

Simultaneous regulation of electrical and thermal transport properties in MnTe chalcogenides via the incorporation of *P*-type Sb₂Te₃

Abdul Basit, Junyou Yang*, Qinghui Jiang, Jiwu Xin, Xin Li, Sihui Li, Suwei Li and Qiang Long

State Key Laboratory of Material Processing and Die & Mould Technology, Huazhong University of Science & Technology, Wuhan 430074, PR China.

Email: jyyang@mail.hust.edu.cn

Fig. SI1: Heat capacity for MnTe + x at% Sb₂Te₃ samples ($x=0, 0.5, 1, 1.5, 2$) samples.

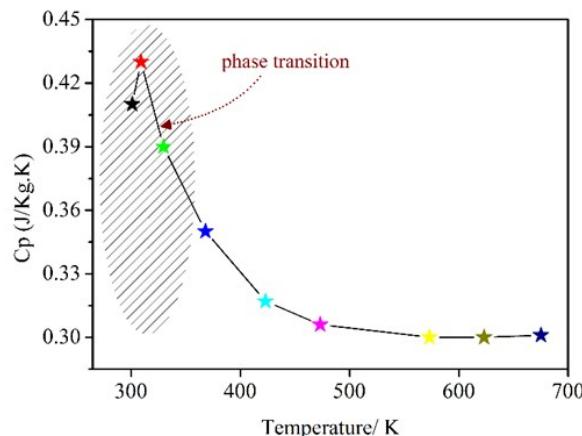


Fig. SI2: SEM and elemental compositions of MnTe + (0.5 and 1) at% Sb₂Te₃ samples.

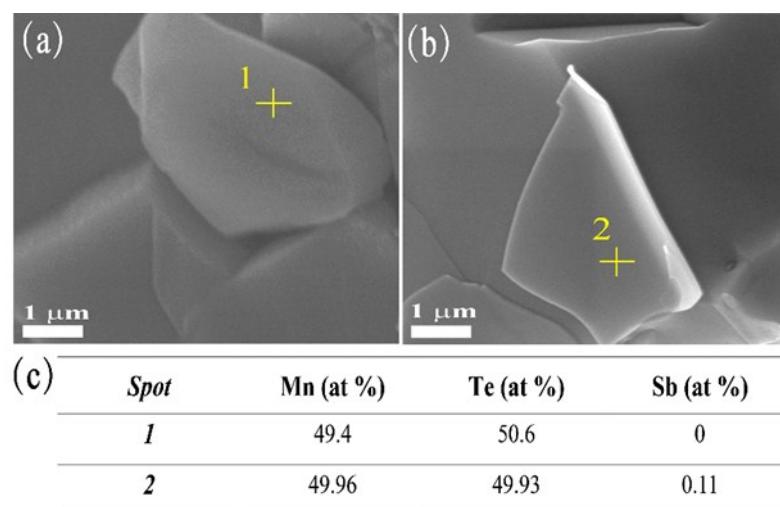


Fig. SI3: SEM and elemental compositions of 1.5 at% Sb₂Te₃ added MnTe sample in

figures (a, b) respectively.

