Anisotropic atomic displacement in layered materials under high pressure

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Transition metal dichalcogenides (TMDs) exhibit fascinating properties, with important applications for nanoelectronics, photonics, sensing, energy storage, and opto-electronics. Compared to well-studied MoS2 with isotropic hexagonal phase, WTe2 forms a distorted octahedral geometry with reduced symmetry that strongly enhances the anisotropy in the unit cell, which further shows astonishing characteristics in optoelectronic and electronic applications. This distorted crystal structure shows fast response to external stimulation, such as pressure, temperature and light pulse, which originated from symmetry transfer among different phases. However, up to date, unambiguous phase transition mechanism remains controversial. Even, there is few report about high pressure single crystal diffraction of TMD.

In this work, by means of high pressure single crystal diffraction we found that W and Te atoms showed anisotropic atom displacement along the in-plane and out-plane direction under different pressure regions, which provides new insight into the sliding mechanism and diverse physical properties under high pressure.