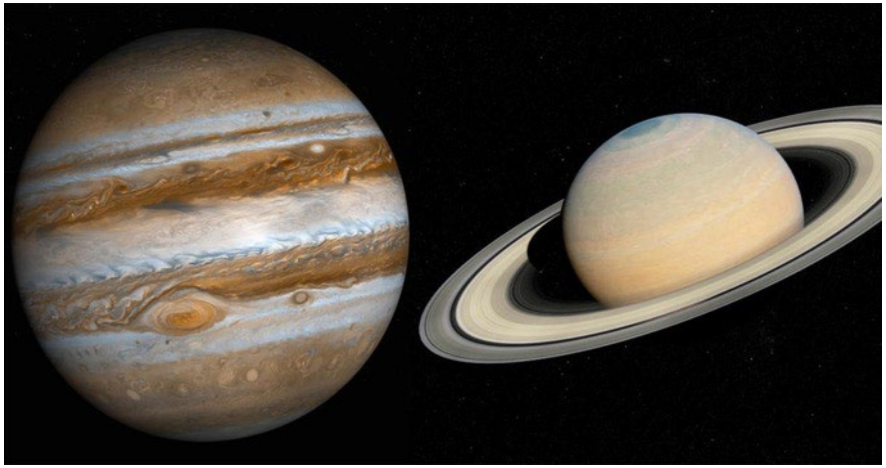
The study of noble gas in warm dense matter conditions is relevant for planetary science



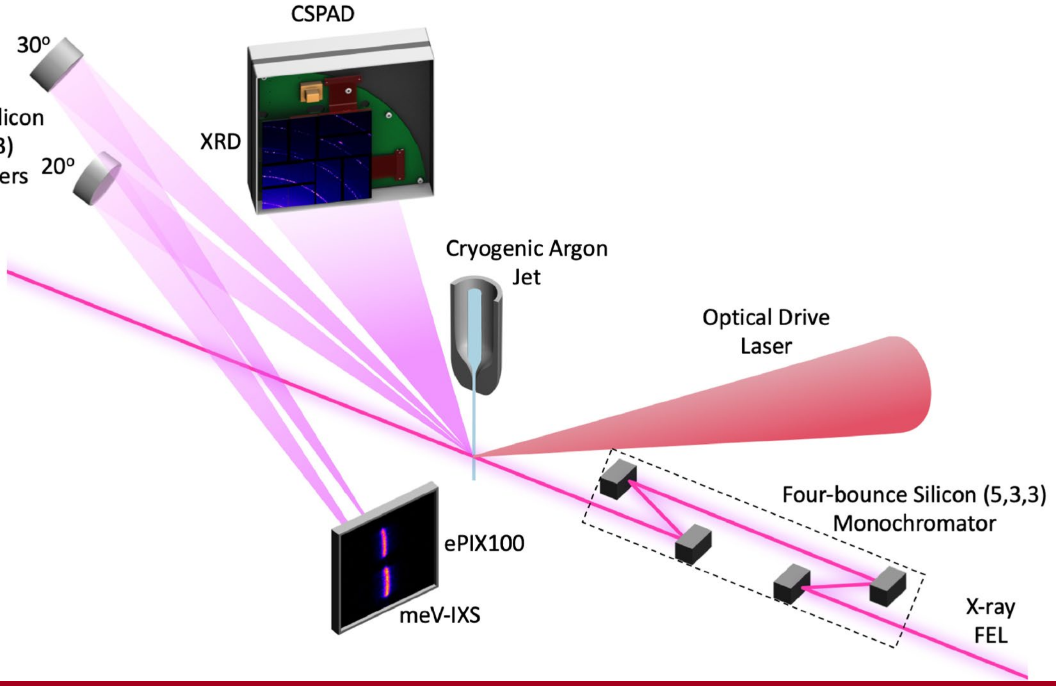
McWilliams et al., PNAS, 112, 7925 (2015)



Argon is a prototypical system for understanding the behavior of noble element at extreme conditions.

