Supplementary Information

Regulation of Ge Vacancies through Sm Doping boosting Superior Thermoelectric Performance in GeTe

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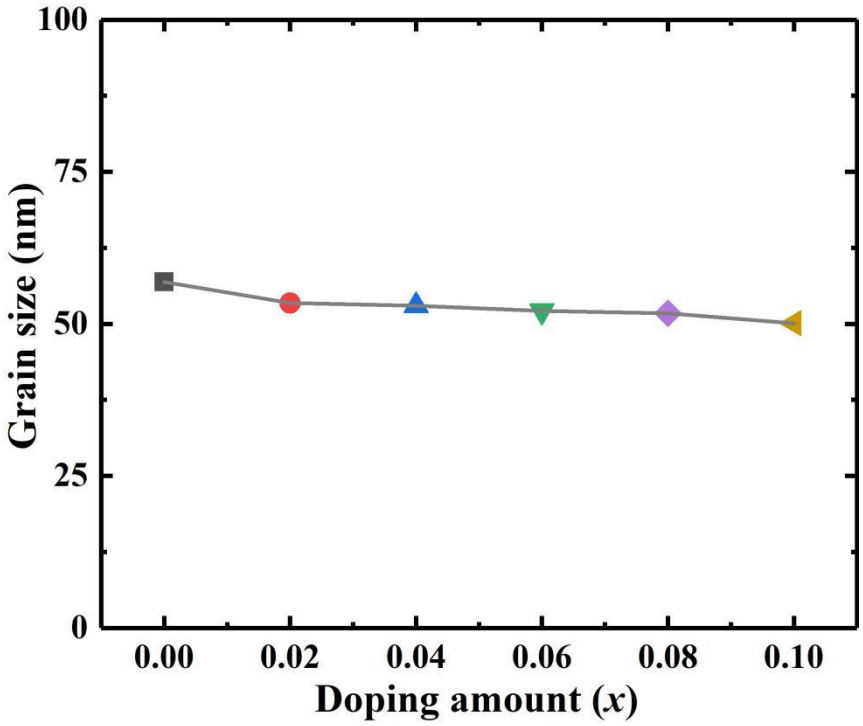

Figure S1. Grain size evaluated by XRD measurements for $Ge_{1-x}Sm_xTe$ samples.

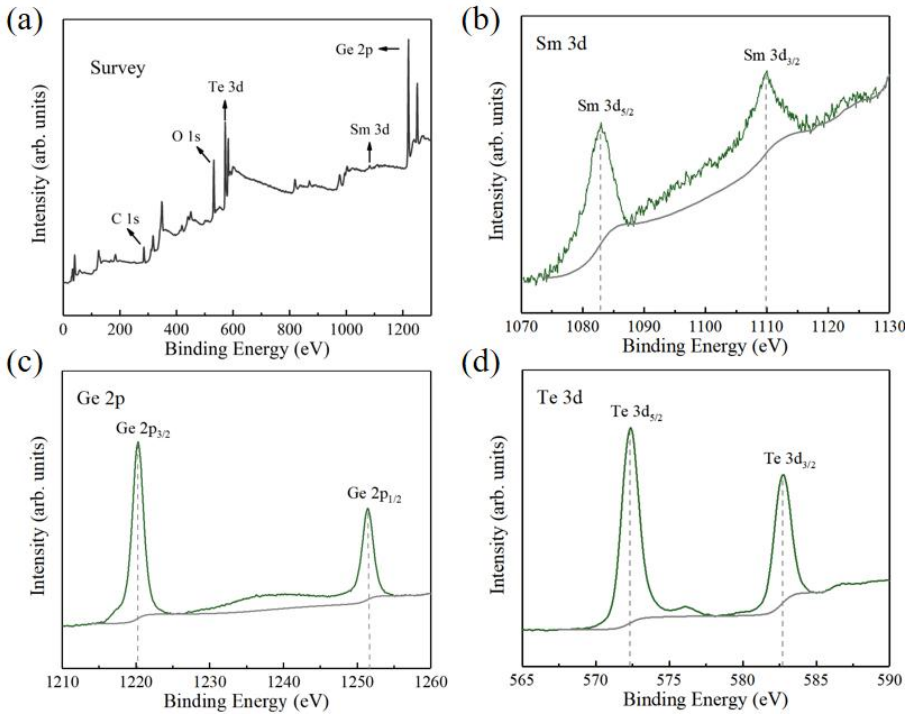

Figure S2. X-ray photoelectron spectroscopy results for $Ge_{0.94}Sm_{0.06}Te$: (a) fully scanned spectrum; (b) Sm 3d; (c) Ge 2p; and (d) Te 3d.

