Supplementary materials

Ultrahigh overall-performance phase-change memory by yttrium dragging

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Supplementary Notes

The protocol for generating an amorphous model

Three models of amorphous Sb_2Te_3, $Y_{0.037}Sb_{2-0.037}Te_3$ (abbreviated to $Y_{3.7\%}$-Sb-Te), and $Y_{0.087}Sb_{2-0.087}Te_3$ (abbreviated to $Y_{8.7\%}$-Sb-Te) were generated using AIMD for simulation boxes with periodic boundary conditions. The total number of atoms in each model was 180. The density of the three models was 5.65 g/cm^3 for Sb_2Te_3 [1], 5.62 g/cm^3 for $Y_{3.7\%}$-Sb-Te [2], and 5.55 g/cm^3 for $Y_{8.7\%}$-Sb-Te, respectively. 180-atom rocksalt models of Sb_2Te_3, $Y_{3.7\%}$-Sb-Te, and $Y_{8.7\%}$-Sb-Te, in which the Y atoms substitute for Sb atom in the cation sites, were first heated at 3000 K over 20 ps for disordering, then equilibrated at 1000 K over 30 ps to obtain a liquid structure. Subsequently, the liquid model was quenched down to 300 K using an annealing formula. The annealing expression is $T_{end} = T_{start} \times \alpha^{time}$, in which α is the annealing factor. The α parameter is 0.99998 in this work, and the average quenching rate is about 9 K/ps. The obtained amorphous models were equilibrated at 300 K for 270 ps. Then, the trajectories on the last 250 ps were used to study the evolution of the internal structural stress.

1. S. Caravati, M. Bernasconi and M. Parrinello, *Phys. Rev. B*, 2010, **81**, 014201.
2. Y. Zhou, L. Sun, G. M. Zewdie, R. Mazzarello, V. L. Deringer, E. Ma and W. Zhang, *J. Mater. Chem. C*, 2020, **8**, 3646-3654.

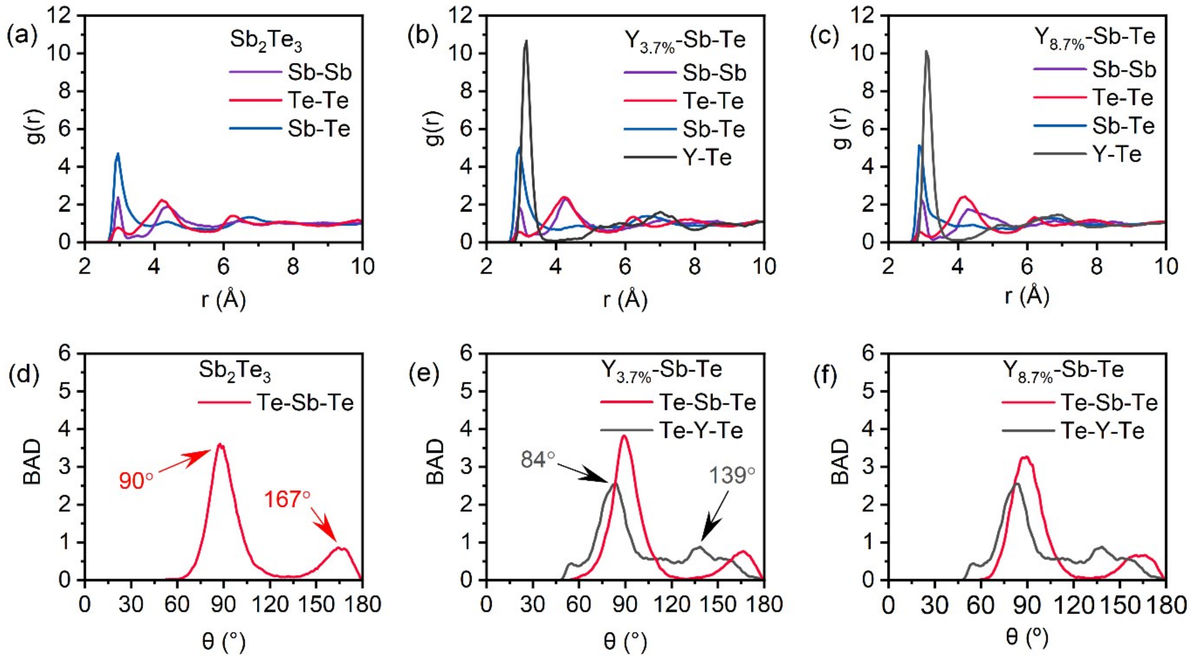

Fig. S1. (a)-(c) The radial distribution function, *g*(r), of Sb_2Te_3, $Y_{3.7\%}$-Sb-Te, and $Y_{8.7\%}$-Sb-Te glasses. The cutoff radius for calculating coordination numbers was 3.4 Å for Sb-Te, 3.3 Å for Sb-Sb, 3.2 Å for Te-Te, 3.4 Å for Y-Te, 3.3 Å for Y-Sb, and 3.3 Å for Y-Y, which is the first minimum in the *g*(r); (d)-(f) The bond-angle distribution of Sb_2Te_3, $Y_{3.7\%}$-Sb-Te, and $Y_{8.7\%}$-Sb-Te glasses. The main angle of Te-Sb-Te units is 90 º and 167 º, whereas the main angle of Te-Y-Te is 84 º and 139 º, indicating the different local motifs around Y and Sb atoms.

