High Pressure Raman Spectroscopy of $IrTe_2$ up to 25.9 GPa: Spectroscopic Mapping of Lattice Destabilization and Amorphization

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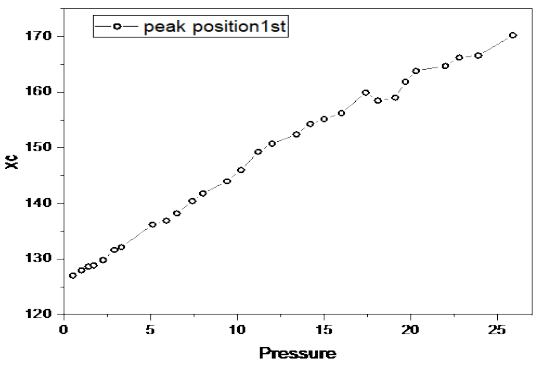
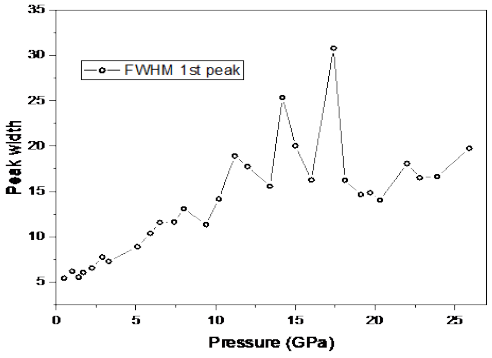
Abstract

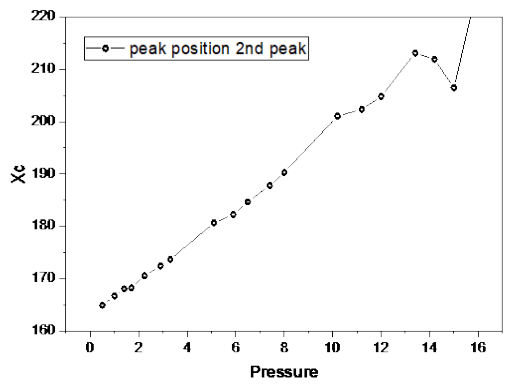
The transition metal dichalcogenide $IrTe_2$ exhibits a fascinating, closely competing phase landscape governed by exotic charge-ordering, local structural dimerizations, and superconductivity. While macroscopic boundaries and long-range structural modifications have been previously mapped using X-ray diffraction techniques, a continuous, localized spectroscopic investigation under high static pressures remains essential to understanding local structural reconstructions and atomic-scale distortions. In this work, we present a detailed high-pressure Raman scattering study of single crystalline $IrTe_2$ executed continuously up to a maximum pressure of 25.9 GPa at room temperature using a diamond anvil cell (DAC).

At ambient conditions, the recorded spectra are dominated by two prominent, well resolved Raman active optical phonon modes located near 128 cm^{-1} and 165 cm^{-1}, assigned to the E_g in-plane shear and A_{1g} out-of-plane symmetric stretching modes, respectively. Under increasing pressure, the reduction of interatomic distances induces a primary blue shift in the peak positions (ω) toward higher wavenumbers. From 0.5 GPa up to approximately 3.3 GPa, both the E_g and A_{1g} modes exhibits a highly linear, tightly constrained pressure dependence (dω/dP). However, around 5.1 GPa, distinct anomalies emerge in the phonon frequency slopes and full width at half maximum (FWHM) profiles for both modes, providing clear spectroscopic confirmation of the macroscopic transition to the low symmetry dimerized phase.

Crucially, a severe structural destabilization is tracked between 10 GPa and 14 GPa. Within this regime, the crystal lattice undergoes an intense structural instability, where the stretching mode exhibits a massive broadening anomaly with the FWHM exceeding 128 cm^{-1} at 13.4 GPa accompanied by a sharp frequency softening beyond this point. Upon further pressure elevation above 17.4 GPa and extending up to 25.9 GPa, the sharp crystalline modes completely merge into a singular, highly diffuse, and heavily broadened multi-phonon band. This behavior provides direct spectroscopic evidence of an extreme, pressure induced lattice amorphization, which serves as a definitive experimental benchmark for the high pressure phase diagram of correlated 5d transition metal dichalcogenides.







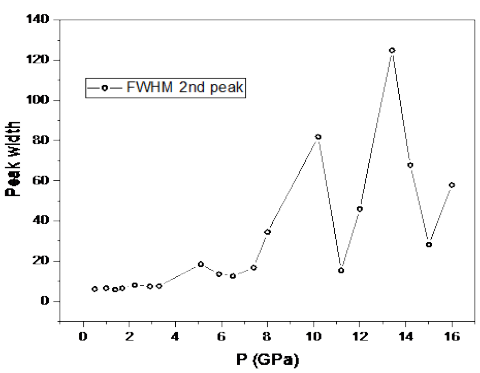


Figure 1: Pressure dependence of the phonon peak positions (wavenumbers) and full width at half maximum (FWHM) profiles for the E_g and A_{1g} modes of single-crystalline $IrTe_2$. The data clearly illustrates the initial linear regimes, the dimerization anomaly at 5.1 GPa, and the severe structural destabilization and softening tracking beyond 13.4 GPa.