

ARTICLE

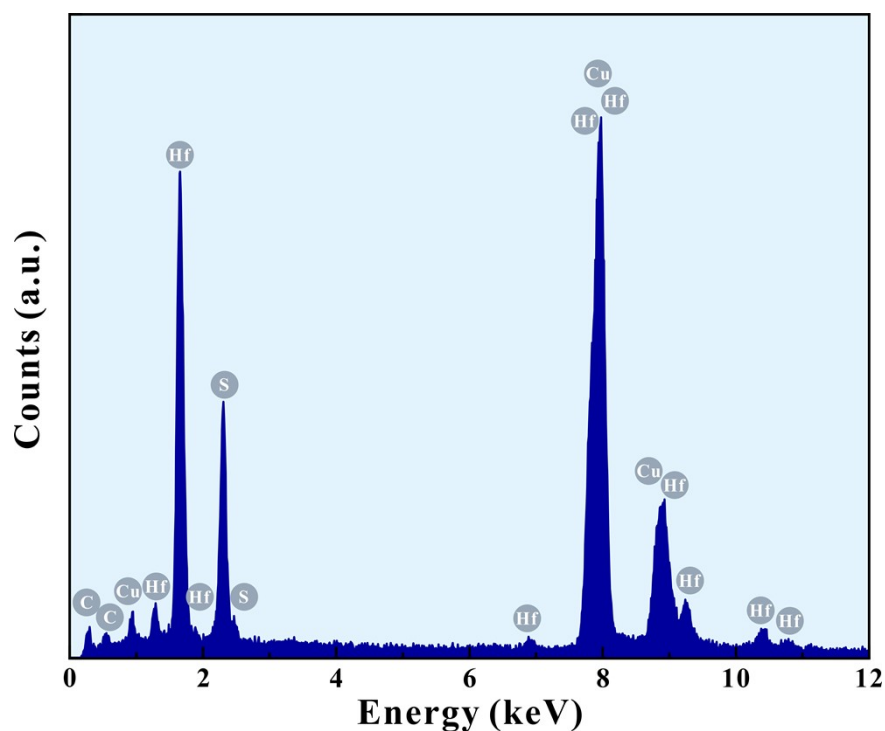
High-pressure structural phase transitions and metallization in layered HfS_2 under different hydrostatic environments up to 42.1 GPa

Received 22th April 2022,
Accepted 00th January 20xx

DOI: 10.1039/x0xx00000x

Meiling Hong,^{ab} Lidong Dai,^{*a} Haiying Hu,^{*a} Xinyu Zhang,^{ab} Chuang Lj^{ab} and Yu He^{ab}

Supplementary Figures and Table

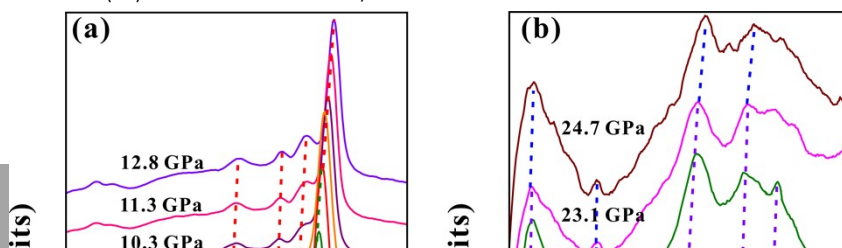


Supplementary Figure 1. Transmission electron microscope equipped with an energy dispersive X-ray spectroscopy (TEM-EDS) of the starting HfS_2 sample.

