Supporting Information

Enhancement of thermoelectric properties in Ag_2Te semiconductors through In-doping induced resonant levels and multi-valley degeneracy

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Theoretical calculation for carrier mobility

The carrier mobility is based on the deformation potential theory. In this work, the tensile and compressive elastic constants along the (100) direction . The correlations are expressed as follows,[1, 2]

$$\mu = \frac{2^{3/2}\pi^{1/2}\mathrm{h}^4 eC_{ii}}{3m_b^{*5/2}(k_B T)^{3/2}E_l^2}$$

where e denotes the electronic charge, $\hbar$ denotes the reduced Planck constant, C_{ii} denotes the elastic constant along the (100) direction, m^* b denotes the band effective mass and E_l denotes the deformation potential.

$$C_{ii} = \frac{\partial^2 E / \partial(\varepsilon)^2}{0.5V}$$

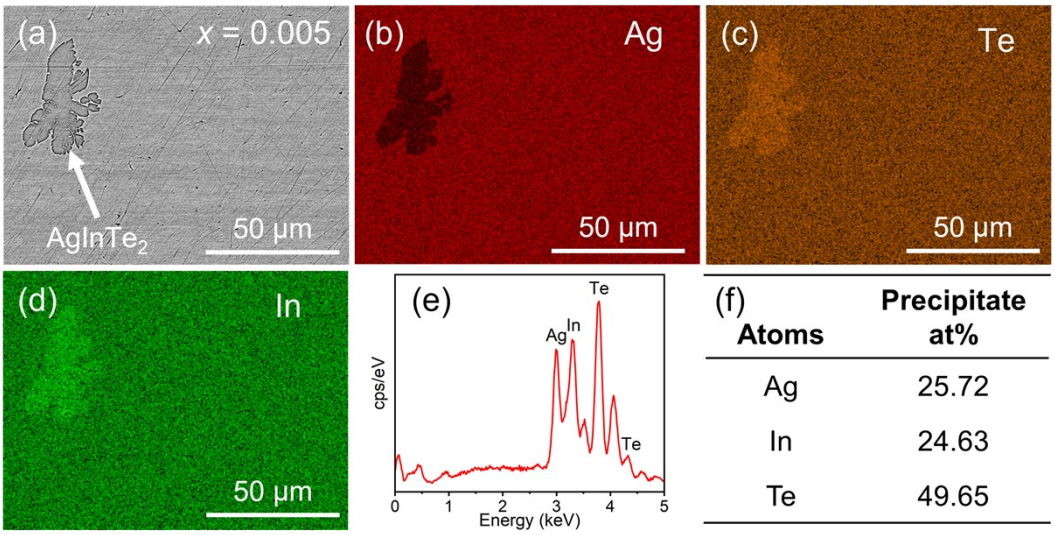
where E and ε denote the deformation energy and the strain under tension or compression along the (100) direction, respectively, V denotes the initial volume without deformation.

$$m_b^* = \mathrm{h}^2 / \frac{\partial^2 E}{\partial(k)^2}$$

where E is the energy band and k is the reciprocal lattice path.

$$E_l = \frac{\partial E}{\partial \varepsilon}$$

Where E and ε are the energy of the CBM or VBM and the strain under tension or compression along the (100) direction, respectively.



(f)

Atoms	Precipitate at%
Ag	25.72
In	24.63
Te	49.65

Fig. S1 Backscattering-electron (BSE) image of $Ag_{1.995}In_{0.005}Te$ sample and (b)-(d) corresponding elemental mappings of Ag, Te and In, respectively. (e) EDS point analysis spectra and (f) EDS point analysis of Te-rich precipitates.

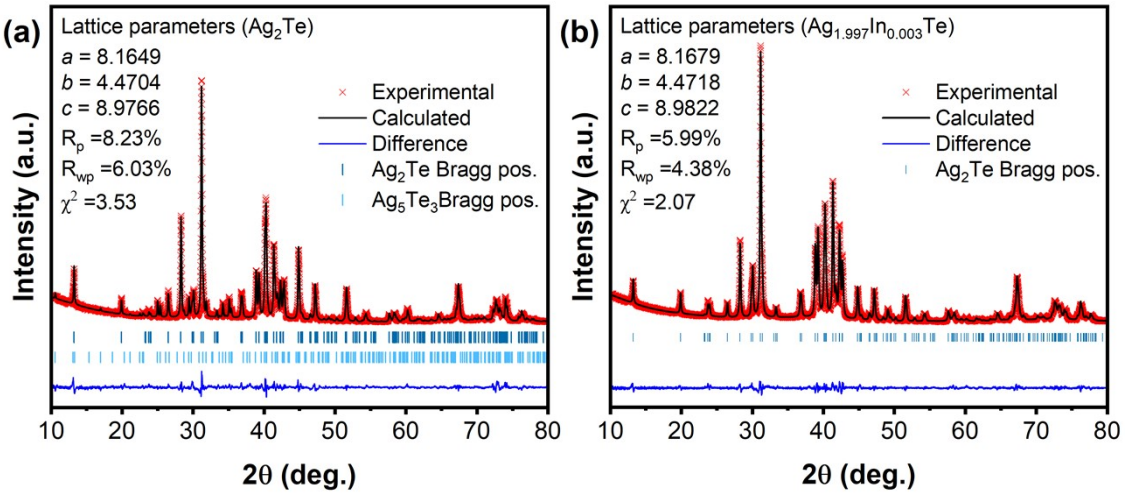


Fig. S2 Rietveld refinement profiles for (a) undoped Ag_2Te and (b) $Ag_{1.997}In_{0.003}Te$

