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Outstanding CdSe with Multiple Functions Leads to High Performance of GeTe Thermoelectrics

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Thermoelectric materials can achieve the direct conversion between electricity and heat, which has drawn extensive attention in recent decades. Understanding the chemical nature of band structure and microstructure is essential to boost the thermoelectric performance of given materials. Herein, CdSe alloying promotes the evolution of multiple valence bands in GeTe, resulting in the contemporaneous appearance of band convergence and density of state distortion, which benefits the sharply enhanced effective mass from 2.3 m_0 to 5.0 m_0 . The carrier mobility and effective mass are well optimized via CdSe alloying, contributing to the ultrahigh weighted mobility of ≈199 cm² V⁻¹ s⁻¹ at 300 K in CdSe-alloyed GeTe. Accordingly, a superior power factor of \approx 41 μ W cm⁻¹ K⁻² is attained at 673 K. Meanwhile, the nanoprecipitates, strain, and mass field fluctuations introduced by CdSe alloying result in a significantly decreased lattice thermal conductivity. A highest figure of merit (ZT) of \approx 2.3 at 673 K and the ultrahigh ZT_{ave} of \approx 1.46 at 303-773 K are achieved in CdSe-alloyed GeTe. This work illustrates that the charge and phonon transport properties of GeTe can be simultaneously optimized through integrating band engineering and all-scale defects incorporation via CdSe alloying.

1. Introduction

Thermoelectric (TE) technology is identified to be an ecofriendly technology, enabling the reversible conversion between heat and electricity.^[1–3] The thermoelectric efficiency of materials can be evaluated by the dimensionless figure of merit, namely $ZT = S^2 \sigma T / (\kappa_{ele} + \kappa_{lat})$, where *S* represents Seebeck

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coefficient, σ represents electrical conductivity, *T* represents working temperature in Kelvin, κ_{ele} denotes electronic thermal conductivity, and κ_{lat} denotes lattice thermal conductivity.^[4,5] Extensive efforts are devoted to decoupling these correlative parameters.^[6]

Electrically, the strategies of band convergence,^[2] band alignment,^[4,7] densityof-states (DOS) distortion,^[8,9] modulation doping,^[10] enhancing the symmetry of crystal^[11] and quantum confinement^[12] are successfully established to equilibrate the Seebeck coefficient (S) and the electrical conductivity (σ) in favor of a superior power factor (PF).^[13] It is well known that the enhanced band degeneracy due to band convergence could increase the effective mass a bit without degrading the carrier mobility. And DOS distortion, which improves the band effective mass, is a feasible strategy with risks for deteriorating the carrier mobility.^[14] It is clear that the optimal balance between the

effective mass and the carrier mobility is beneficial for the electrical performance of TE materials. This relationship primarily depends on the weighted mobility, $\mu W = \mu_{\rm H} (m^*/m_{\rm e})^{3/2}$, where $\mu_{\rm H}$ represents the carrier mobility, m^* represents the DOS effective mass, and $m_{\rm e}$ represents the unit electron mass.

Thermally, intensifying the phonon scattering is considered to be an effective method to decrease the thermal conductivity (κ_{lat}), which is generally classified into incorporating extra phonon scattering centers^[15] and seeking inherent low lattice thermal conductivity materials.^[16,17] The latter representing materials might have a complex crystal structure,^[1] heavy constituent elements,^[18] intense lattice anharmonicity,^[19] and soft chemical bonding.^[20] And the extra phonon scattering sources include point defects, nanoprecipitates, grain boundaries, and so on.^[21] To date, state-of-the-art TE materials, including Zintl phase,^[22] half-Heusler,^[23] skutterudite,^[24] SiGe,^[25] chalcogenides,^[8,26] and Bi₂Te₃-based compounds,^[27] etc., exhibit prominent thermoelectric performance.