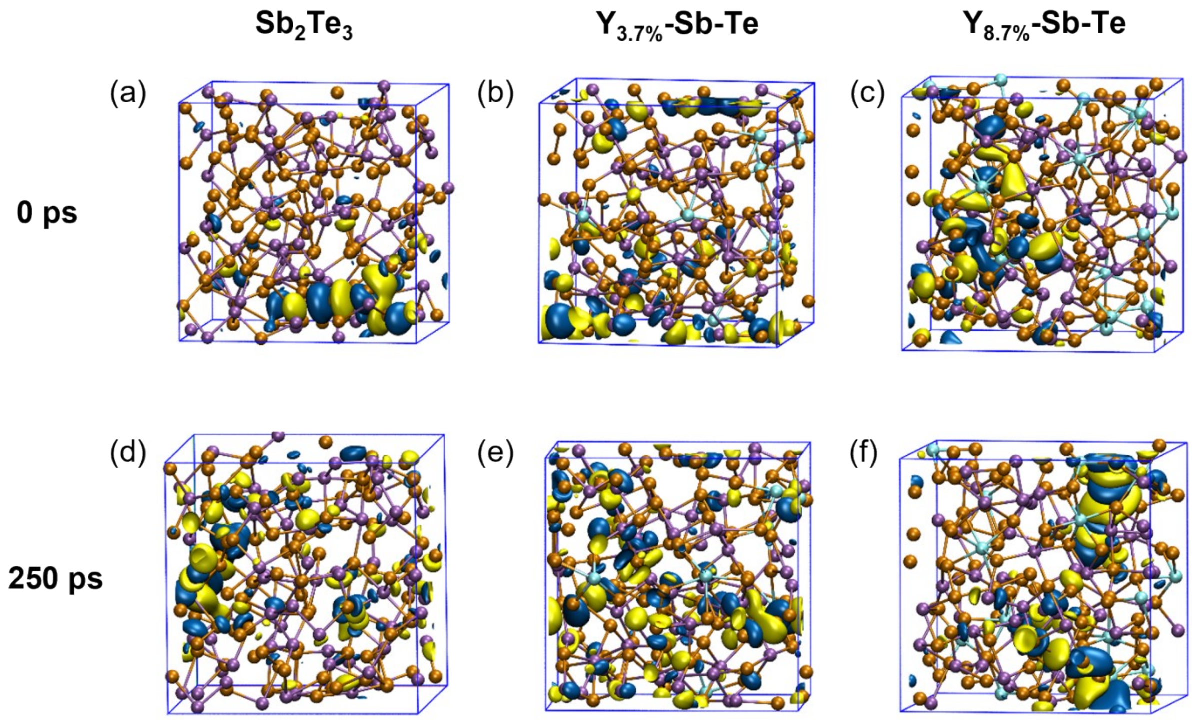

Fig. S2. Isosurfaces for the lowest unoccupied conduction-band state for Sb_2Te_3, $Y_{3.7\%}$-Sb-Te, and $Y_{8.7\%}$-Sb-Te glasses at 0 ps (a)-(c) and 250 ps (d)-(f), with positive values shown in yellow, and negative values in blue. The isosurface value is ± 0.015 e/bohr^3. Sb atoms are shown in purple, Te atoms are shown in orange, and Y atoms are shown in navy blue.

