

# High Thermoelectric Performance Achieved in Sb-doped GeTe by Manipulating Carrier Concentration and Nanoscale Twin Grains

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## Research Article

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# Abstract

Lead-free and eco-friendly GeTe shows a promising candidate for mid-temperature thermoelectric application. However, a low Seebeck coefficient due to its intrinsically high holes concentration that induced by Ge vacancies, and a relatively high thermal conductivity result in an inferior thermoelectric performance of pristine GeTe. However, extrinsic atoms Sb, Bi, and Y could play a crucial role in regulating the holes concentration of GeTe because of their relatively high solubility. Here we investigate the thermoelectric performance of the GeTe upon Sb doping, and demonstrate a high maximum  $zT$  value up to 1.88 could be achieved in Ge<sub>0.90</sub>Sb<sub>0.10</sub>Te as a result of the significant suppression in thermal conductivity while holding a high power factor. Where the maintained high power factor is due to the markable enhancement in  $S$ , which could be attributed to the significant suppression of holes concentration and the valence band convergence upon Sb doping; while the low thermal conductivity stems from the suppression of electronic thermal conductivity due to the increase in electrical resistivity and the lowering of lattice thermal conductivity through strengthening the phonons scattering by the lattice distortion, dislocations, and twin boundaries. Aside from the excellent thermoelectric performance, Ge<sub>0.90</sub>Sb<sub>0.10</sub>Te also shows good reproducibility, as well as thermal stability. This work confirms the Ge<sub>0.90</sub>Sb<sub>0.10</sub>Te is a superior thermoelectric material for practical application.

