Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A.

SUPPORTING INFORMATION

Synergistic optimization of thermoelectric performance of Sb doped GeTe with strained domain and domain boundaries

Khasim Saheb Bayikadi[a], Chien Ting Wu[b], Li-Chyong Chen[c,d], Kuei-Hsien Chen[c,e*], Fang-Cheng Chou[c,d*], Raman Sankar[a,c*]

[a] Institute of Physics, Academia Sinica, Nankang, Taipei, Taiwan 11529.

[b] Taiwan Semiconductor Research Institute, Hsinchu Science Park, Hsinchu 300, Taiwan.

[c] Centre for Condensed Matter Sciences, National Taiwan University, Taipei 10617, Taiwan.

[d] Center of Atomic Initiative for New Materials, National Taiwan University, Taipei 10617, Taiwan.

[e] Institute of Atomic and Molecular Sciences, Academia Sinica, Taipei 10617, Taiwan.

Corresponding Authors

***Email: sankarraman@gate.sinica.edu.tw (R Sankar), chenkh@pub.iams.sinica.edu.tw (K H Chen), fcchou@ntu.edu.tw (F C Chou)**

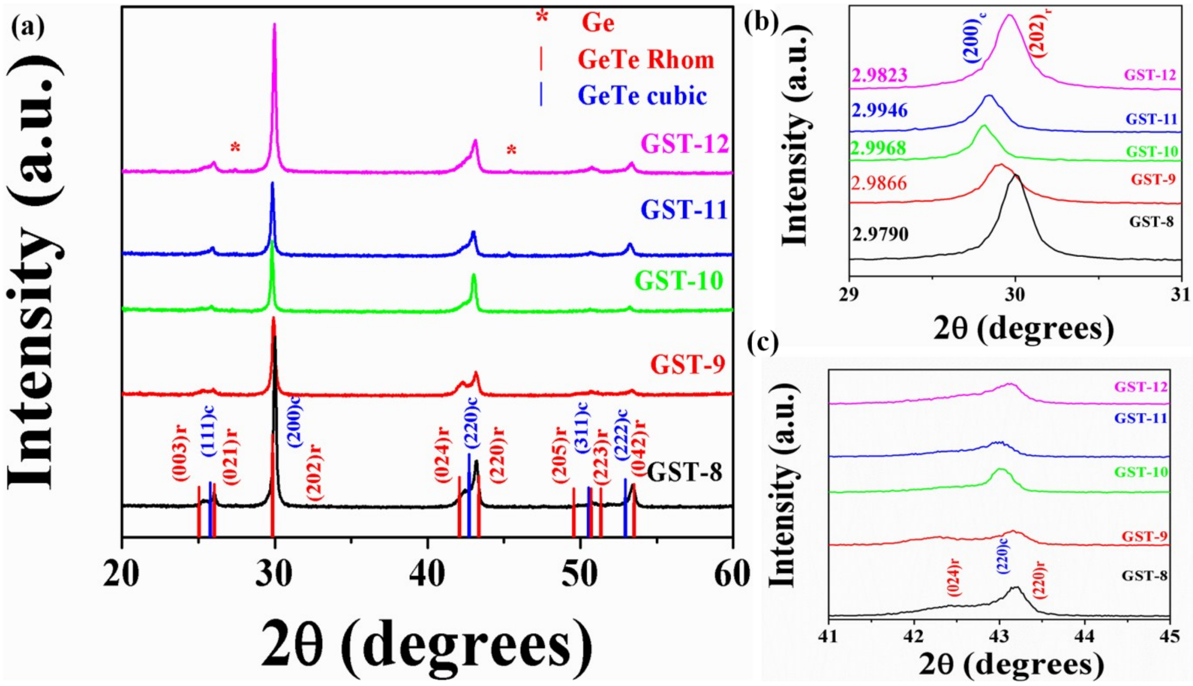

Figure S1: (a) XRD patterns for the GST compounds. (b) $(202)_r$ peak shifting, and (c) characteristic peaks between 40-45 ^{o}.