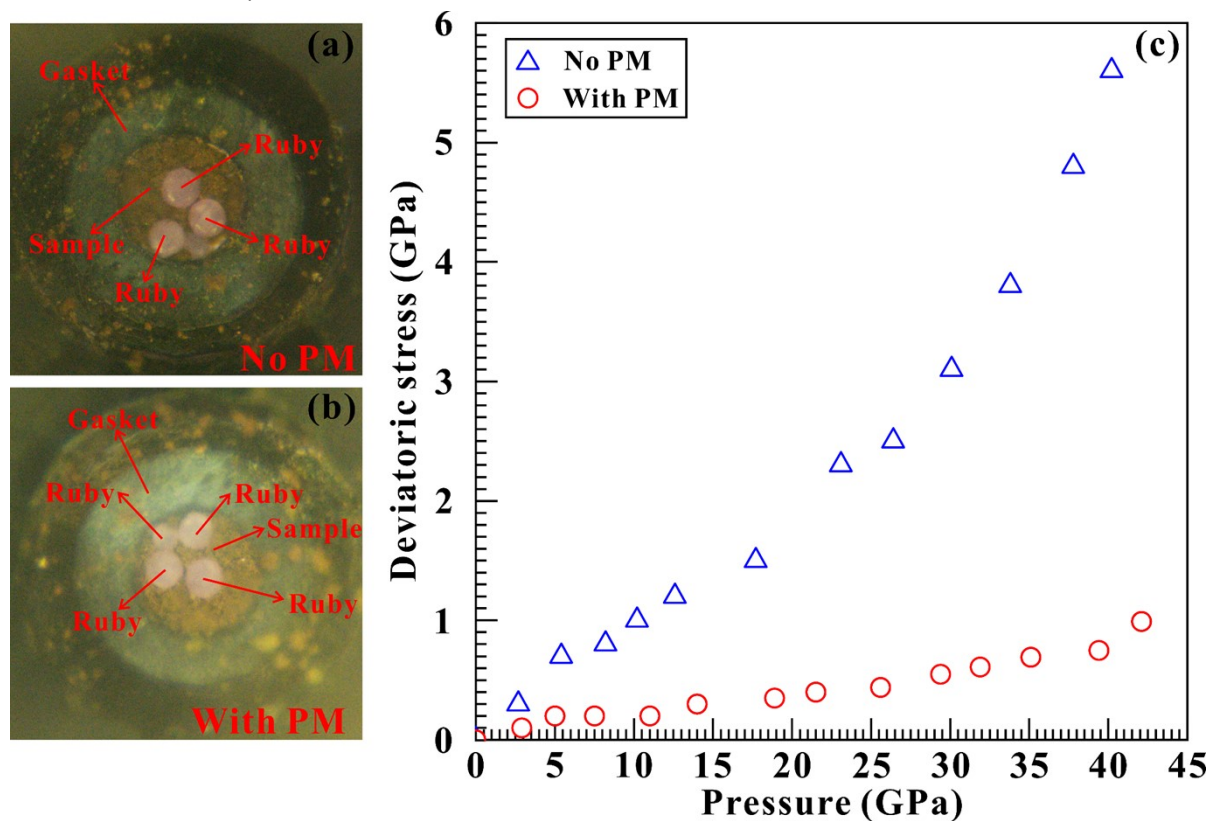
^a Key Laboratory of High-temperature and High-pressure Study of the Earth's Interior, Institute of Geochemistry, Chinese Academy of Sciences, Guiyang, Guizhou 550081, China. Email: dailidong@vip.gyig.ac.cn, huhaiying@vip.gyig.ac.cn