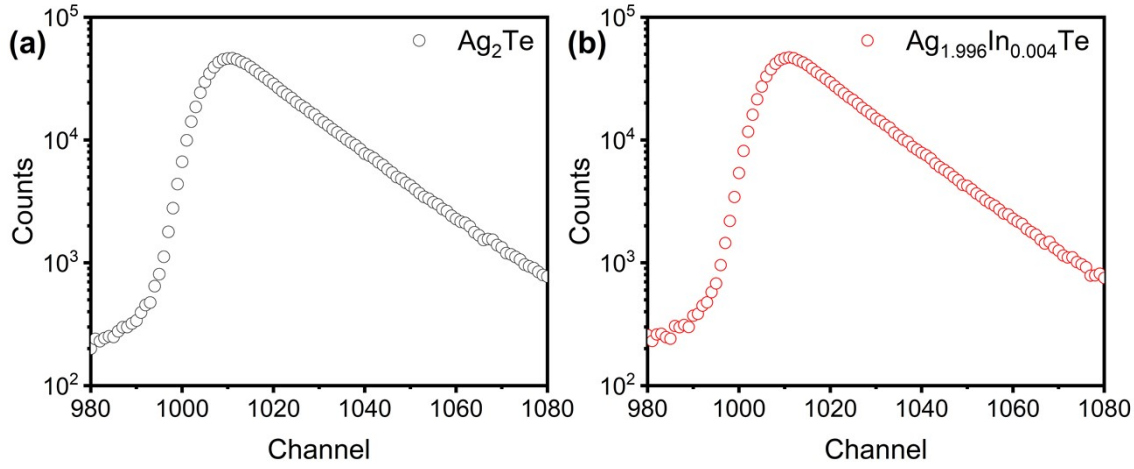


Fig. S3 Positron annihilation lifetime (PAL) spectra of (a) undoped Ag_2Te and (b) $Ag_{1.996}In_{0.004}Te$. (20 ps per channel)

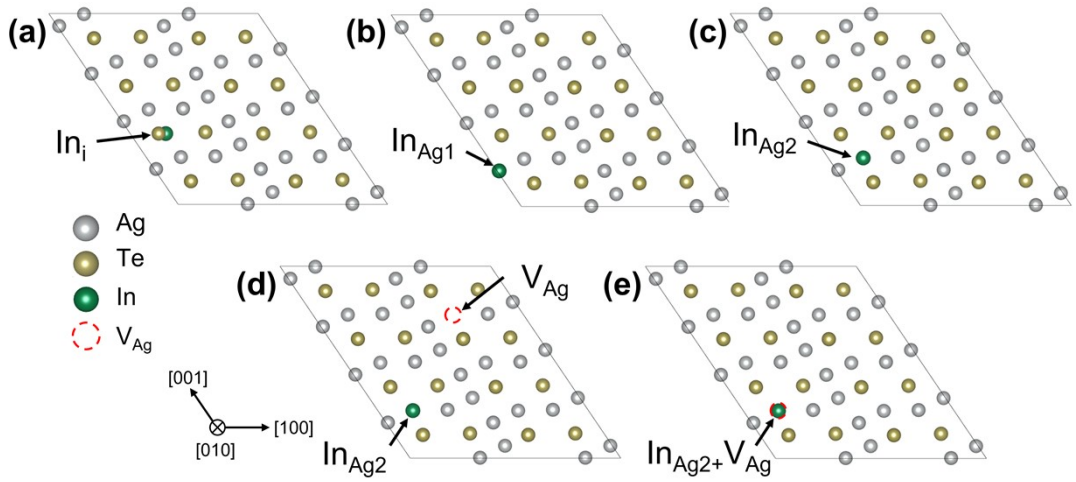


Fig. S4 The structural drawings for different defects.

