

Persistence of the $R3m$ Phase in Powder GeTe at High Pressure and High Temperature

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Fig. S1 X-ray diffraction patterns of GeTe plotted against pressure in the first experimental run with silicone oil as the pressure transmitting medium. The inset shows the relationships of the FWHM of peaks a—e versus pressure for GeTe.

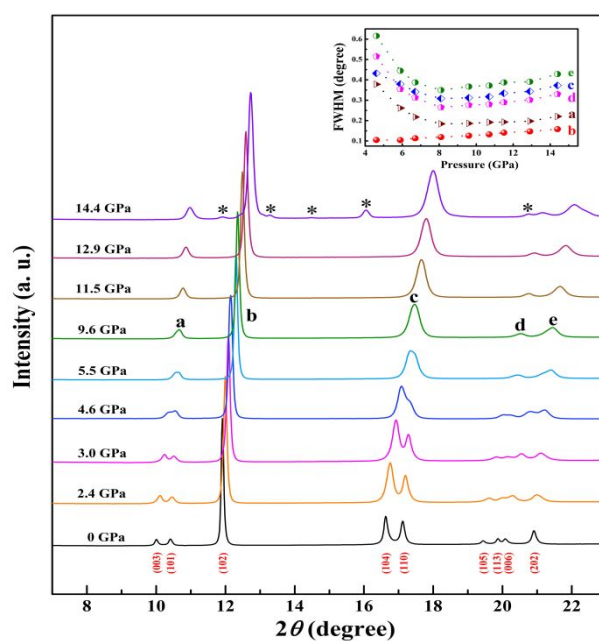


Fig. S2 Typical Rietveld refinement results of α -GeTe under ambient conditions. The

black open circles and red solid line represent the experimental and simulated data, respectively, and the blue solid lines at the bottom are the residual intensities. The solid short vertical bars indicate the peak positions.

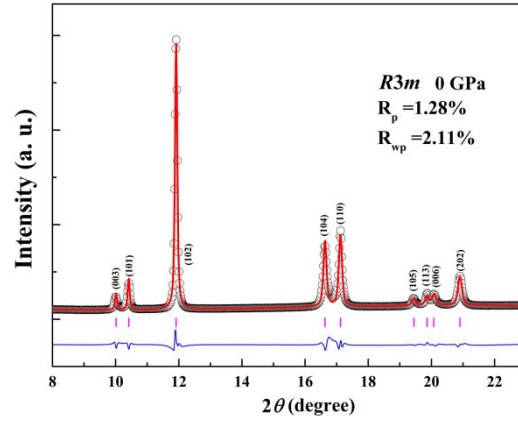


Fig. S3 (a) Calculated total energy versus volume for the $R3m$ and B1 phases of GeTe, the inset shows the total energy of the two structures in the volume range 45–50 Å³. (b) Enthalpy difference (relative to $R3m$ phase) of two structures as functions of pressure in GeTe. The total energy and enthalpies are given per formula unit.