## Full Text

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## Figures

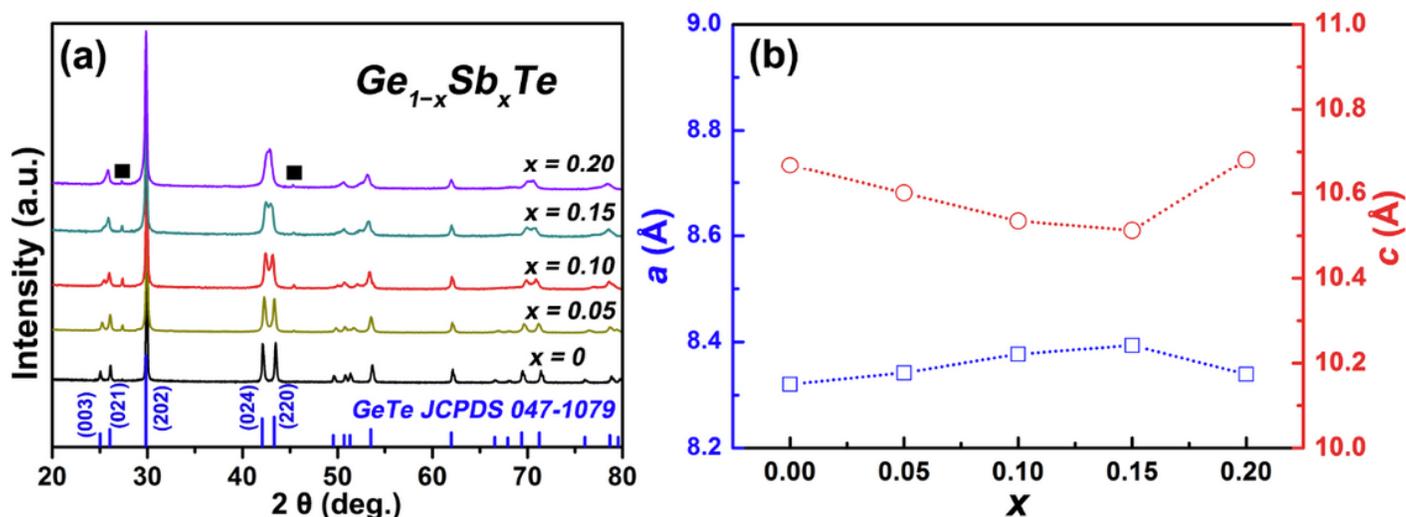
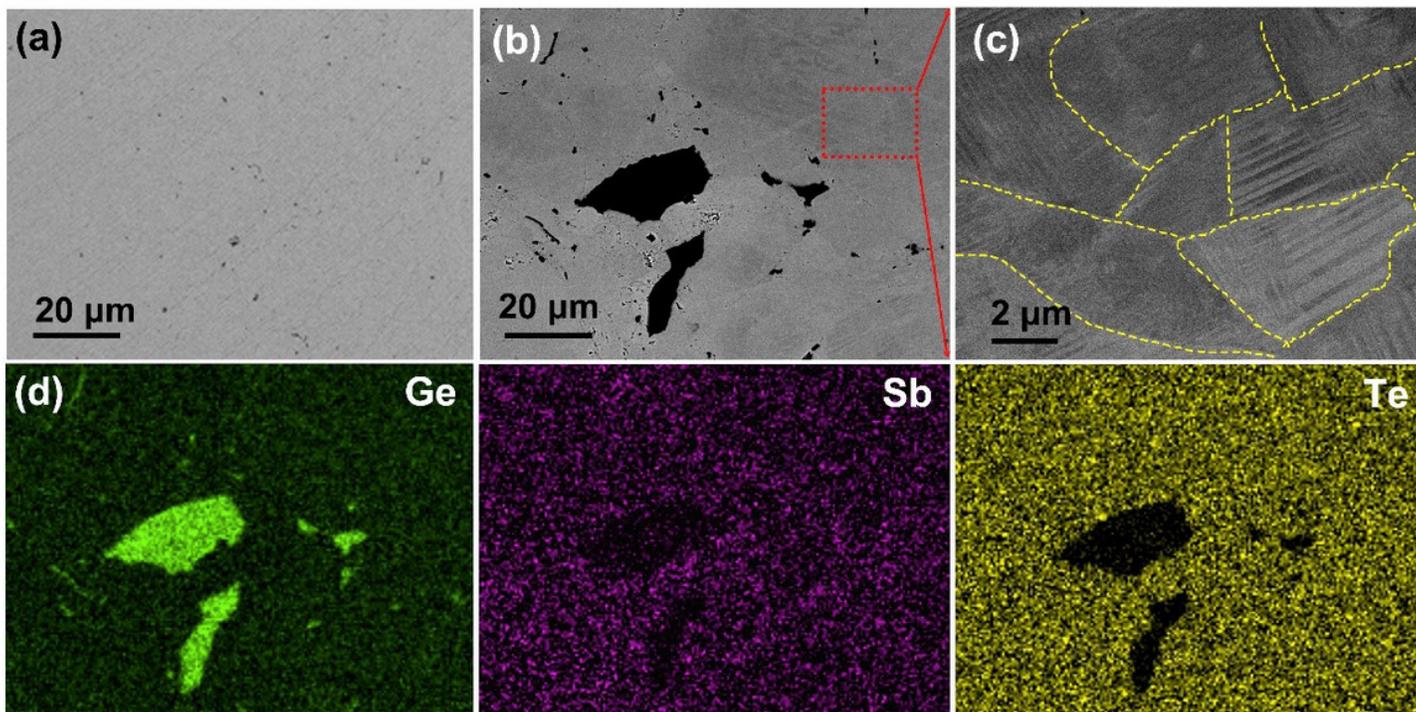


Figure 1

(a,b) Powder XRD patterns and lattice parameters  $a$  and  $c$  of Ge<sub>1-x</sub>Sb<sub>x</sub>Te. Where the black square (■) represents Ge precipitates.



