Invited Lecture

Half a Century of High-Pressure Single Crystal Diffraction: From Laboratory Pioneers to Synchrotron Multigrain Crystallography

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Fifty years ago, Dr. Leo Merrill and Professor Bill Bassett developed a miniature Diamond Anvil Cell for single crystal diffraction (Merrill and Bassett, 1974). They used this simple but innovative tool to determine the crystal structure of $CaCO_3$-II, a high-pressure polymorph of one of Earth's most common minerals that cannot be retained at ambient conditions. This groundbreaking device enabled systematic exploration of crystal chemistry under non-ambient conditions, leading to increasingly accurate structure refinements of materials under static compression with laboratory equipment.

Over the past three decades, this technique has also been successfully applied at synchrotron sources to determine structures following first-order phase transitions. Recent studies have uncovered unique structural details of materials across a wider range of pressures and temperatures.

This presentation reviews the evolution and current state of single crystal diffraction under extreme conditions. Through examples from Ca-carbonates, alkali carbonates, Fe-oxides, and Mg-silicates, we highlight how modern techniques now allow for the structural determination of unquenchable phases and tiny single crystal domains within multigrain and multiphase samples after chemical reactions.