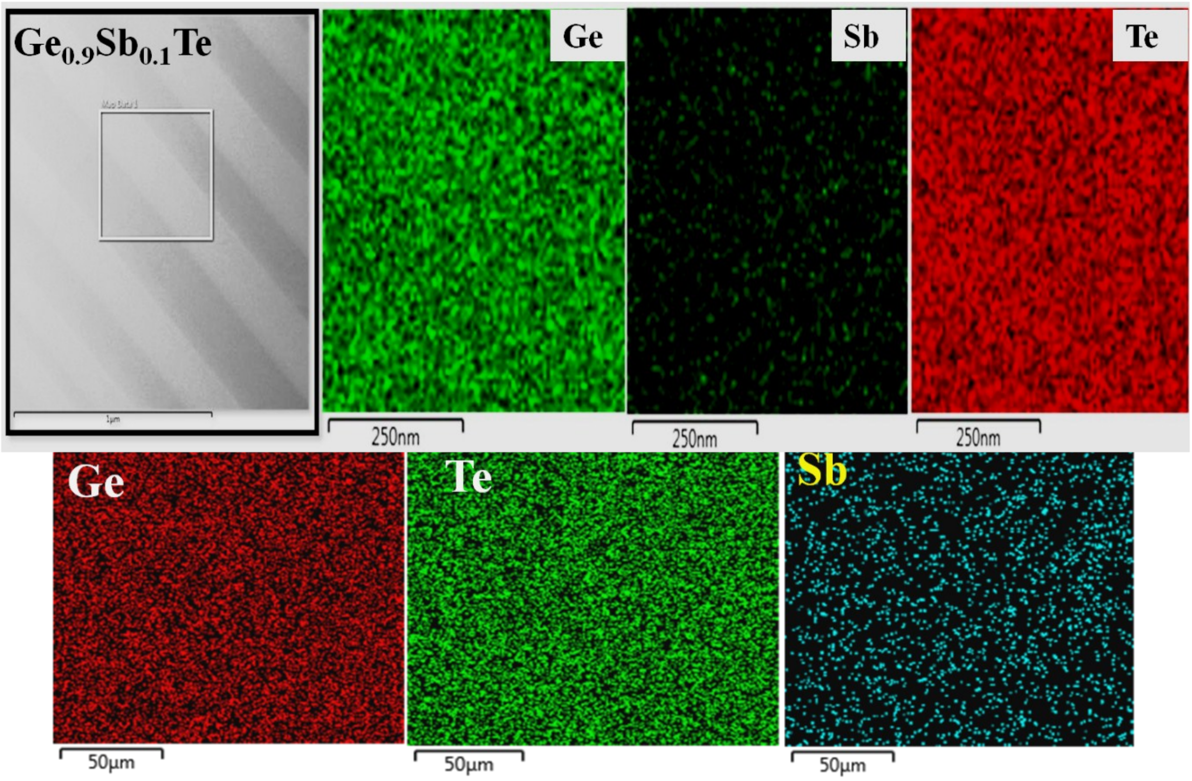

Figure S2: FE-SEM image for the elemental mapping of $Ge_{0.9}Sb_{0.1}Te$. The individual mapping for Ge, Sb, and Te confirms that no Ge precipitate present in the 50 µ length scale.

Figure S3: TEM image for the elemental mapping for $Ge_{0.9}Sb_{0.1}Te$ at 250 nm scale, no Ge precipitants is confirmed.