**Figure 2**

BSE images of the pristine GeTe (a) and Ge<sub>0.90</sub>Sb<sub>0.10</sub>Te (b); (c) magnified ECC image of Ge<sub>0.90</sub>Sb<sub>0.10</sub>Te taken on the region marked by the red dotted rectangle in Fig. 2b; (d) elemental mapping images taken on the region that displayed in Fig. 2b.

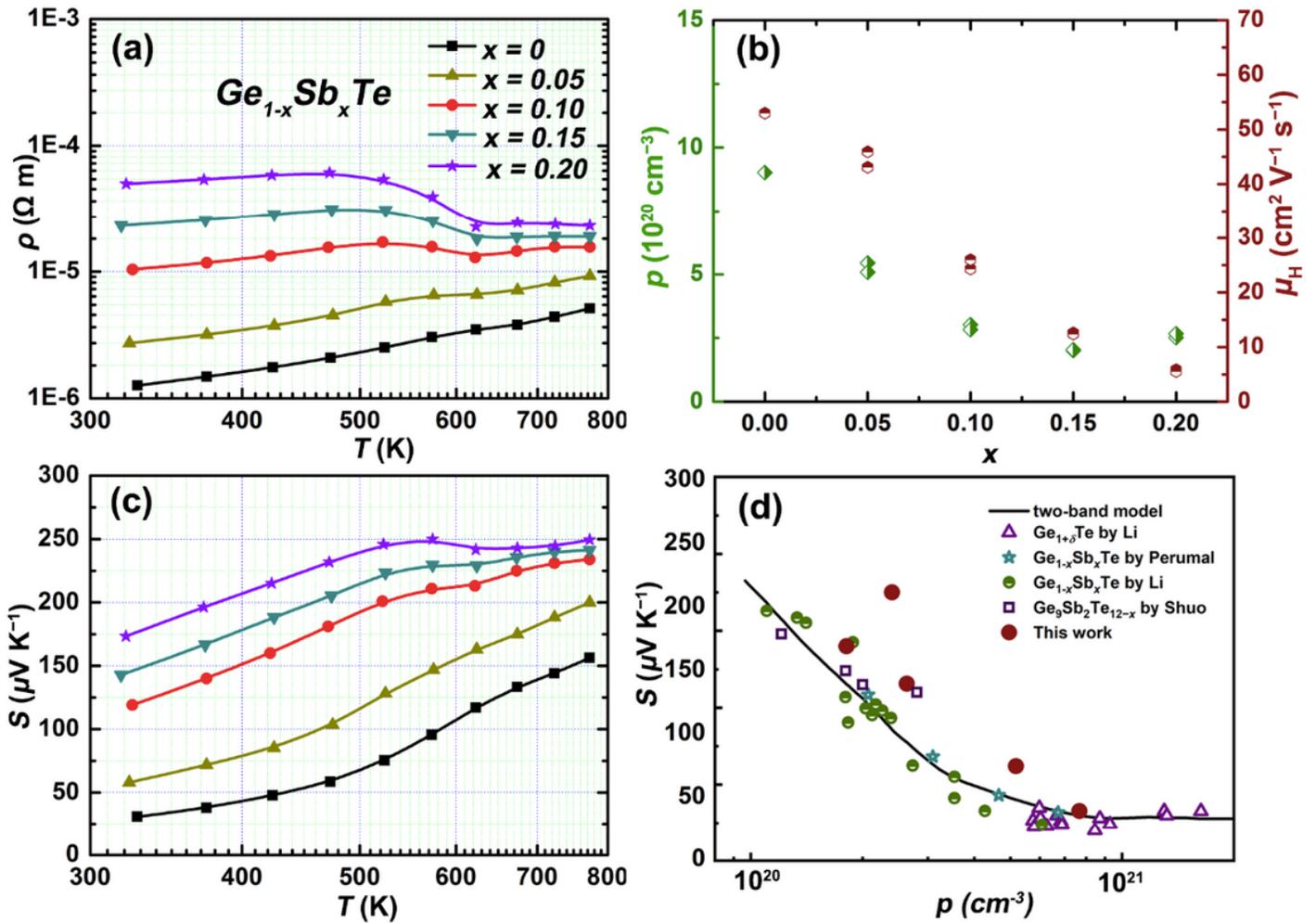


Figure 3

Electrical properties of  $\text{Ge}_{1-x}\text{Sb}_x\text{Te}$ : (a) electrical conductivity; (b) carrier concentration and mobility as a function of the Sb content  $x$  at room temperature; (c) Seebeck coefficient; (d) Pisarenko plot.