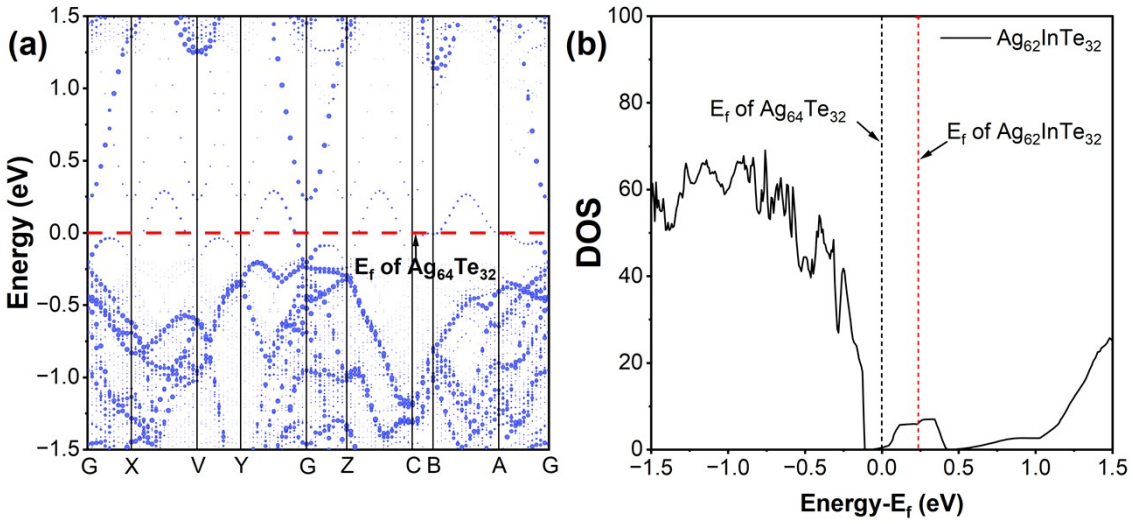


Fig. S5 (a) The band structure of $Ag_{62}InTe_{32}$. (b) The total DOS for $Ag_{62}InTe_{32}$. The black and red lines represent the E_f positions of $Ag_{64}Te_{32}$ and $Ag_{62}InTe_{32}$, respectively.

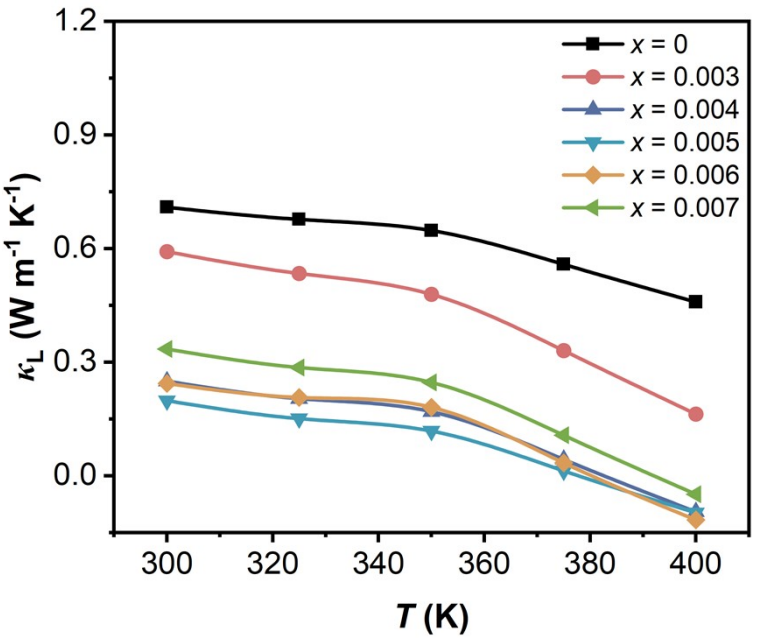


Fig. S6 Temperature dependence of lattice thermal conductivity for $Ag_{2-x}In_xTe$ (x = 0-0.007) samples.

Table S1 Positron annihilation lifetime parameters of Ag_2Te and $Ag_{1.996}In_{0.004}Te$ samples.

Compositions	τ_1 (ps)	I_1 (%)	τ_2 (ps)	I_2 (%)	τ_3 (ps)	I_3 (%)	τ_{avg} (ps)
Ag_2Te	151	6.8	306	92.8	1420	0.4	299.916
$Ag_{1.996}In_{0.004}Te$	197	16.5	301	83.1	1042	0.4	286.804

Table S2 DFT-calculated elastic constants (C_{ii}), band effective masses (m^* b), deformation potentials (E_l) and carrier mobility (μ). (using the tensile and compressive elastic constants along the (100) direction)

Compositions	C_{ii} (Pa)	m^* b (kg)	E_l (J)	μ (cm^2 v^{-1} s^{-1})
$Ag_{64}Te_{32}$	6.742×10^{10}	2×10^{-31}	-1.96×10^{-18}	1214.6
$Ag_{63}InTe_{32}$	6.402×10^{10}	1.65×10^{-31}	-2.22×10^{-18}	1452.6

References

1. H. Wang, Y. Z. Pei, A. D. LaLonde and G. J. Snyder, *Proc. Natl. Acad. Sci. U. S. A.*, 2012, **109**, 9705-9709.
2. J. Bardeen and W. Shockley, *Phys. Rev.*, 1950, **80**, 72-80.