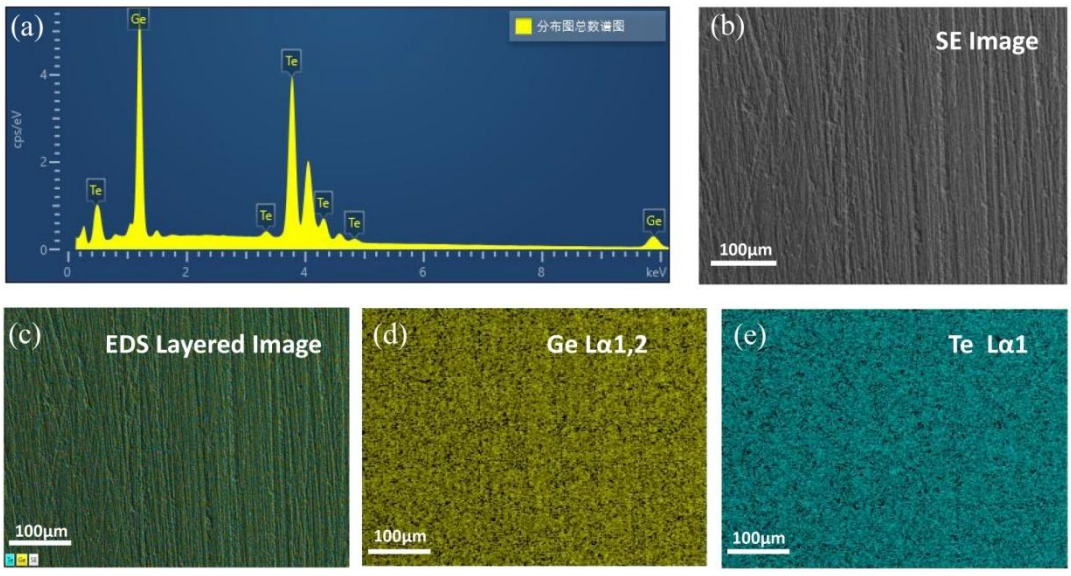

Figure S3. Energy dispersive X-ray spectroscopy (EDS) results for pristine GeTe.

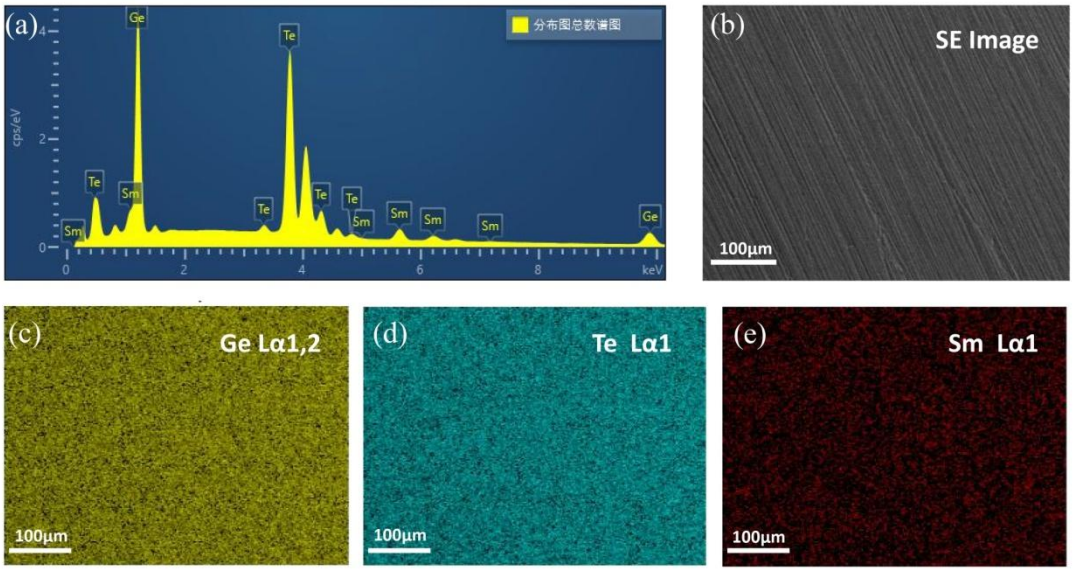

Figure S4. Energy dispersive X-ray spectroscopy (EDS) results for $Ge_{0.92}Sm_{0.08}Te$.