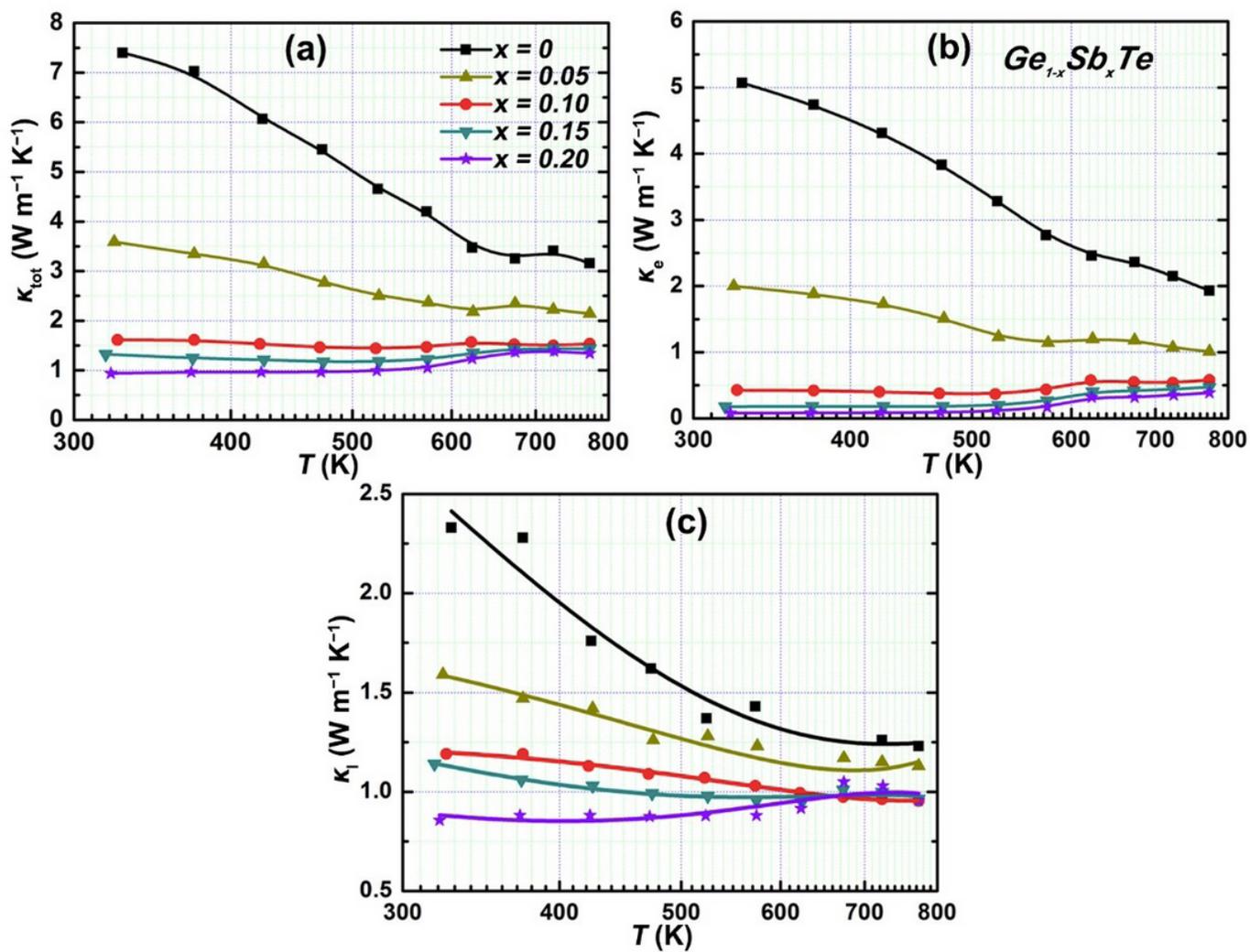
