Supplementary Information

Pressure-induced metallization and electronic transition in two-dimensional ferroelastic semiconductor of Nb$_2$SiTe$_4$ under different hydrostatic environments

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AFFILIATIONS

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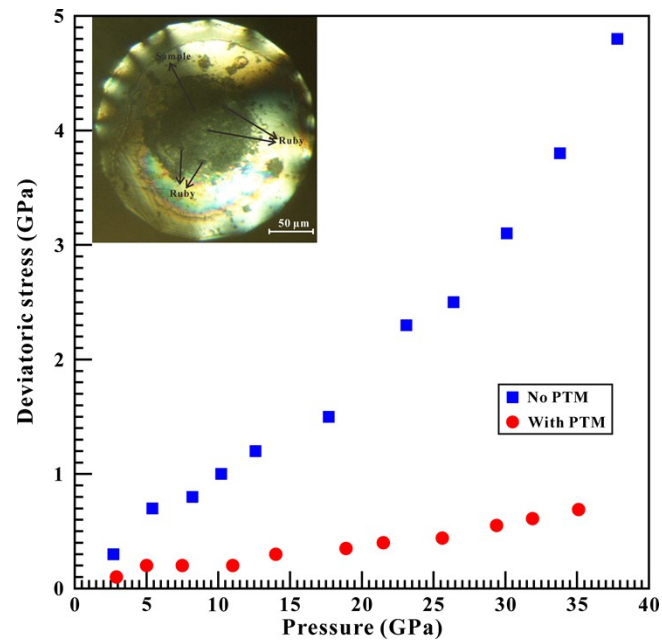
Fig. S1 The relationship between deviatoric stress and pressure under different hydrostatic environments. Inset: the optical image of the sample chamber in a diamond anvil cell. Herein, the signal of PTM stands for pressure transmitting medium.
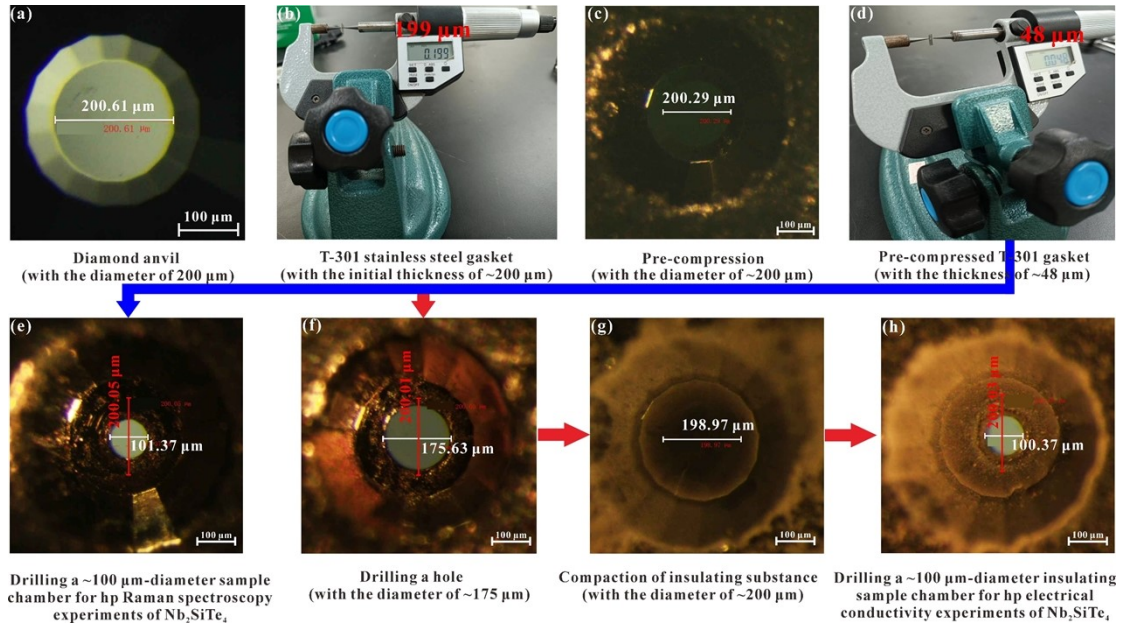
Fig. S2 The detailed procedures on the high-pressure Raman spectroscopy and electrical conductivity experiments of Nb$_2$SiTe$_4$. Herein, the symbol of ph denotes high pressure.