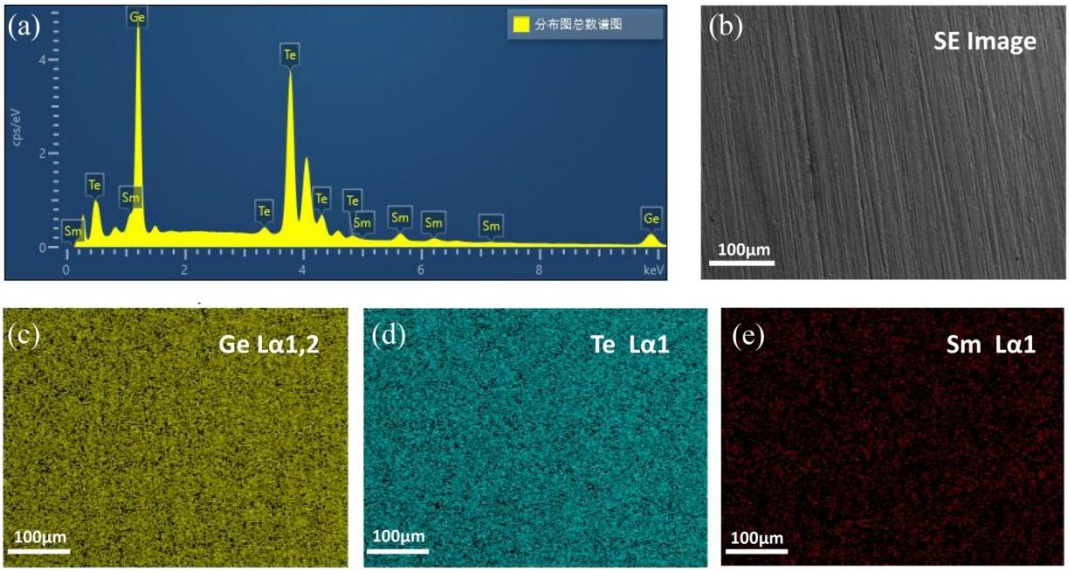

Figure S5. Energy dispersive X-ray spectroscopy (EDS) results for $Ge_{0.90}Sm_{0.10}Te$.