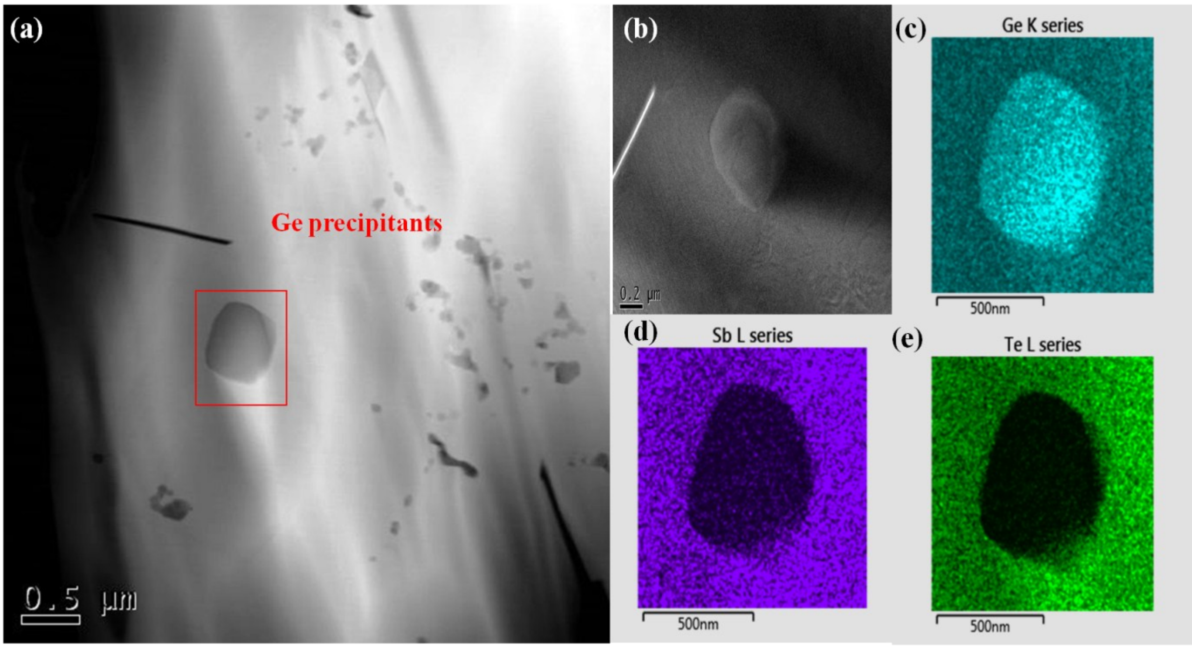

Figure S4: TEM image and elemental mapping of $Ge_{0.88}Sb_{0.12}Te$. Ge precipitate is identified, as verified from (c) to (e).

