

Advancing crystallography with high-pressure single-crystal diffraction techniques

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High-pressure instrumentation such as diamond anvil cells enables the synthesis and study of novel materials with extraordinary properties. By subjecting samples to extreme pressures and temperatures—typically tens to hundreds of GigaPascal and thousands of Kelvin—it becomes possible to access a wide range of thermodynamically stable and metastable states of matter, and to induce the formation of crystalline compounds with bonding configurations unattainable under ambient conditions.

Historically, structural characterization under such conditions has been limited by significant experimental challenges, including restricted angular access, strain effects, poor crystallinity, and multiphase mixtures. However, recent developments are transforming the field. The advent of synchrotron X-ray sources with ultra-high-flux and micron-focused beams, coupled with high-resolution detectors and new algorithms capable of processing multigrain single-crystal diffraction datasets, now allows precise structure determination from individual submicron crystallites within polycrystalline samples.

This methodological shift—treating polycrystalline samples as ensembles of microcrystals rather than a “bad powder”—has begun to revolutionize high-pressure crystallography and holds significant promise for ambient-pressure applications as well, particularly for samples that are difficult to grow as large single crystals. In this talk, I will present the current capabilities and limitations of these methods, and highlight examples from my recent research.