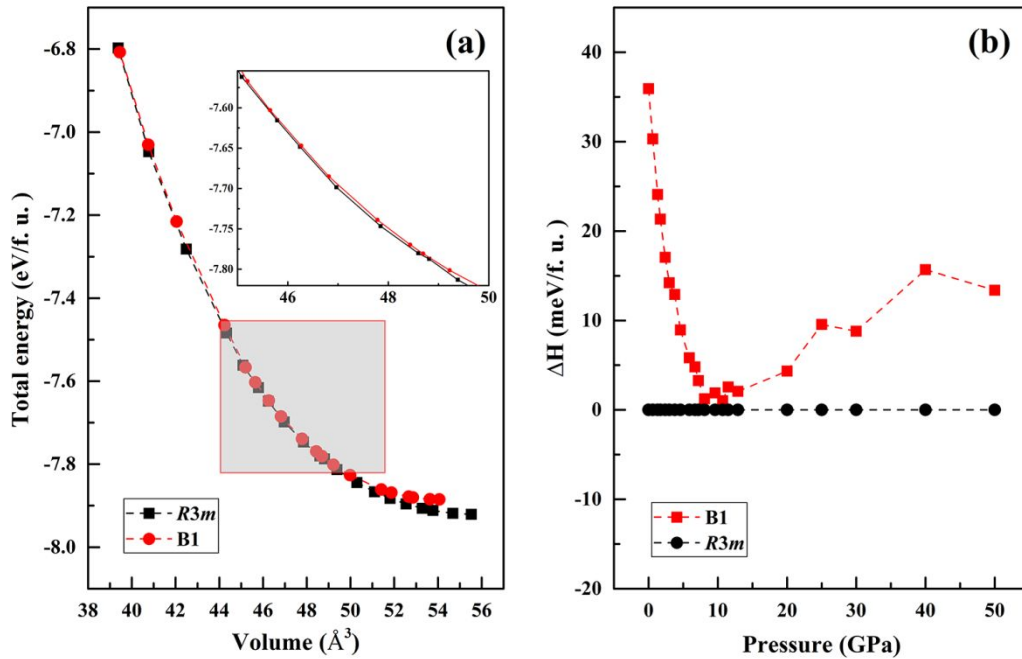


Table S1 The full unit cell results versus pressure for the $R3m$ phase of GeTe in the first experimental run with Ne as the pressure transmitting medium.

P (GPa)	a	$\sigma(a)$	c	$\sigma(c)$	V	$\sigma(V)$	$u(\text{Te})$	$u(\text{Ge})$	σ
2.2	4.14976	2.48E-4	10.31585	9.09E-4	153.844	0.073	0.24174	0.76163	3.64E-04
3.5	4.11931	3.74E-4	10.18314	0.00197	149.645	0.034	0.23322	0.76074	3.25E-04
4.9	4.08695	3.59E-4	10.06457	0.00193	145.588	0.049	0.23237	0.75952	2.59E-04
7.1	4.04371	3.32E-4	9.95594	0.00175	140.985	0.145	0.23075	0.75894	3.67E-04
10.1	4.00049	3.06E-4	9.85082	0.0016	136.530	0.097	0.23044	0.75711	4.32E-04
13.4	3.96094	2.82E-4	9.73832	0.0015	132.316	0.083	0.23107	0.75601	3.75E-04

Table S2 The full unit cell results versus pressure for the $R3m$ phase of GeTe in the second experimental run with silicone oil as the pressure transmitting medium.

P (GPa)	a	$\sigma(a)$	c	$\sigma(c)$	V	$\sigma(V)$	$u(\text{Te})$	$u(\text{Ge})$	σ
0.0	4.16661	3.13E-04	10.66107	0.00132	160.287	0.043	0.76613	0.23815	3.14E-04
0.6	4.16157	3.18E-04	10.63065	0.00151	159.442	0.064	0.76541	0.23752	4.27E-04
1.3	4.15305	7.03E-04	10.5819	0.00187	158.063	0.069	0.76468	0.23725	4.99E-04
1.7	4.14309	0.0011	10.51931	0.00281	156.375	0.105	0.76343	0.23699	4.27E-04
2.4	4.13612	0.00113	10.4611	0.00283	154.896	0.107	0.7631	0.2369	5.33E-04
3.0	4.12784	0.00157	10.40012	0.00415	153.467	0.053	0.7627	0.23674	5.25E-04
3.8	4.12057	5.18E-04	10.31984	1.90E-04	151.746	0.01	0.76137	0.23611	4.47E-04
4.6	4.10848	3.52E-04	10.28015	0.00145	150.277	0.054	0.76103	0.23548	3.04E-04
5.5	4.09809	6.32E-04	10.18819	0.00202	148.18	0.077	0.7585	0.23443	2.94E-04
6.7	4.09136	0.0015	10.16078	0.00274	147.324	0.051	0.75791	0.22996	4.62E-04
7.2	4.08113	0.00178	10.11018	0.00174	145.831	0.069	0.75629	0.22995	3.88E-04
8.1	4.05952	0.0086	10.01508	0.00253	142.934	0.072	0.74798	0.22996	6.97E-04
9.6	4.03749	0.00484	9.95981	0.00986	140.606	0.079	0.74749	0.22952	5.47E-04
10.7	4.02197	0.00674	9.92527	0.01329	139.042	0.065	0.74795	0.22958	3.34E-04
11.5	4.00686	0.00432	9.88563	0.01227	137.449	0.039	0.74734	0.22959	7.09E-04
12.9	3.98892	0.00412	9.83628	0.01839	135.541	0.087	0.74669	0.23001	5.28E-04