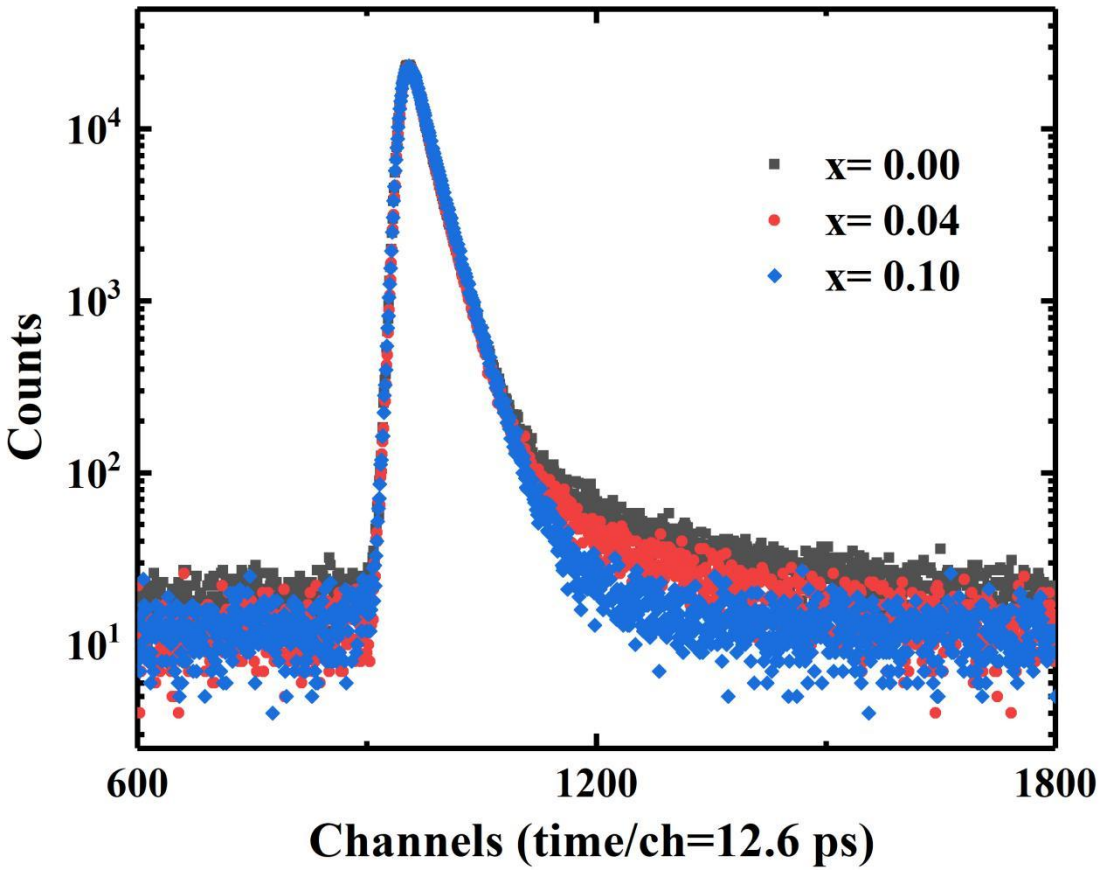

Figure S6. PAL spectrums for $Ge_{1-x}Sm_xTe$ samples.

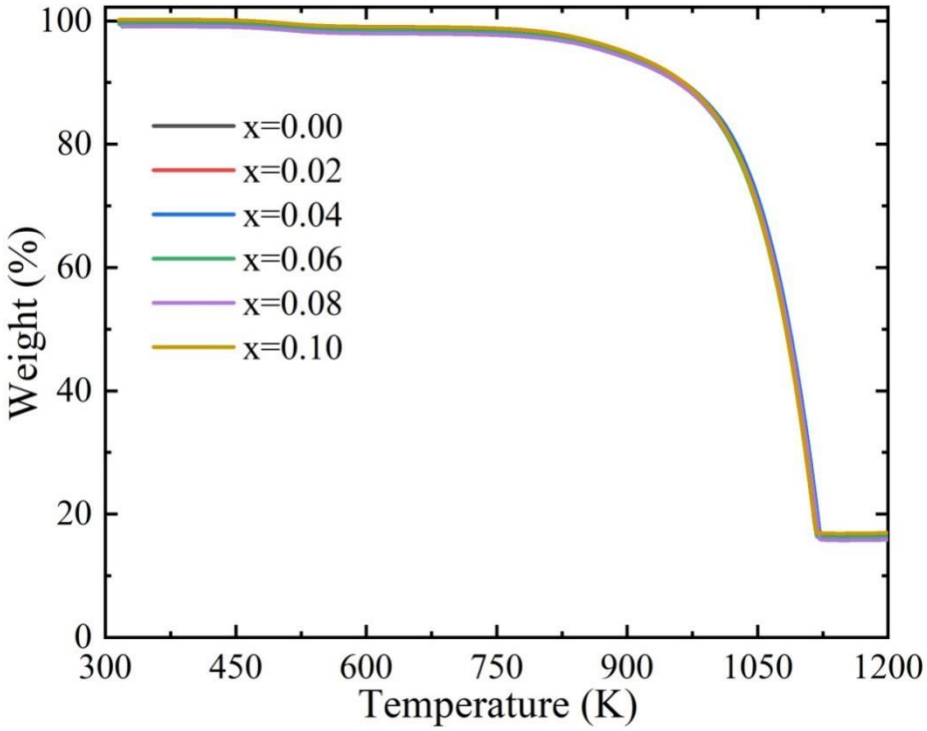

Figure S7. TG curves for $Ge_{1-x}Sm_xTe$ samples.

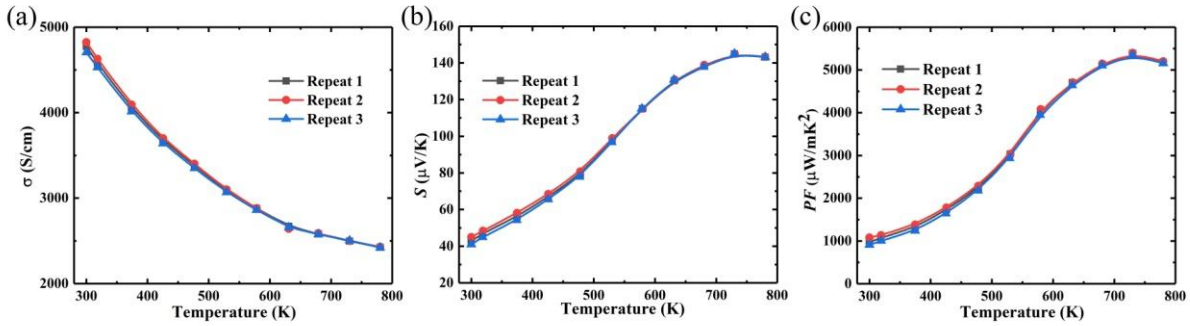

Figure S8. The reproducibility of electric transport properties as a function of temperature for the $Ge_{0.94}Sm_{0.06}Te$ sample during three times measurements: (a) Electrical conductivity σ; (b) Seebeck coefficient S; (c) Power factor PF.