High-resolution inelastic scattering on shock compressed Argon at MEC, LCLS

McBride E. E. *et al.* (In prep.)
McBride, E. E., *et al. Rev. Sci. Inst.* **89**, 10 (2018)
Kim, J *et al. Rev. Sci. Inst.* **89**, 10K105 (2018)



Laser parameters:

- Duration: $120\ ps$ (chirped)
- Wavelength: $800\ nm$
- Energy: $400\ mJ$
- Spot size: $50\ \mu m$ FWHM

X-ray parameters:

- Energy: $7.492\ keV$
- Energy: $400\ \mu J$
- Spot size: $5\ \mu m$ FWHM

High resolution inelastic X-ray scattering requires the accumulation of many X-ray shots due to the small inelastic X-ray cross section.

- High repetition rate driver laser
- Self refreshing target using a cryogenic Argon jet

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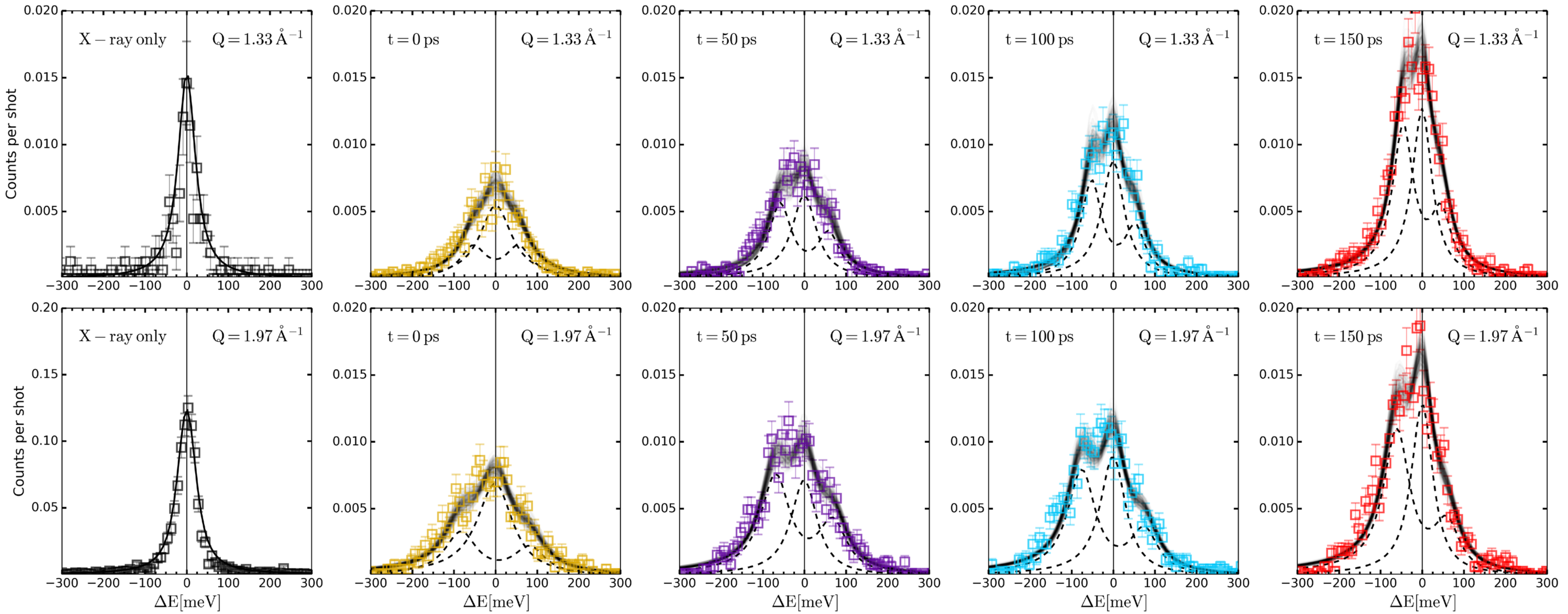
The temperature is obtained from the asymmetry of the spectrum

Time evolution of the high-resolution inelastic spectrum of laser compressed Argon



Fits obtained using Markov Chain Monte Carlo procedure

As a function of time delay , the spectrum becomes more asymmetric and narrower indicative of a cool down and a change in the mode dispersion relation.