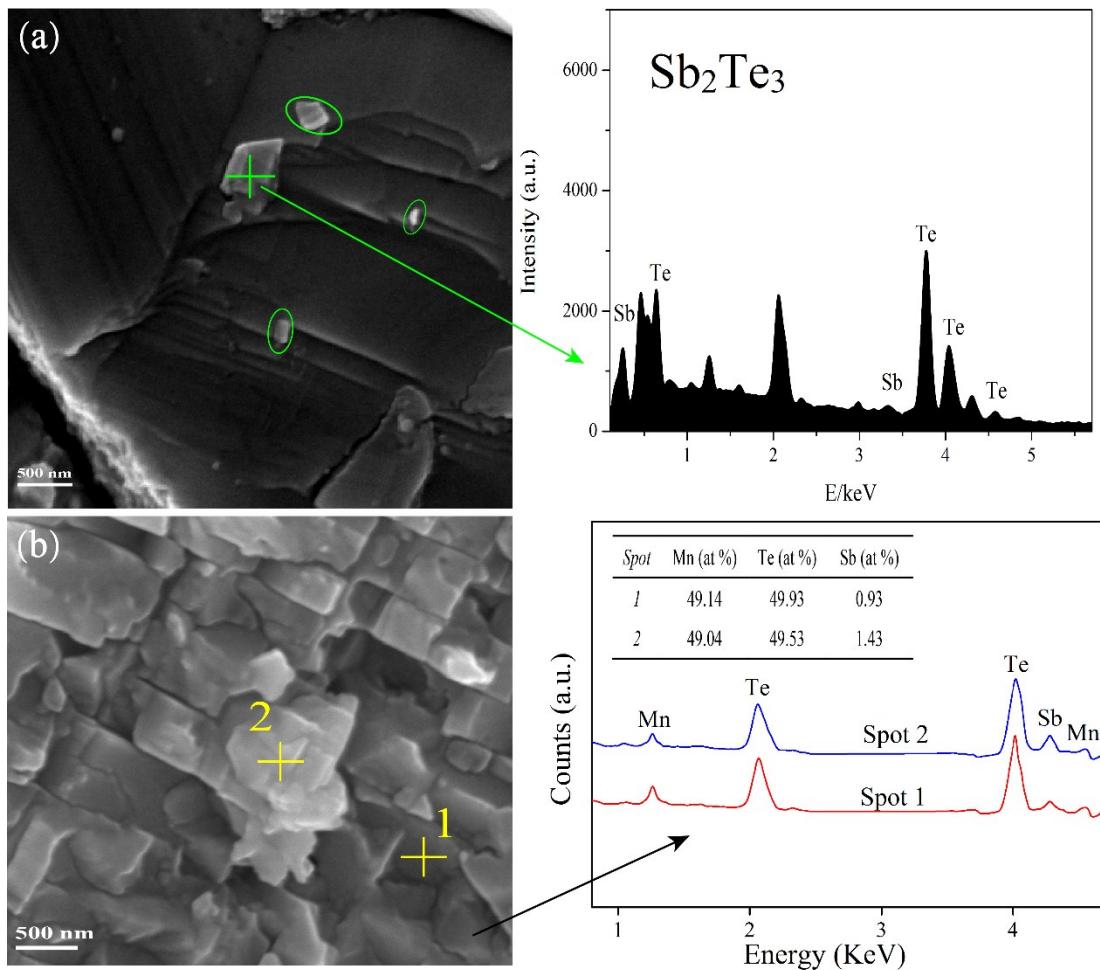


Fig. SI4: HRTEM of MnTe + 1.5at% Sb₂Te₃ sample.

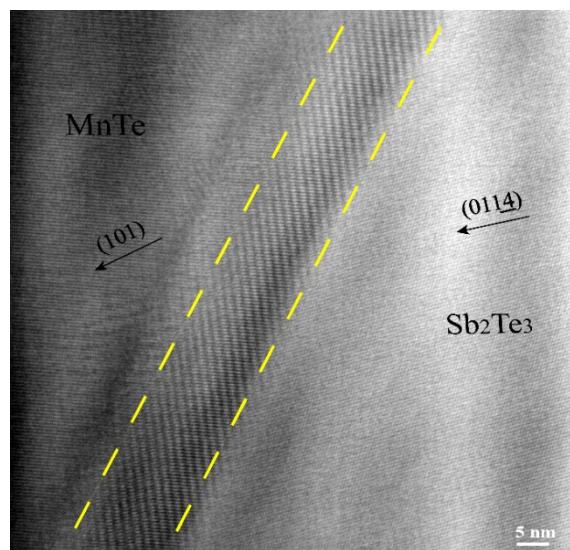
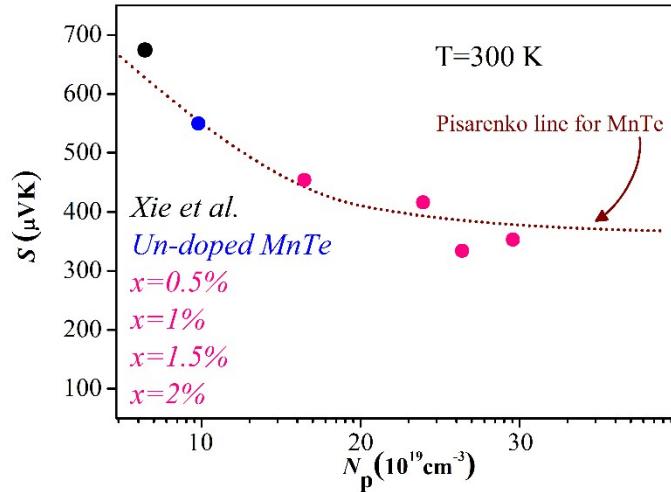


