## **Supporting Information**

Zhang et al. 10.1073/pnas.1014085108

<



Fig. S1. The carrier density of Bi<sub>2</sub>Te<sub>3</sub> single crystal at ambient and 1.0 GPa, respectively, showing a slight increase with pressure.



Fig. S2. The Rietveld refinements of the crystal structure for Bi<sub>2</sub>Te<sub>3</sub> at 4.0 GPa at room temperature. The cross and red line correspond to that for experiment and refinement, respectively, while the blue is the difference.



Fig. S3 The crystal structure of  $Bi_2Te_3$ .

OGPa	atom		site		х	у	Z
	Bi		6c		0	0	0.400 (0.44)
	Te1 Te2		3a		0	0	0.0 (0.0)
			6с		0	0	0.2095 (0.2094)
	Bi-Te1 (Å)	Bi-Te2 (Å)	Te1-Bi-Te1 (°)	Te1-Bi-Te2 (°)	d1 (Å)	d2 (Å)	d3 (Å)
	3.2551	3.0808	84.805	90.874	2.0434	1.7515	2.6243
	a = b = 4.390 (4.400) Å, c = 30.497 (30.335) Å, $lpha$ = 90°, $eta$ = 90°, $\gamma$ = 120°						
4GPa	a atom Bi Te1 Te2		site 6c 3a		x	у	Z
					0	Ō	0.4030 (0.401)
					0	0	0.0 (0.0)
			6с		0	0	0.2059 (0.2055)
	Bi-Te1 (Å)	Bi-Te2 (Å)	Te1-Bi-Te1 (°)	Te1-Bi-Te2 (°)	d1 (Å)	d2 (Å)	d3 (Å)
	3.1845	2.9731	83.331	90.802	2.0411	1.6924	2.2989
$a=b=4.234$ (4.237) Å, $c=29.296$ (29.262) Å, $lpha=90^\circ,eta=90^\circ,\gamma=120^\circ$							

Table S1. The crystal structure data of  $Bi_2Te_3$  at ambient and 4.0 GPa at room temperature

The theoretically relaxed lattice constants and internal atomic sites are listed in parenthesis. The interlayer distance d1, d2, and d3 are defined in the structure