Supplementary Materials: Phase-change-induced martensitic deformation and slip system in GeSbTe

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Supplementary Figure Captions

Figure S1. HRTEM image of an as-grown GST film with no crystallized regions.

Figure S2. (a) HRTEM images of the monoclinic phase, which has an FCC angle of 90°, after annealing at 220 °C. (b) Corresponding FFT diffraction patterns of this crystal, showing γ of 80.7° and monoclinic (200) and (020) lattice spacings of 3.06 and 2.99 Å, respectively. (c) HRTEM image of another monoclinic phase, showing an FCC angle of 90°, after annealing at 220 °C. (d) FFT diffraction patterns obtained from the crystal shown in (c), showing γ of 81.0° and monoclinic (200) and (020) lattice spacings of 3.18 and 3.10 Å, respectively.

Figure S3. (a) HRTEM images of the monoclinic phase, which has an FCC angle of 90°, after annealing at 220 °C. (b) Corresponding FFT diffraction patterns of this crystal, showing γ of 81.1° and monoclinic (200) and (020) lattice spacings of 3.03 and 3.02 Å, respectively. (c) HRTEM image of another monoclinic phase, showing an FCC angle of 90°, after annealing at 220 °C. (d) FFT diffraction patterns from the crystal shown in (c) with a γ angle of 87.8° and monoclinic (200) and (020) lattice spacings of 3.18 and 3.00 Å, respectively.

Figure S4. Volume shrinkage (\(\delta v\)) of the crystallized region of radius \(R_a\) within an amorphous matrix of radius \(R_b\). The crystallized region and the amorphous matrix are concentrically spherical in shape.

Figure S5. Images of the geometrically optimized \(4a\times4b\times4c\) GST structure with deformation angles (\(\gamma\)) of (a) 86°, (b) 78°, (c) 74°, and (d) 66°, which have the same configurations as those shown in Figs. 4(c)–(e). The red-dashed boxes correspond to a \(2a\times2b\) cell of the GST structure.

Figure S6. (a) HRTEM images of FCC crystal with slip system in the FCC (111) plane along the \([\bar{T}10]\) direction. (b) Corresponding Fourier-transformed diffraction patterns, showing FCC[100] and FCC[010] interplanar spacings of 2.99 and 3.07 Å, respectively, and an angle of 88.6° between these planes. (c) Side view of successive atomic motion in the FCC crystal during slip along \([\bar{T}10]\) in the (111) plane from 1 to 10. The green arrow indicates the direction of the slip.

Figure S7. Total DOS of GST materials for various values of γ ranging from 90 to 66°, as obtained by VASP simulation. The vertical dotted line indicates the Fermi level (\(E_F\)) of the DOS.
The gap below $E_F$ at 90° indicates the semimetallicity of the FCC crystal structure. After deformation, this gap is filled by electron states except at the angle of 70°.
Figure S1
Figure S2

(a) and (c) show high-resolution images of the material's surface, with a scale bar of 2 nm at the top and 1 nm at the bottom. The images display a clear lattice structure, indicating well-ordered atomic arrangements.

(b) and (d) present the corresponding electron diffraction patterns with a scale bar of 2 nm at the top and 5 nm at the bottom. The diffraction patterns are marked with the Miller indices M (020) and M (200), along with their respective lattice spacings of 2.99 Å, 3.06 Å, 3.18 Å, and 3.10 Å. The angles shown are 80.7° and 81.0°.

Fig. S2 Jang et al.
Figure S3

(a) M (020) 3.02 Å
(b) M (200) 3.03 Å
(c) M (020) 3.00 Å
(d) M (200) 3.18 Å

Fig. S3 Jang et al.
Figure S5

Fig. S5 Jang et al.
Figure S6

(a) FCC [110] 2 nm 2 nm

(b) FCC [100] 2.99 Å 3.07 Å

88.6° 88.6°

FCC [010]

(c) (111)(111) [110] [110]

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Fig. S6 Jang et al.
Figure S7

Fig. S7 Jang et al.