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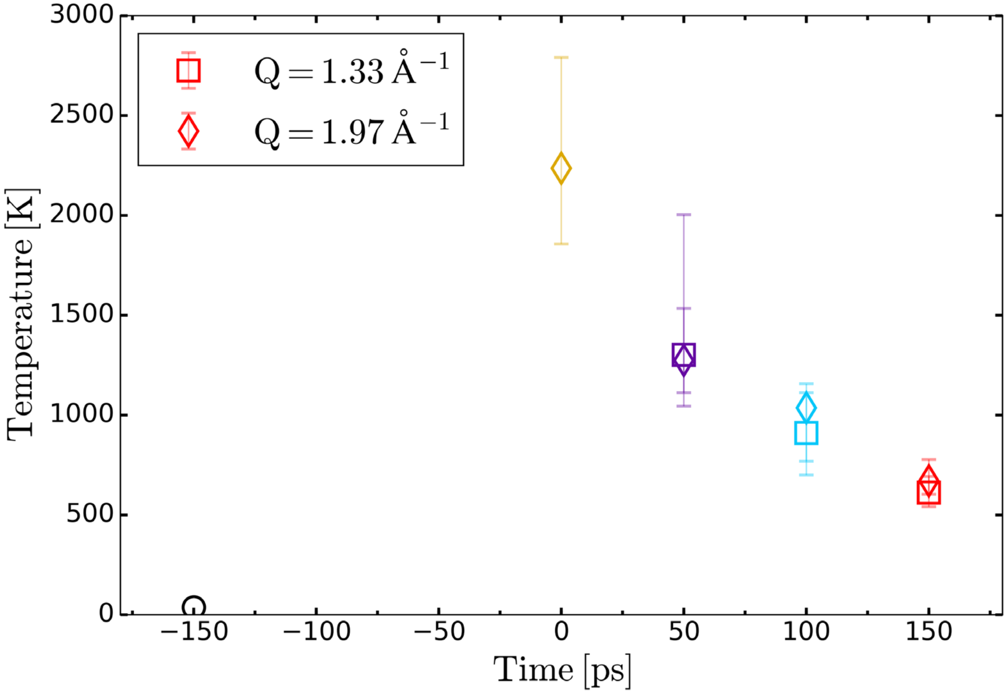
The temperature is obtained from the asymmetry of the spectrum

Evolution of the measured temperature as a function of probe delay



The temperatures measured with the two analysers are consistent and indicate a cool of the system in the ~100 ps time scale.

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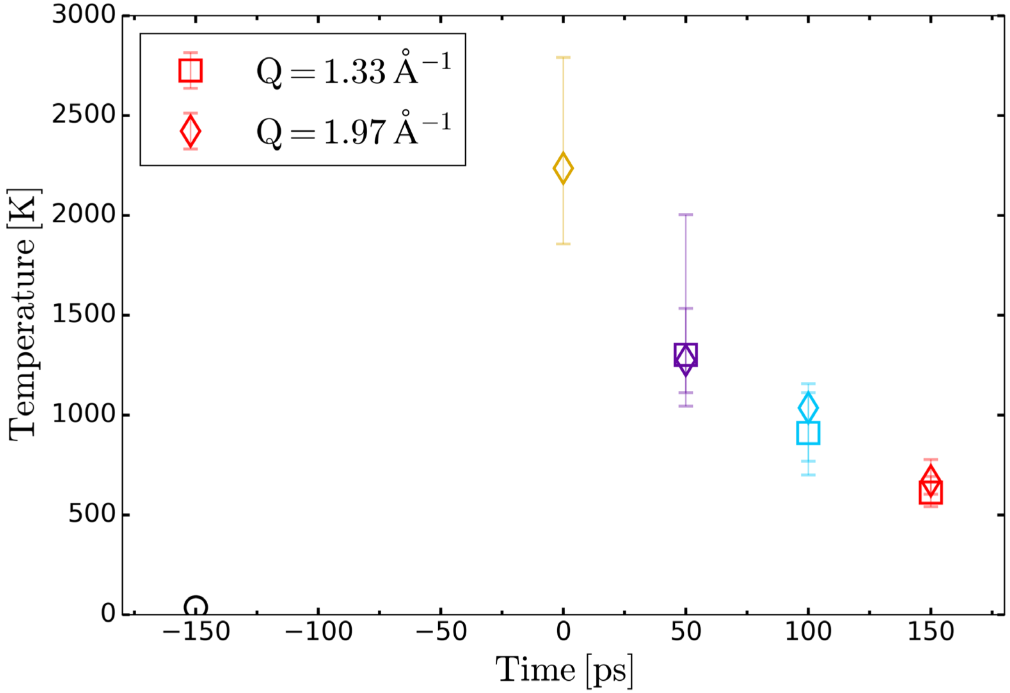
The temperature is obtained from the asymmetry of the spectrum

