Pressure-Induced Optical Anisotropy of HfS_2

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In this work, we study the transition metal dichalcogenide (TMD) hafnium disulfide (HfS_2) by Raman scattering (RS) under high-pressure (HP). HfS_2 has been quote to the development of thermoelectric and optoelectronic devices. [1] We probed the polarization of the scattered beam, as well as the angle-resolved polarized RS (ARPRS), which provides us the in-plane anisotropy of the crystal. The HP was stablished with the aid of a diamond anvil cell (DAC).

Under hydrostatic conditions, the RS lineshape shows a systematic blueshift of the spectral features (Fig. (a)). However, to the non-hydrostatic regime (P>6.5 GPa), seven new peaks emerge in the spectrum. The simultaneous observation of both ambient and HP features, suggests the coexistence of different phases. The ARPRS reveals that the isotropy angular dependence of HfS_2 (*e.g.* A_{1g} mode in Fig. (b)) is lost in the non-hydrostatic regime, showing a huge in-plane anisotropy under P=7.4 GPa (Fig. (c)).

In conclusion, we proposed that the original 1T-HfS_2 is distorted by the non-hydrostatic component, leading to the orthorhombic crystal structure. Simultaneously, a new phase appeared, which was related to a distorted *Pnma* structure. [2] Our findings point how the non-hydrostatic environment facilitated the emergence of a new phase in HfS_2 at lower pressure compared to hydrostatic one. Furthermore, ARPRS excited by λ=561 nm shows a more complex dependence, highlighting the role of resonant effects in ARPRS experiments.

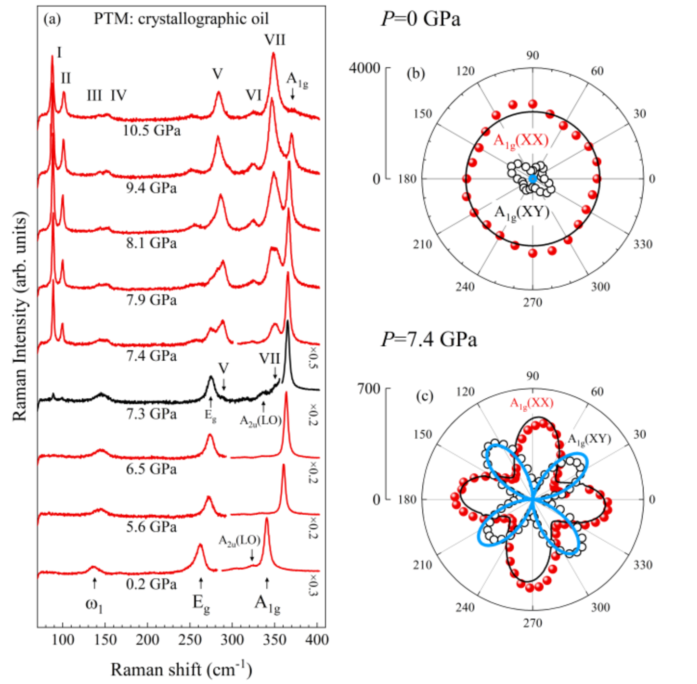

Figure: The evolution of the RS spectra in HfS_2 during the compression (a) and the ARPRS angular dependence of A_{1g} under P=0 GPa (b) and 7.4 GPa (c). The measurements were taken under λ=633 nm excitation.

[1] Deobrat Singh and Rajeev Ahuja, *ACS Applied Energy Materials 2* (9), 6891-6903 **(2019)**.
[2] Zhang Shihui, Wang Hailun, *et al.*, Physical Review Materials 7, 104802 (2023).