Fig. SI5: Pisarenko relation between S and carrier concentration of MnTe + x at%

Sb_2Te_3 samples ($x=0, 0.5, 1, 1.5, 2$) samples.



SI Table. 1: Lorenz number, carriers concentration and mobility of $\text{MnTe} + x$ at% Sb_2Te_3 samples.

Nominal			
composition	$L (10^{-8} \text{ W}\Omega\text{K}^{-2})$	$n_H (\text{cm}^{-3})$	$\mu_H (\text{cm}^2 \cdot \text{V}^{-1} \cdot \text{s}^{-1})$
$x=0$	1.4902	8.99E18	9.37632
$x=0.5$	1.4945	5.99E19	7.98316
$x=1$	1.5029	2.67E20	3.26835
$x=1.5$	1.518	4.65E20	2.37632
$x=2$	1.5111	7.51E20	1.8056

SI6:

Approximating a single parabolic band model [1], the Lorenz number (L) was carried out by the following equation;

$$L = \left(\frac{k_B}{e}\right)^2 \left[\frac{(r+7/2)F_{r+5/2(\varphi)}}{(r+3/2)F_{r+1/2(\varphi)}} - \left\{ \frac{(r+7/2)F_{r+3/2(\varphi)}}{(r+3/2)F_{r+1/2(\varphi)}} \right\}^2 \right]$$

Fermi integration $F_n(\varphi)$:

$$F_n(\varphi) = \int_0^\infty \frac{x^n}{1+e^{x-n}} dx$$

Here, r is the scattering parameter ($r = -1/2$) and φ ($=E_F/k_B T$) is the reduced Fermi energy which can be derived with the help of measured Seebeck coefficient followed by Single band approximation:

$$S = \pm \frac{k_B}{e} \left\{ \frac{(r + 5/2)F_{r+3/2(\eta)}}{(r + 3/2)F_{r+1/2(\eta)}} - \varphi \right\}$$

And hence this approximation were made for all MnTe + x at% Sb₂Te₃ ($x = 0, 0.5, 1, 1.5$ and 2) samples to calculate L, as given below in Fig. SI6:

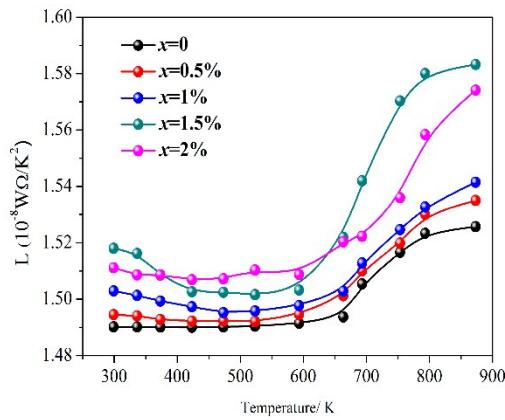


Fig. SI6: The calculated Lorenz number.

Reference

- [1] W. Xie, S. Populoh, K. Gałzka, X. Xiao, L. Sagarna, Y. Liu, M. Trottmann, J. He and A. Weidenkaff, J. Appl. Phys., 2014, 115, 103707.