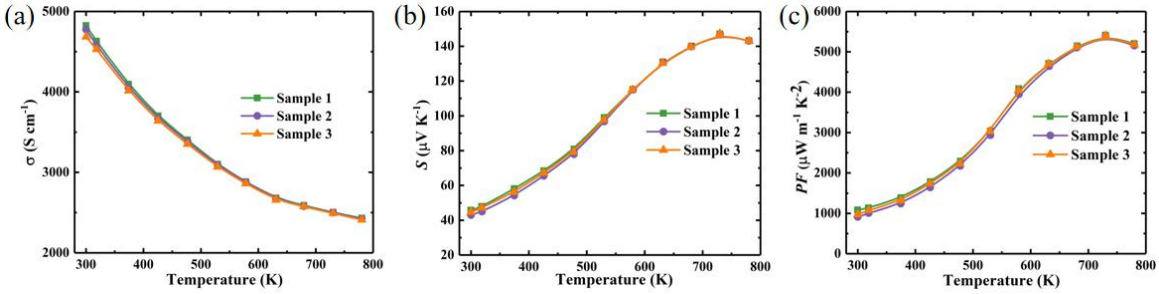

Figure S9. The reproducibility of electric transport properties as a function of temperature for three $Ge_{0.94}Sm_{0.06}Te$ samples prepared by the same synthesis process: (a) Electrical conductivity σ; (b) Seebeck coefficient S; (c) Power factor PF.

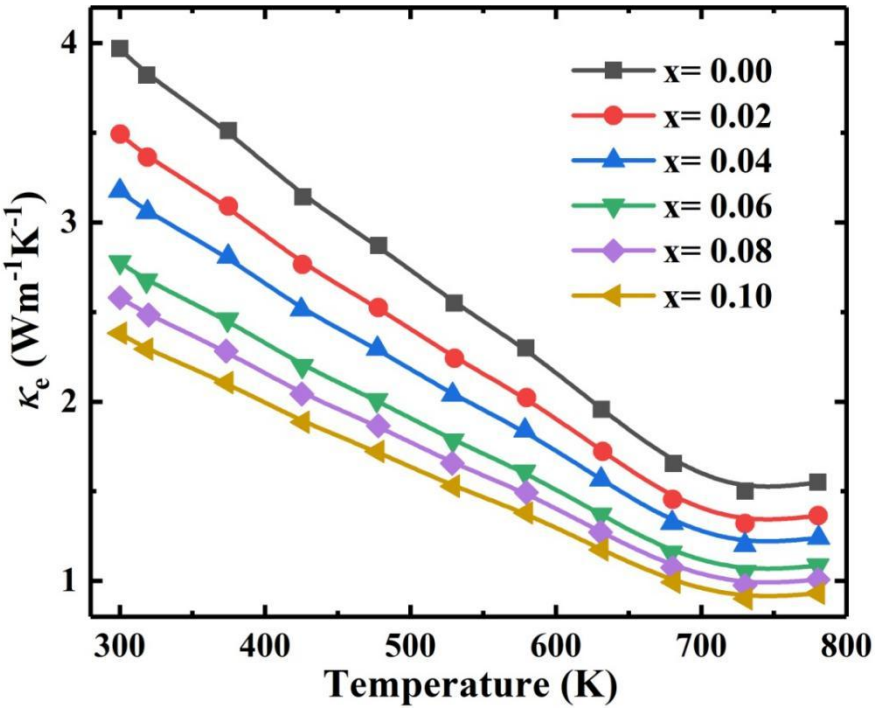

Figure S10. Electronic thermal conductivity as a function of temperature for $Ge_{1-x}Sm_xTe$ samples.