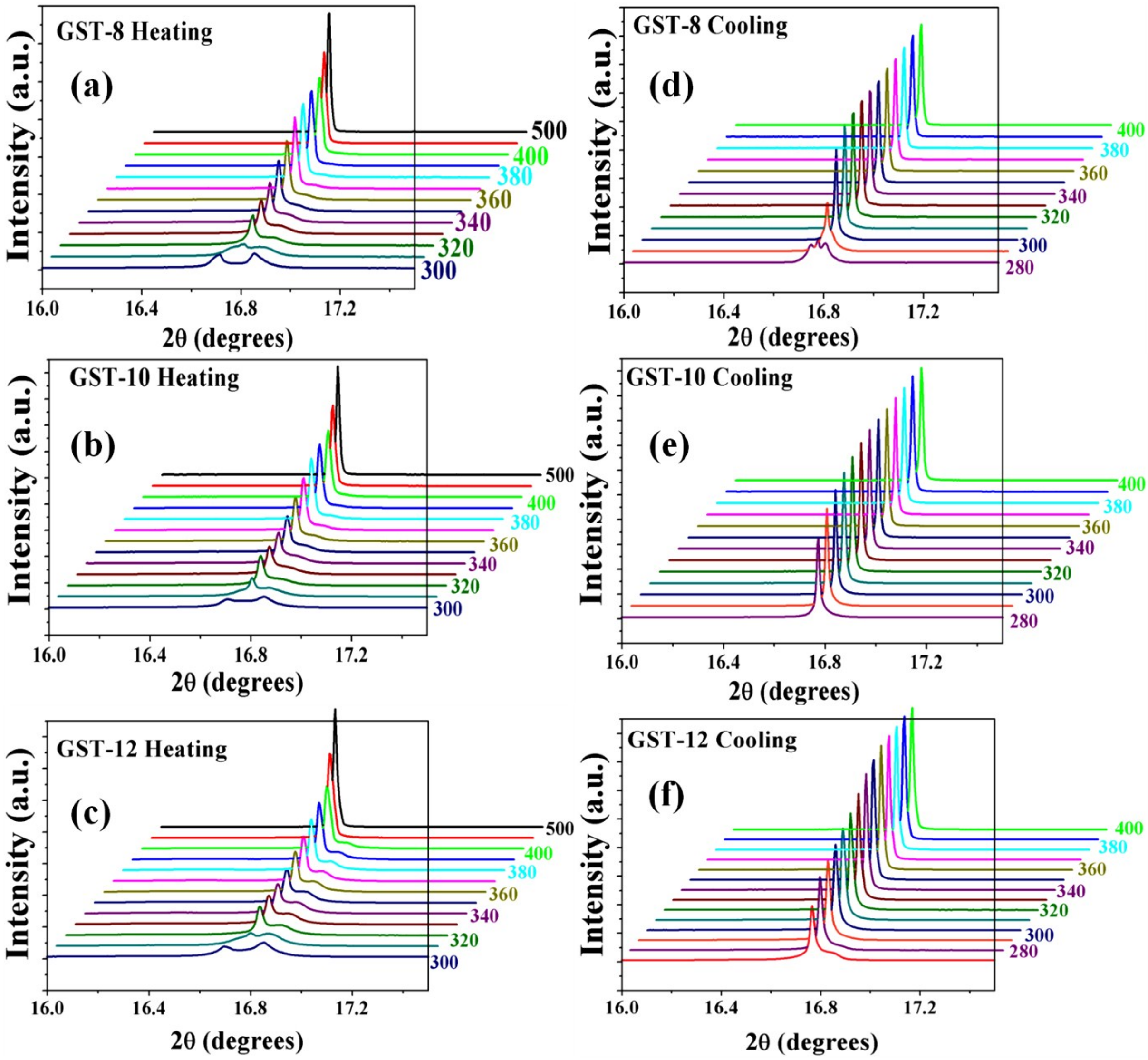

Figure S5: High temperature synchrotron XRD analysis for the GST- 8, 10, and 12 samples upon (a)-(c) warming and (d)-(f) cooling. The wavelength of the incident synchrotron X-ray is 0.62 Å.