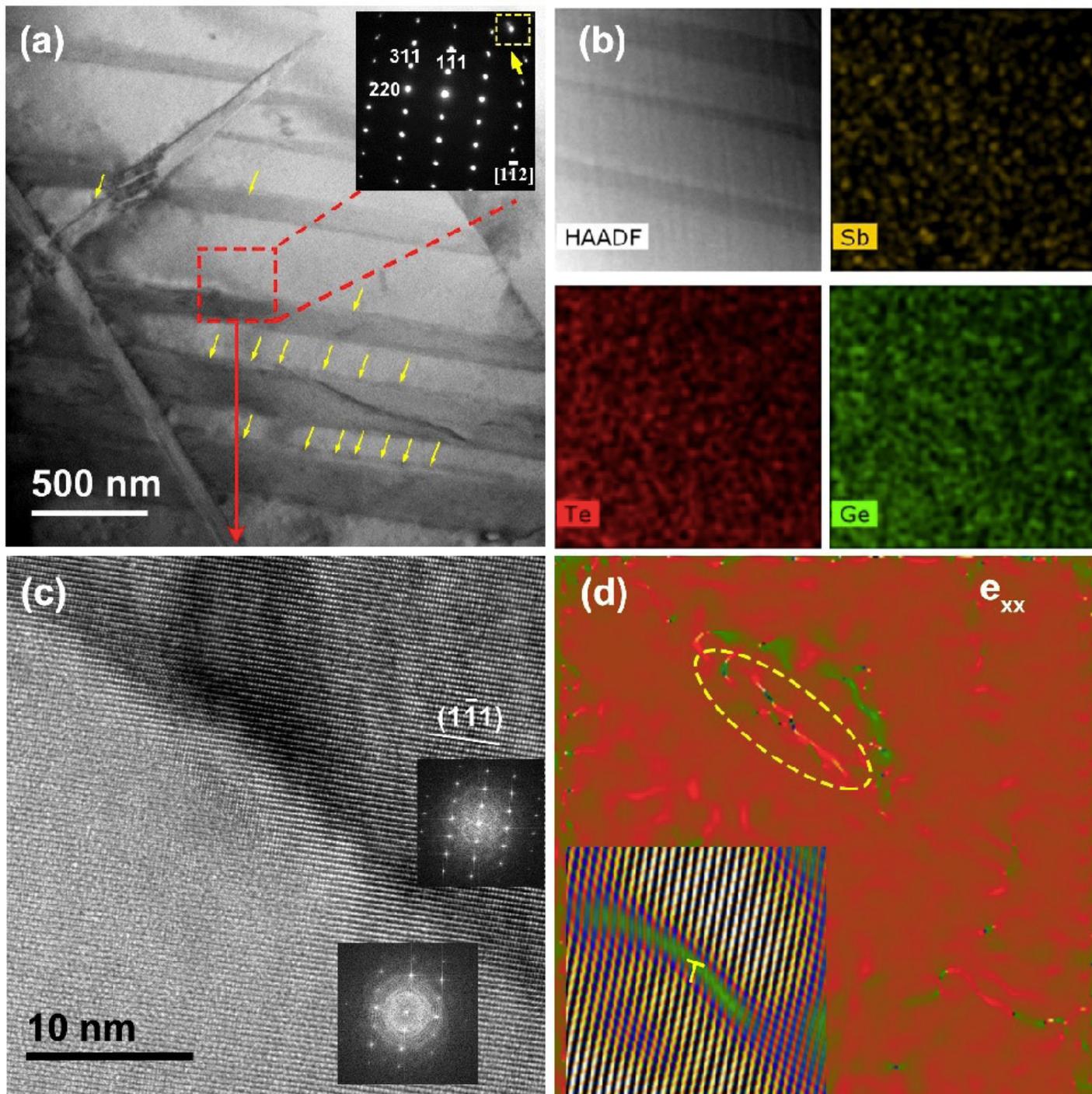


