Time-resolved diffraction at an X-ray free-electron laser: femtosecond pump–probe and MHz studies at extreme conditions

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X-ray free-electron lasers (XFELs) enable diffraction experiments in regimes that are difficult or impossible at storage-ring sources: femtosecond time resolution, very high peak brightness, and—in the case of the European XFEL—pulse trains that support MHz-class data acquisition. In this keynote, I will discuss how these capabilities are being used at the HED-HiBEF instrument at the European XFEL to advance time-resolved structural science under extreme conditions, with an emphasis on diffraction and total scattering approaches that connect naturally to the powder-diffraction community.

First, I will focus on high-repetition-rate (MHz) diffraction from diamond anvil cells, where MHz diffraction and efficient detectors enable statistically robust mapping of phase boundaries and transient/metastable states. As recent examples, I will present *in situ* diffraction of the pressure-induced α→ε transition in iron at intermediate strain rates, demonstrating how time-resolved diffraction constrains transformation pathways and kinetics beyond static compression data sets [1]. Further results include multiple freezing–melting pathways in high-density ice via ice XXI at room temperature [2], and the synthesis and crystallographic characterization of gold hydride at high pressure and temperature [3].

Secondly, I will highlight single-shot and pump–probe diffraction of laser-driven shock compression, where structural transitions can be captured on femtosecond-to-nanosecond timescales. Recent results include structural motifs in superionic water, including mixed close-packed ordering [4]. I will further discuss the emergence of ultrafast total scattering and pair distribution function (PDF) measurements at XFELs, which extend beyond Bragg diffraction to local structure in disordered and nanoscale systems [5], and I will relate these methods to studies such as *in situ* diffraction of liquid carbon at extreme conditions [6].

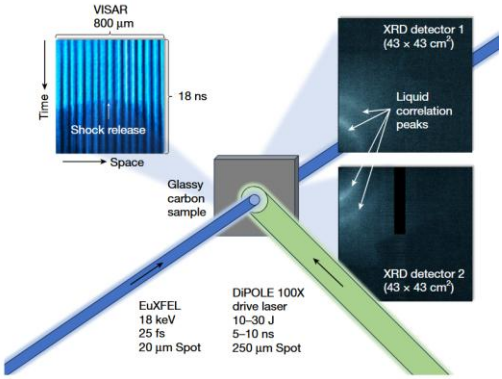


Figure 1. | *Schematic of the experimental setup in ref. [6].*

Overall, the talk will outline practical measurement concepts (setup and drivers, target chamber geometry, detectors, data reduction) and show how femtosecond and MHz diffraction at XFELs is becoming a complementary, quantitative toolset for phase-transition science across crystalline, partially ordered, and liquid states.

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[6] Kraus, D. *et al.*, Nature (2025). 642, 351–355.