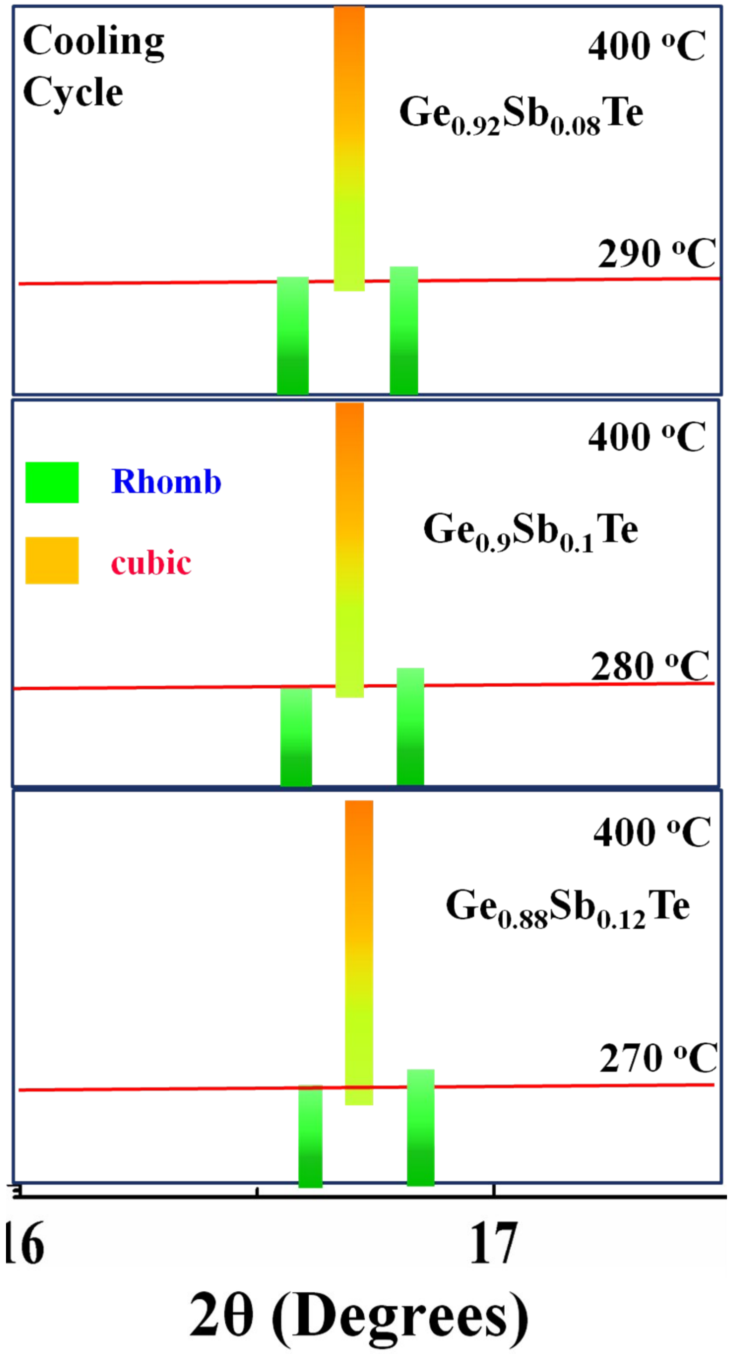

Figure S6: Based on the cooling cycle data shown in Fig. 5S, the temperature and Sb doping dependence is analysed to show the evolution of rhombohedral-to-cubic reversible phase transformation.