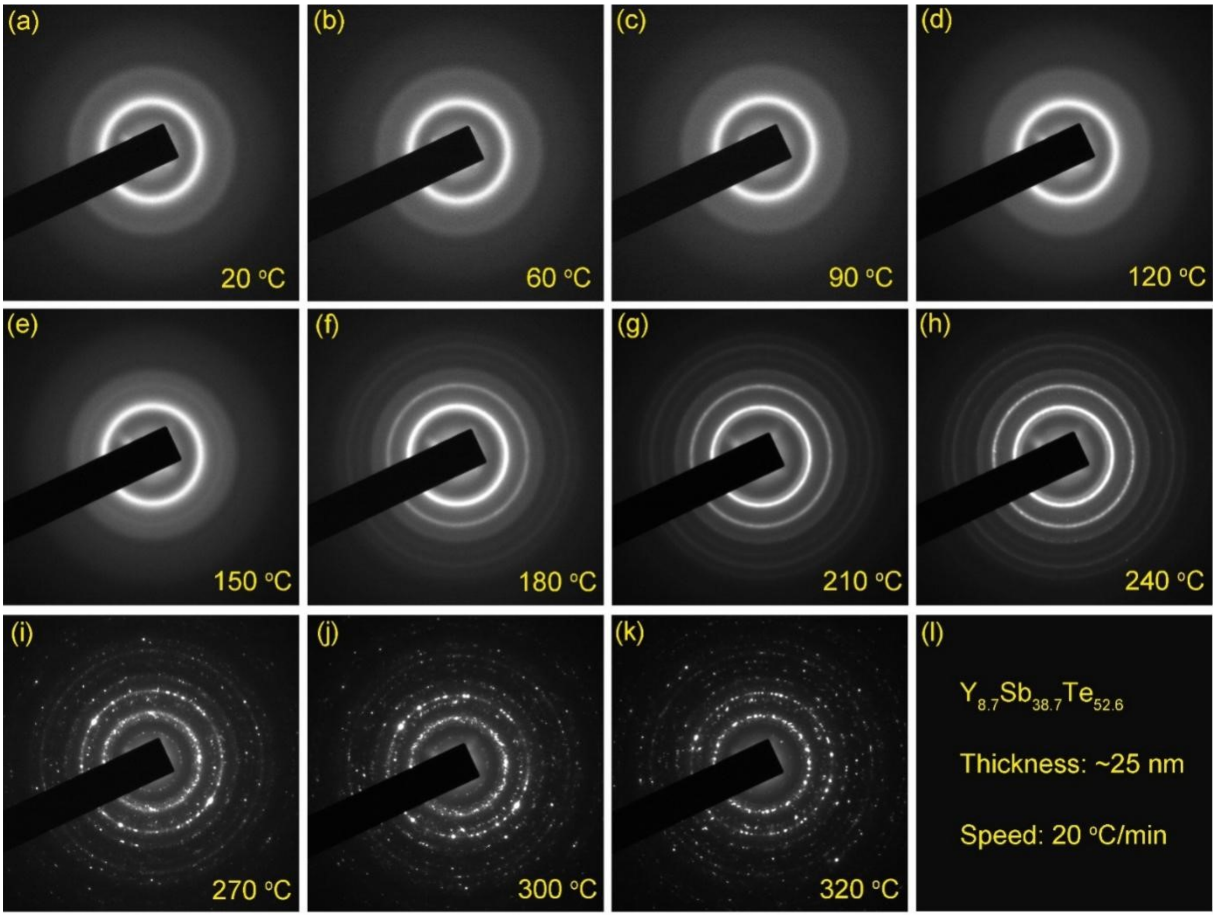

Fig. S3. TEM diffraction patterns of a $Y_{8.7}Sb_{38.7}Te_{52.6}$ film upon *in situ* thermally-induced crystallization. The transition temperature from the amorphous to the cubic phase (T_c) is ~ 180 ^{o}C, and that from the cubic to the hexagonal phase is about 270 ^{o}C.

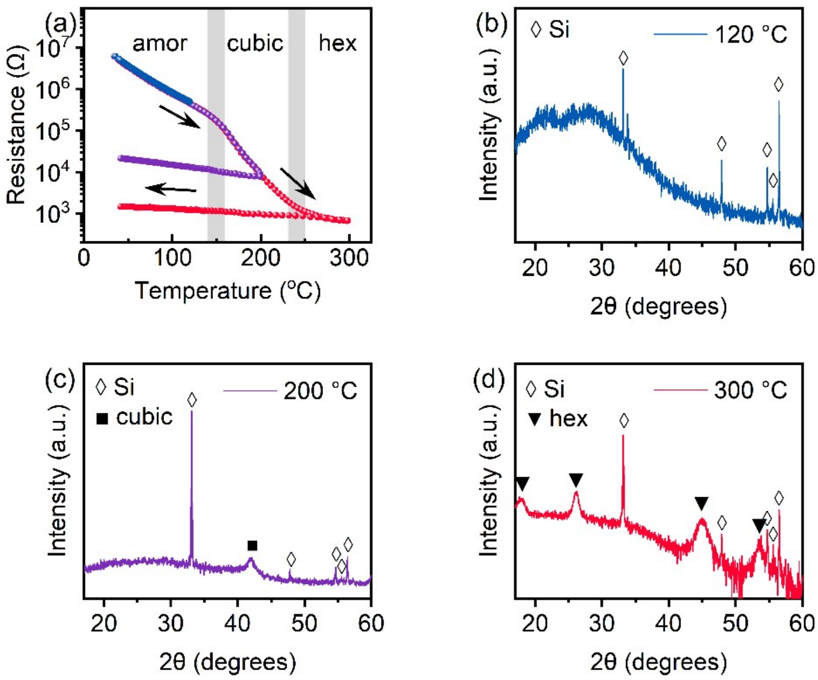

Fig. S4. (a) Temperature dependence of the electrical resistance (*R*-*T*) of ~40 nm-thick $Y_{8.7}Sb_{38.7}Te_{52.6}$ films with different cut-off temperatures (120 °C, 200 °C, and 300 °C, respectively); (b)-(d) XRD patterns of the three $Y_{8.7}Sb_{38.7}Te_{52.6}$ films after *R*-*T* measurements in (a).