Evolution of the measured temperature as a function of probe delay



Principle of detailed balance

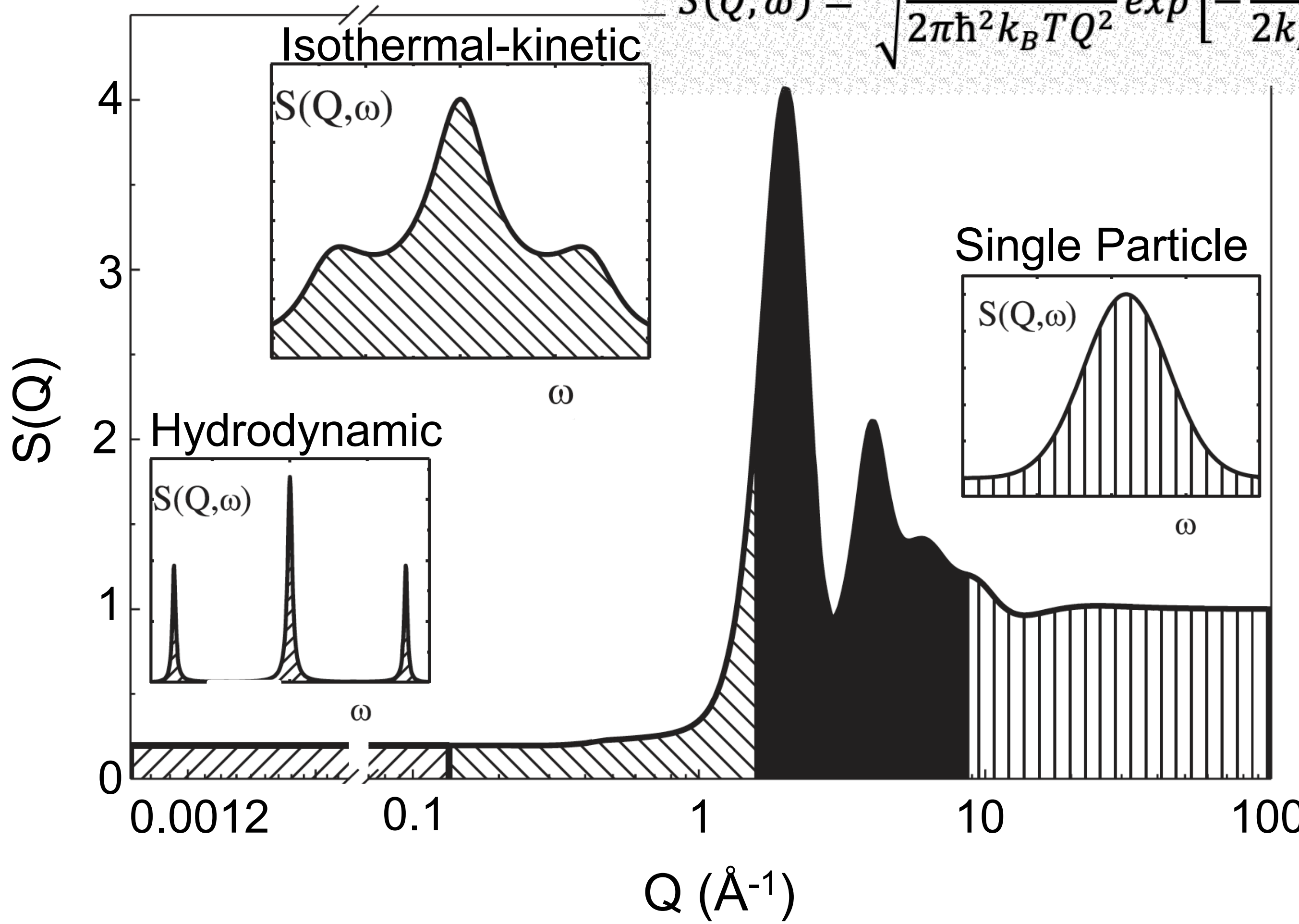
$$\frac{S(-\hbar\omega, -Q)}{S(\hbar\omega, Q)} = e^{\hbar\omega/k_B T}$$

The asymmetry vanishes for “high” temperatures.