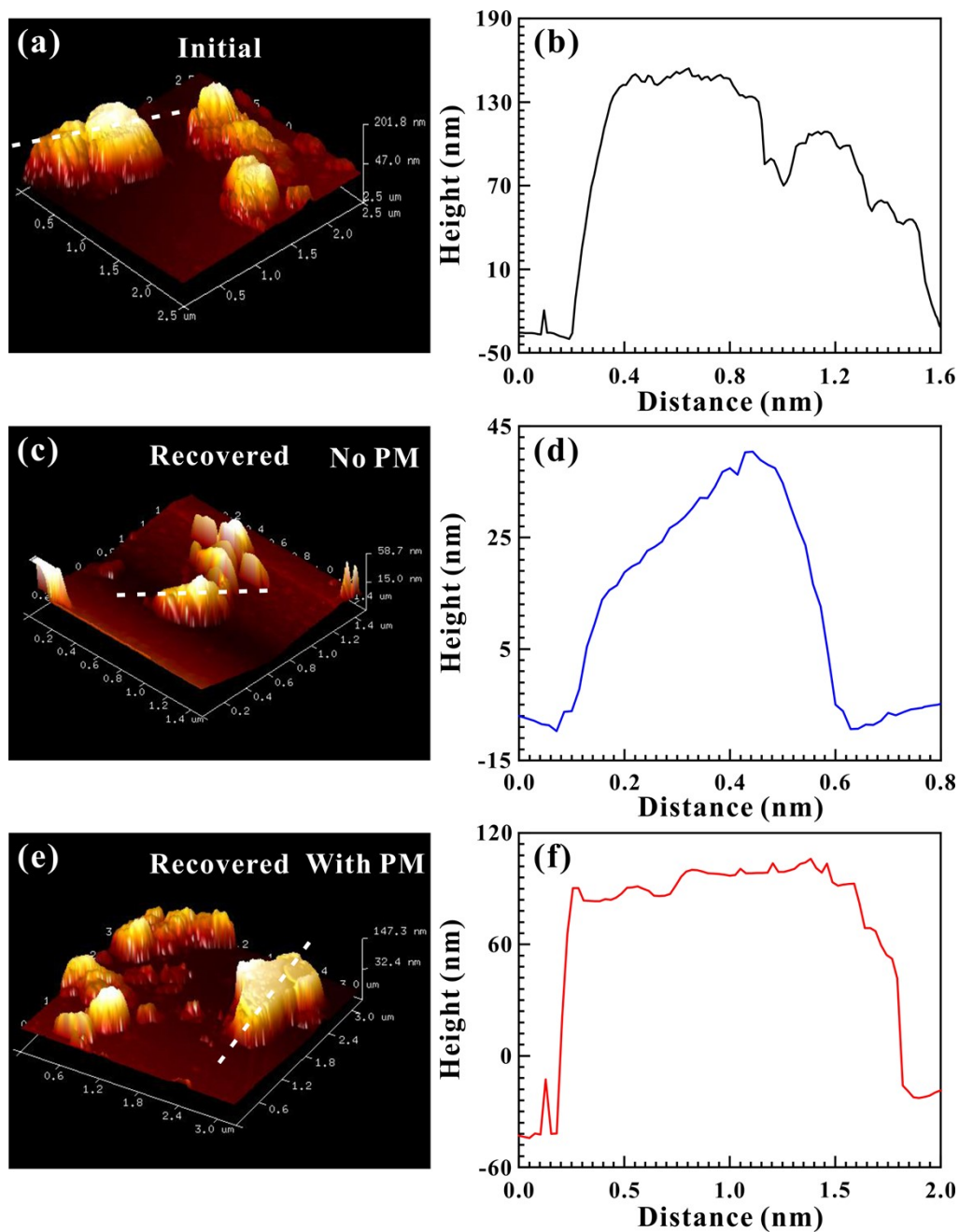
^b University of Chinese Academy of Sciences, Beijing 100049, China

Electronic Supplementary Information (ESI) available. See DOI: 10.1039/x0xx00000x



Supplementary Figure 3. (a) and (b) represent the optical microscope images of sample chamber under non-hydrostatic and hydrostatic conditions, respectively. In here, PM stands for pressure medium. (c) The relations between deviatoric stress and pressure under different hydrostatic environments.





Supplementary Figure 4. Three-dimensional surface topography images of atomic force microscopy (AFM) and their correspondent distance-height relationships for HfS_2 . Herein, (a) and (b) represent the starting sample; (c) and (d) are the recovered sample decompressed from 38.2 GPa under non-hydrostatic condition; (e) and (f) stand for the recovered sample released from 37.9 GPa under hydrostatic condition. Herein, PM represents pressure medium.

Supplementary Table 1. The relationship between diffraction angle (2θ) and full width at half maximum (FWHM) for HfS_2 .

2θ (°)	FWHM (cm^{-1})
14.99	0.210±0.033
28.31	0.171±0.040
30.38	0.219±0.040
32.22	0.272±0.065
42.07	0.328±0.042
46.37	0.350±0.111
50.18	0.179±0.039
52.70	0.222±0.052
55.28	0.401±0.048
58.66	0.183±0.033
59.87	0.312±0.097
60.95	0.279±0.0908
63.36	0.410±0.062
67.54	0.376±0.100