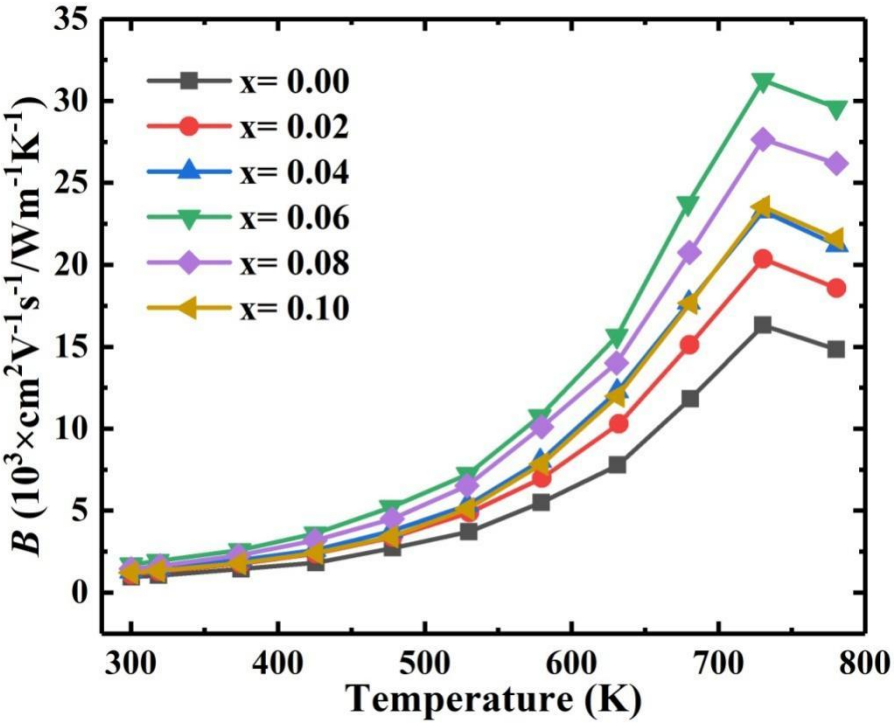

Figure S11. Quality factor *B* as a function of temperature for $Ge_{1-x}Sm_xTe$ samples.

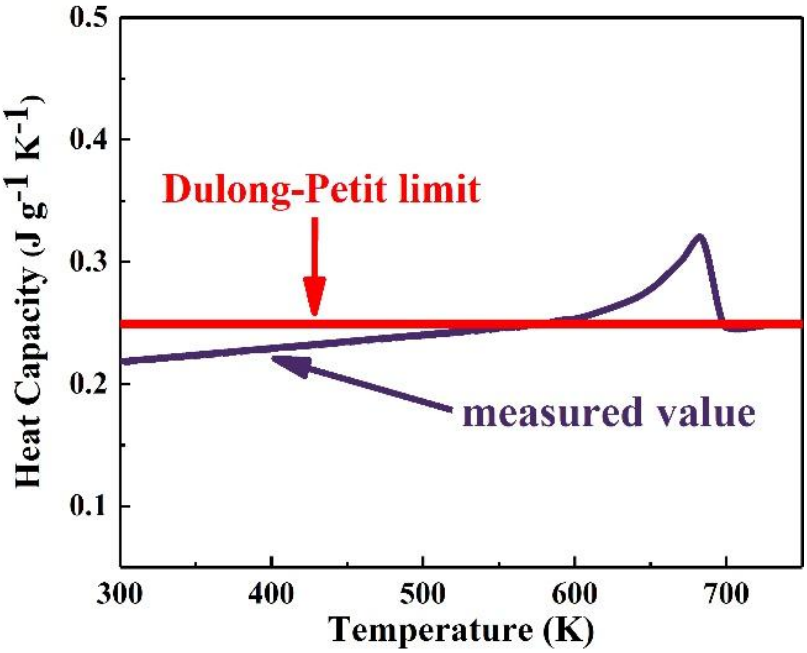

Figure S12. The heat capacity calculated by the Dulong-Petit law and experimentally measured by DSC as a function of temperature for $Ge_{0.94}Sm_{0.06}Te$.

The heat capacity for $Ge_{0.94}Sm_{0.06}Te$ in the temperature range of 300-750 K was measured by using a differential scanning calorimeter (DSC Q20; TA Instruments). The results are depicted above in the Figure S12. The results show that the phase transition temperature of the sample seems to be around 690 K, which is far away from 730 K where the highest zT value appears. Following the widely used way by many other researchers in dealing with heat capacity in GeTe,[1-5] we adopted the value calculated by Dulong-Petit limit, which is an effective approximation for the heat capacity evaluation at temperatures not close to that of phase transition. From the figure it is also clear that at temperatures far away from the phase transition point, the calculated C_p is close to the measured value, especially near 730 K.

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