a.descamps@qub.ac.uk

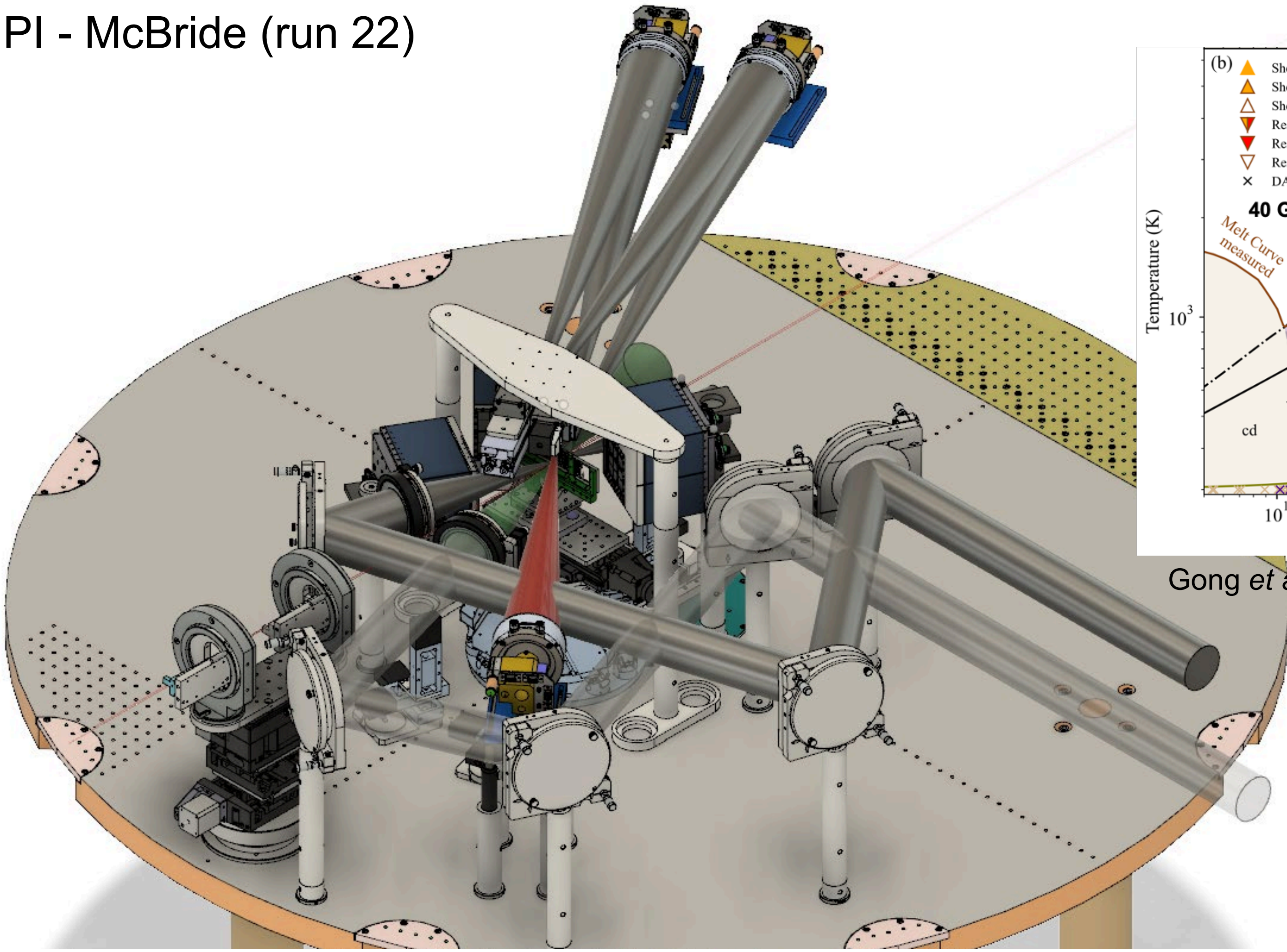
The temperature can also be measured in the single particle regime