Figure 4

Temperature-dependent thermal properties of  $Ge_{1-x}Sb_xTe$ : (a) thermal conductivity; (b) electronic thermal conductivity; (c) lattice thermal conductivity.



**Figure 5**

The microstructure characterization of Ge<sub>0.90</sub>Sb<sub>0.10</sub>Te: (a) a low-magnification bright-field image, the inset is the SAED pattern taken on the marked region; (b) a HAADF image and the corresponding elemental mappings; (c) a HRTEM image from the marked region in Fig. 5a, the insets are the corresponding FFT images; (d) the distribution of strain calculated by GPA, the inset is the corresponding IFFT image.

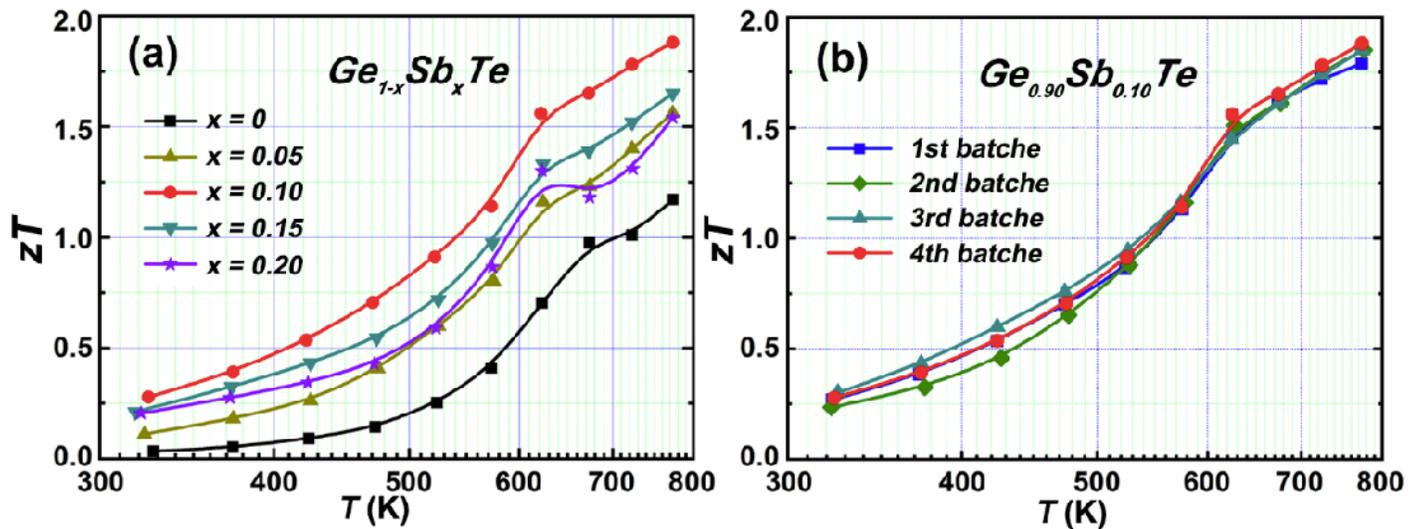


Figure 6

(a)  $zT$  value of  $Ge_{1-x}Sb_xTe$  ( $x = 0, 0.05, 0.10, 0.15, 0.20$ ); (b)  $zT$  value of the different batches samples  $Ge_{0.90}Sb_{0.10}Te$ .

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