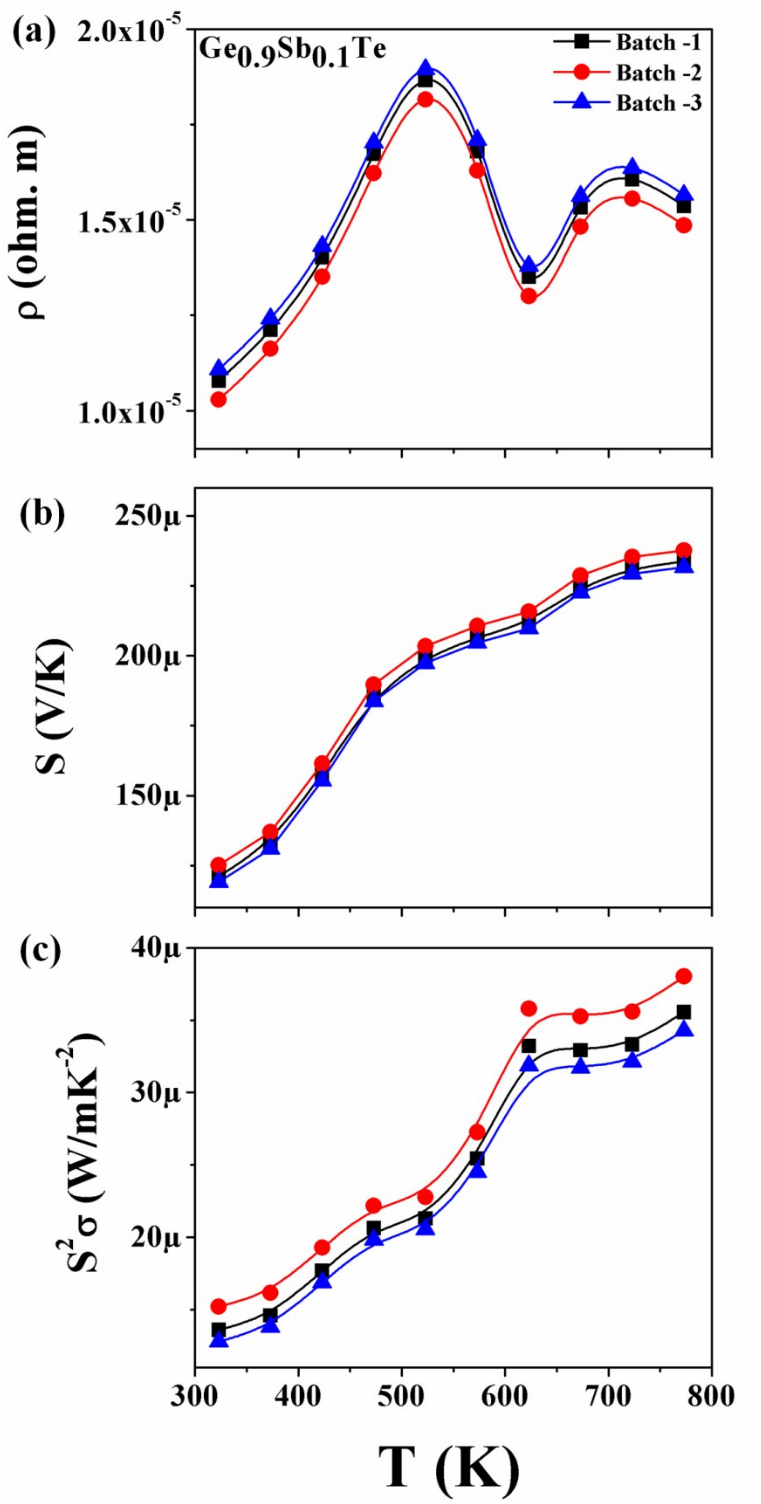

Figure S7: The reproducibility has been checked using two more separately prepared batches of $Ge_{0.9}Sb_{0.1}Te$-900. Temperature dependence of (a) electrical conductivity, (b) Seebeck coefficient, and (c) power factor.

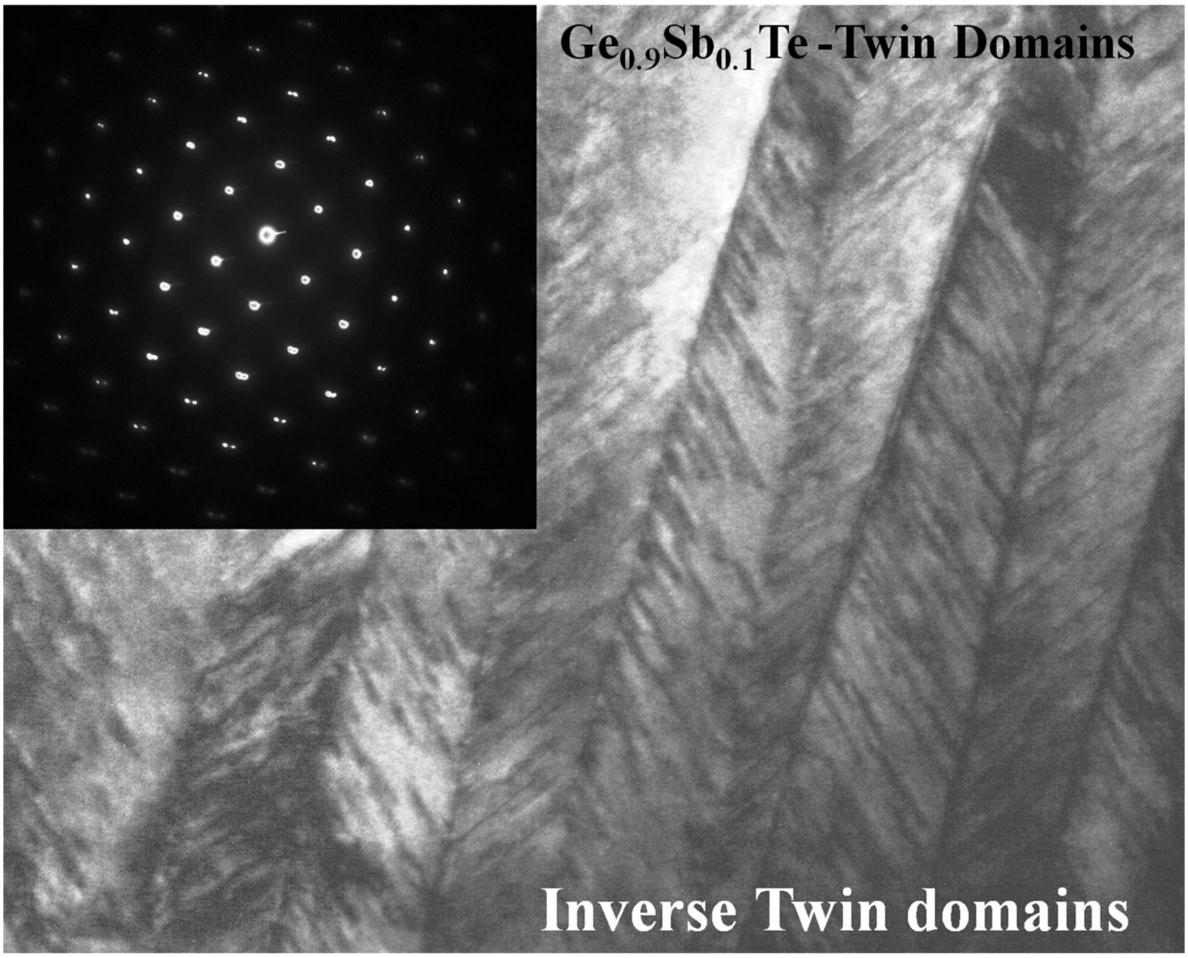

Figure S8: The herringbone structure of $Ge_{0.9}Sb_{0.1}Te$-900 shows twin domains and inverse-twin domain. The inset of shows doublet in the SAED pattern originated from the twin domain.