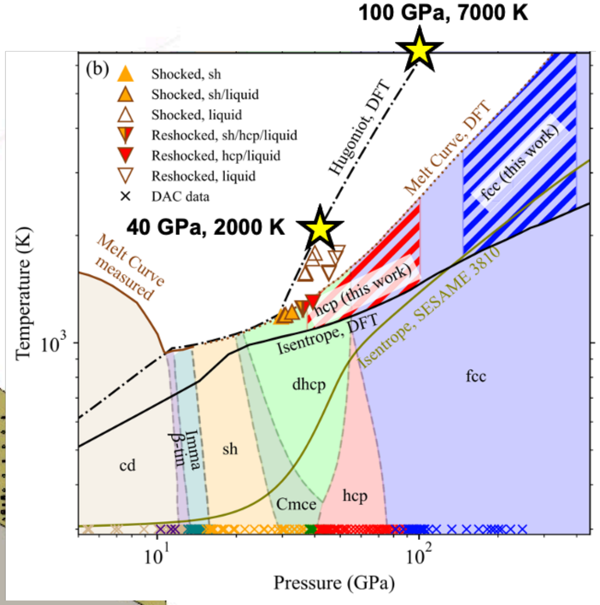
$$S(Q,\omega) = \sqrt{\frac{M}{2\pi\hbar^2 k_B T Q^2}}\, exp\left[-\frac{M}{2k_B T Q^2}(\omega-\omega_r)^2\right]$$



Direct measurement of temperature of shock-compressed silicon using forward and backward scattering at MEC, LCLS

PI - McBride (run 22)

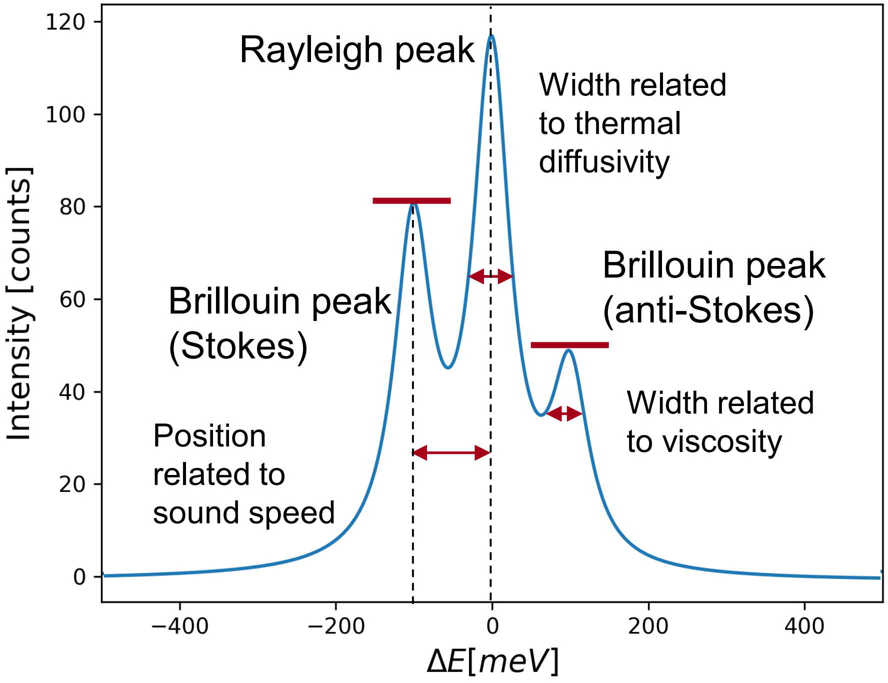




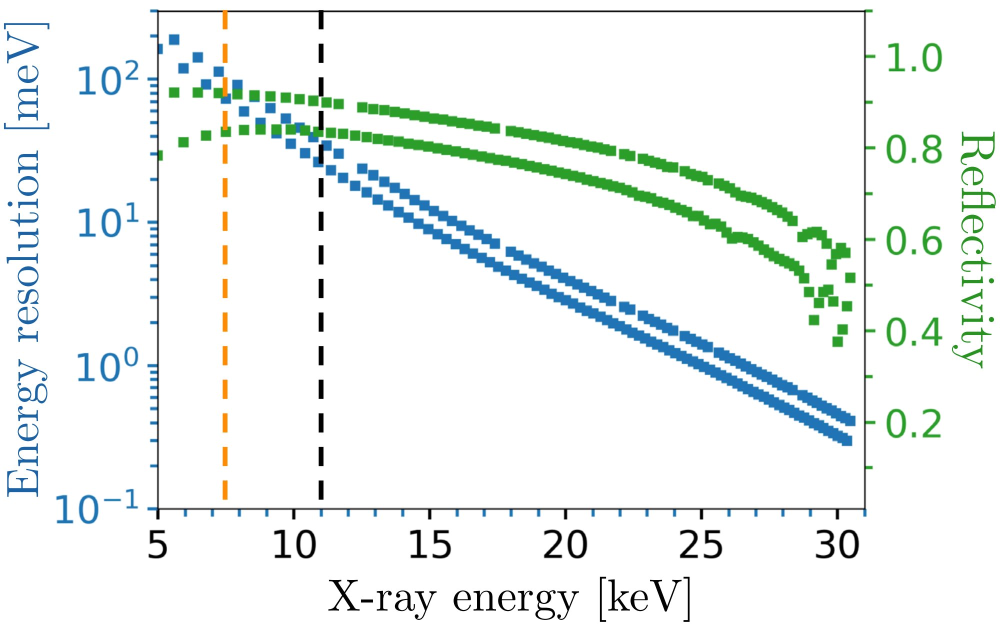
Gong *et al.*, PRL, **130,** 076101 (2023)