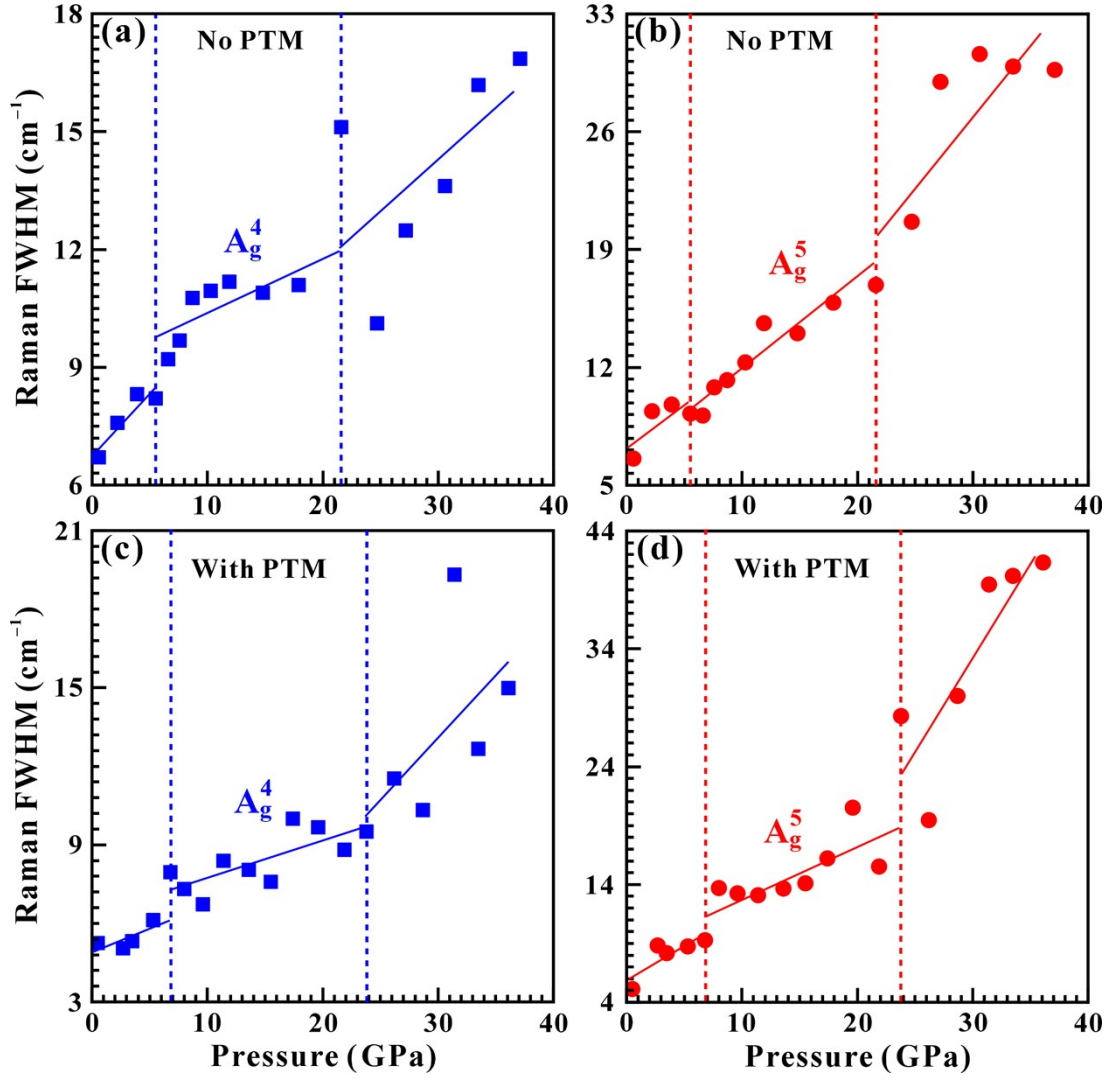
Fig. S3 The evolution of Raman FWHM as a function of pressure for (a) A_g^4 mode and (b) A_g^5 mode under non-hydrostatic condition as well as (c) A_g^4 mode and (d) A_g^5 mode under hydrostatic condition, respectively. Herein, the signal of PTM signifies pressure transmitting medium. The errors in Raman FWHMs are within the size of the symbols. The colored solid and dashed lines are visual guides.
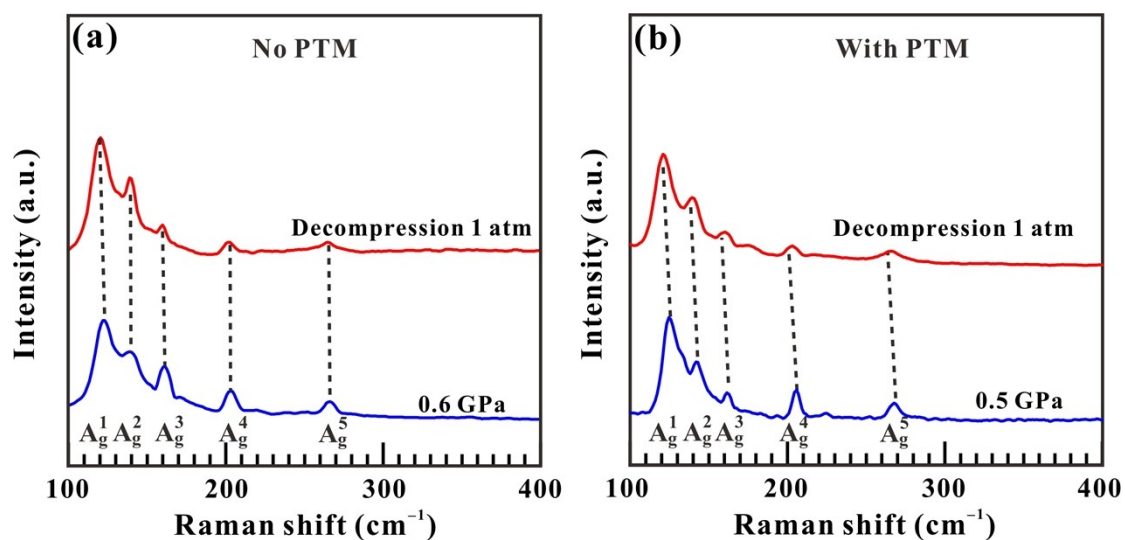
Fig. S4 The comparison of Raman spectra for the starting and recovered samples under (a) non-hydrostatic condition and (b) hydrostatic condition, respectively. Herein, the signal of PTM denotes pressure transmitting medium. The black dashed lines are used to guide to the eyes.

Table S1 Pressure-dependent Raman FWHMs ($\mathrm{d}F/\mathrm{d}P$, cm^{-1} GPa^{-1}) of Nb$_2$SiTe$_4$ upon compression under different hydrostatic environments. Herein, F (cm^{-1}) and P (GPa) represent Raman FWHM and pressure, respectively.

Pressure condition	Pressure range (GPa)	A_g^4	A_g^5
Non-hydrostatic	0.6–3.9	0.32	0.51
	5.5–17.9	0.14	0.55
	21.6–37.1	0.26	0.85
Hydrostatic	0.5–5.3	0.18	0.74
	6.8–21.9	0.14	0.44
	23.8–36.1	0.48	1.60

Table S2 The detailed values of the cross-sectional area of electrodes (S) and the distance between electrodes (L) at five representative pressure points of 0, 5.4, 9.5, 14.1 and 17.0 GPa.

Pressure (GPa)	L (cm)	S (cm^2)
0	0.0050	0.00011217
5.4	0.0048	0.00009059
9.5	0.0046	0.00006998
14.1	0.0043	0.00006011
17.0	0.0041	0.00005422