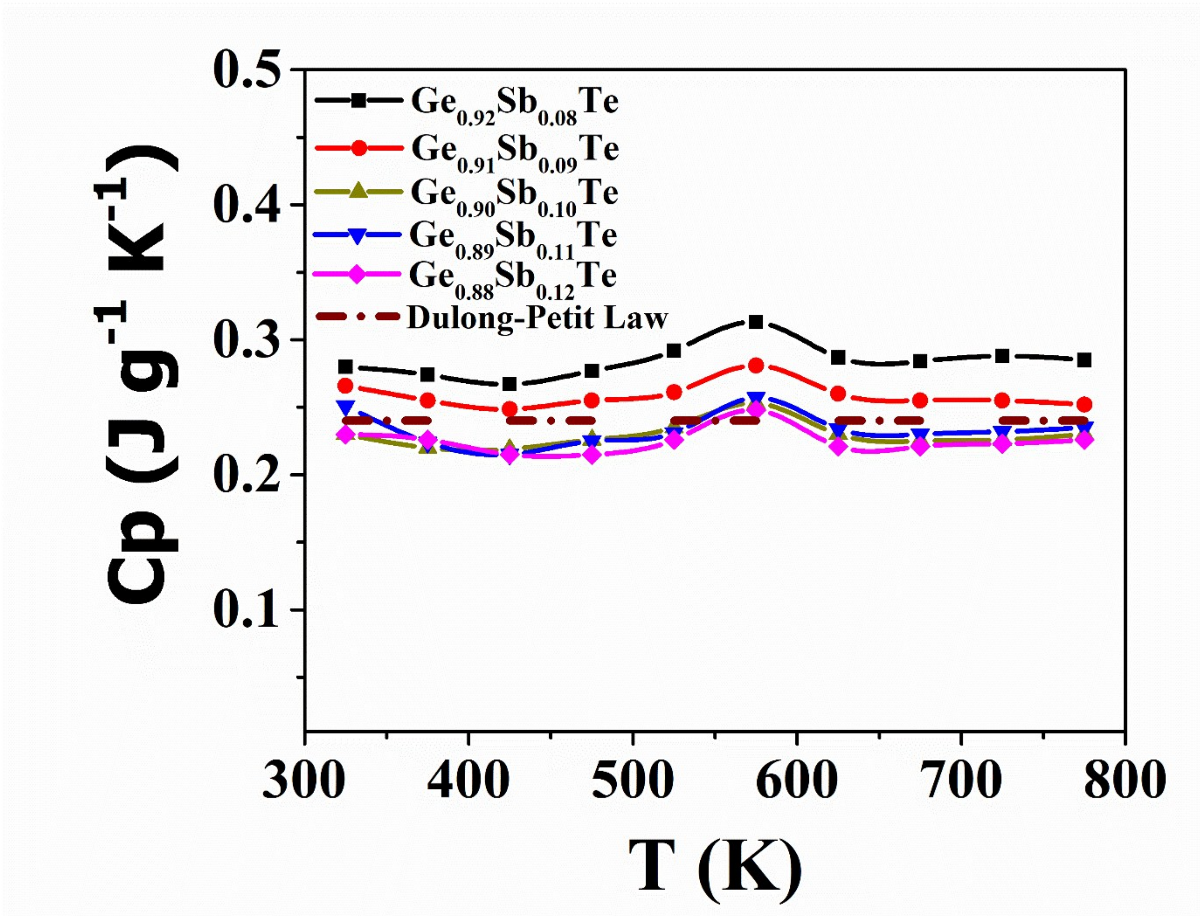

Figure S9. Dulong-Petit Cp and experimentally measured Cp as a function of temperature.