a.descamps@qub.ac.uk

The energy resolution of the spectrometer improves with harder X-rays



Energy resolution and reflectivity of silicon optics

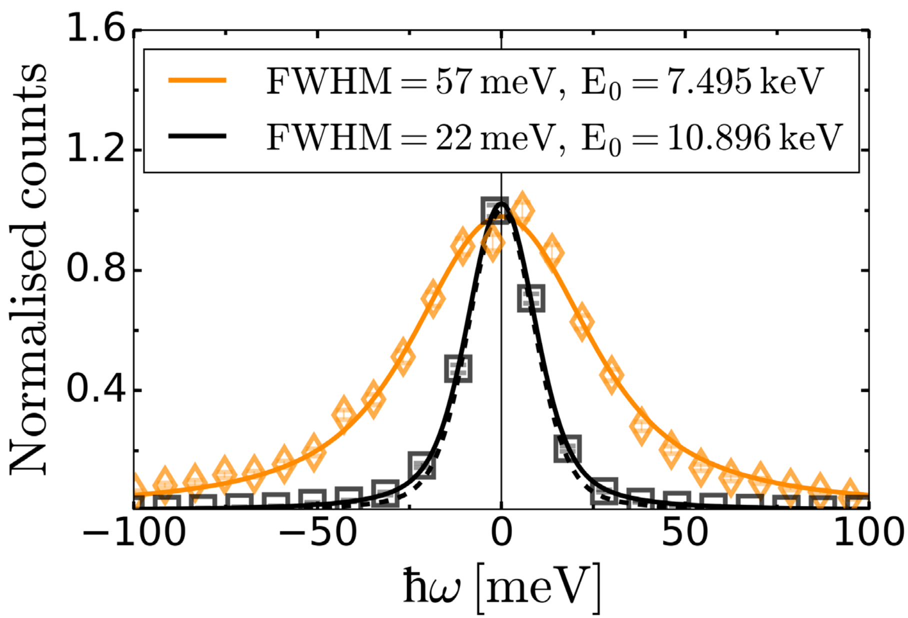


a.descamps@qub.ac.uk

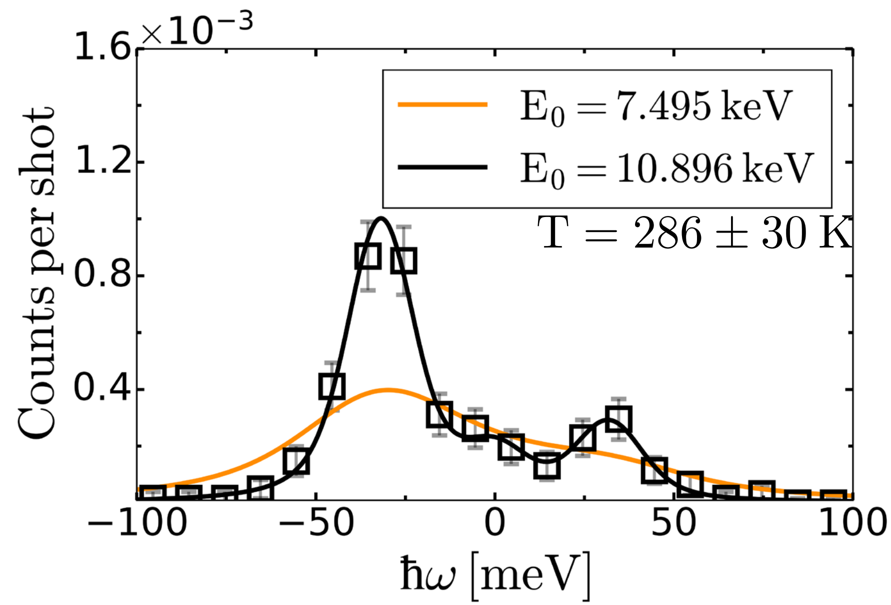
The energy resolution of the spectrometer improves with harder X-rays

Descamps. A *et al. J. Synchrotron Rad. 29, 931 (2022)*

Measured instrument functions at LCLS on 50 µm PMMA



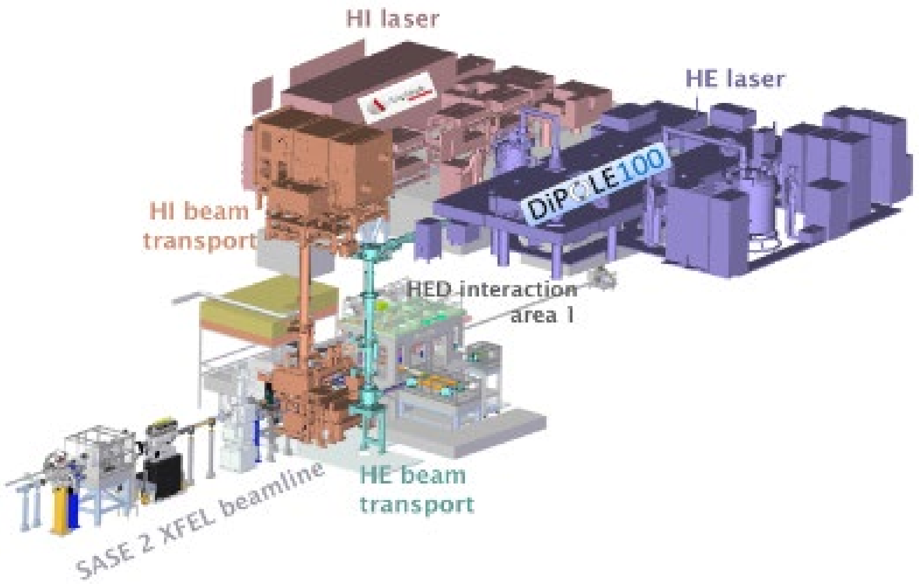
Inelastic spectrum from 10 μm Fe (at ambient conditions)

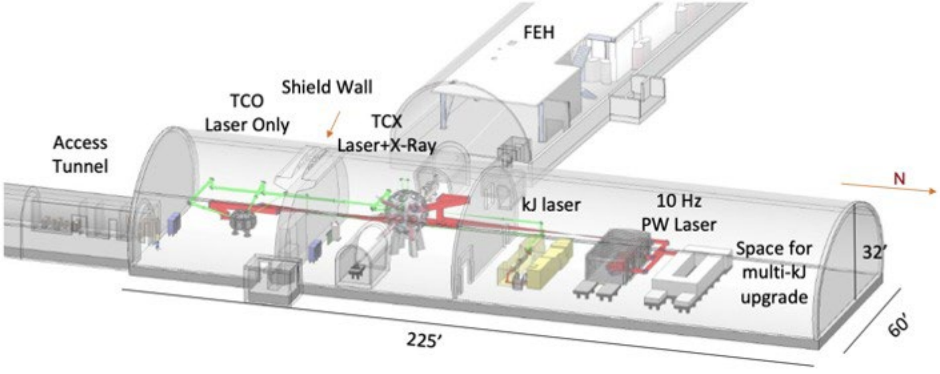


With an improved resolution, one can access materials relevant for planetary science and measure temperature.

a.descamps@qub.ac.uk

The improved energy resolution comes at the cost of lower photometrics





Dipole Laser systems at the HED endstation EuXFEL
DIPOLE-100X: 100 J, 2-15 ns, 10 Hz

MEC Upgrade at LCLS
High rep-rate long pulse (expected): 200 J, 10 ns, 10 Hz

The coupling of hard X-rays Free Electron Lasers and high repetition rate drivers can help compensate for the lower photometrics at higher X-ray energies.