GeTe is proven to be an eminent mid-temperature thermoelectric material.^[28,29] The well-recognized characters of GeTe are multiple valance bands, phase transition, ultrahigh carrier concentration, and high thermal conductivity, which diversify the degrees of freedom to tailor its TE performance.^[30–32] Counter-doping using aliovalent elements, such as Bi, Sb, and In,^[33,34] is a common method to achieve the optimal carrier



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density. Motivated by multiple valence bands (VBs) of GeTe, band engineering, including band convergence,^[35] band alignment,^[36] and DOS distortion,^[34,37] has been widely implemented to optimize the power factor. Coordinating these band engineering effects could favor the charge transport properties of GeTe. Meanwhile, alloying is regarded as an efficient strategy to reduce κ_{iat} , which introduces extra phonon scattering centers, including nanoprecipitates, mass, and strain field fluctuations.^[36,38–40]

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After optimizing the carrier density of GeTe through counter-doped Sb,^[41] here, we further investigate the charge and phonon transport properties of Ge0.2Sb01Te with CdSe alloying. Coupling high-temperature synchrotron radiation X-ray diffraction (SR-XRD) results and the electronic band structure calculations, we find that CdSe alloying gives rise to the decrement of the energy offset between the heavy and light valence band and also produces a DOS distortion. Both the band convergence and the DOS distortion upon CdSe alloying significantly enhance the effective mass from 2.3 m_0 to 5.0 m_0 , resulting in a sharply increased Seebeck coefficient and a rather high weighted mobility. Meanwhile, the impurity level induced by introducing Cd could release holes at high temperature, which favorably maintains the σ in the entire temperature region. Consequently, the peak PF could reach as high as \approx 41 μ W cm⁻¹ K⁻² at 673 K. Additionally, CdSe alloying introduces nanoscale CdSe precipitates, which are observed under scanning transmission electron microscope (STEM), furthermore, massive point defects, including strain and mass field fluctuations, are also introduced by CdSe alloying. Together with these phonon scattering sources, the κ_{lat} is strongly decreased by suppressing the propagation of phonon. Consequently, a superhigh ZT of ≈2.3 at 673 K and an ultrahigh ZT_{ave} of ≈1.46 at 303–773 K are achieved in Ge0.9Sb0.1Te-2%CdSe. The strategies developed in this work of introducing a simple compound in GeTe pave a robust way to achieve extraordinary performance in thermoelectrics.

2. Results and Discussion

The Ge_{0.9}Sb_{0.1}Te matrix with optimal carrier concentration was co-alloyed with Cd and Se. The phase identification in Figure S1a in the Supporting Information shows a rhombohedral-GeTe phase (R3m) with a trace of Ge precipitates. Especially, the characteristic twin peaks of rhombohedral-GeTe in the range of $2\theta = 23^{\circ}-27^{\circ}$ and $2\theta = 41^{\circ}-45^{\circ}$ gradually show a merging trend as increasing the fraction of CdSe, which manifests that the cubic nature of samples is elevated.^[41,42] The result is also verified by differential scanning calorimetry tests, as illustrated in Figure S2a in the Supporting Information. The phase transition temperature of CdSe-alloyed Ge_{0.9}Sb_{0.1}Te samples, manifesting the crystal symmetry of GeTe, shifts to low temperature range with increasing CdSe content. Since the radius difference between Cd and Ge atoms is larger than that between Se and Te atoms, the estimated lattice parameter obtained by XRD refinement slightly increases with rising CdSe fraction, as depicted in Figure S1b in the Supporting Information.

2.1. Electrical Transport Properties in ${\sf Ge}_{0.9}{\sf Sb}_{0.1}{\sf Te}$ with Alloying CdSe

Figure 1 illustrates the electrical transport properties of $Ge_{0.9}Sb_{0.1}Te-x\%CdSe$ (x = 0, 1, 2, 3, 4, 5). In Figure 1a, the electrical conductivity (σ) of the above samples declines with rising CdSe content at ambient temperature. Especially, the electrical conductivity in CdSe-alloyed samples initially exhibits a slight descending trend with rising temperature and then turns to remain nearly constant across all high temperature range (600–773 K). The unique behavior of σ is not typical for GeTe-based materials and will be discussed later. The Seebeck coefficient (*S*) of CdSe-alloyed samples significantly enhances from 134 to 211 μ V K⁻¹ at ambient temperature, as depicted in Figure 1b. The overall *S* of CdSe-alloyed samples is higher than the CdSe-free sample in the entire test temperature range. Since the degenerated σ is recompensated by the highly elevated Seebeck coefficient, a peak PF of ~41 μ W cm⁻¹ K⁻² is attained at 673 K.

Hall measurements are performed to reveal the behavior of electrical conductivity at room temperature. Interestingly, the carrier density $(n_{\rm H})$ experiences a slight increment, varying from $\approx 1.76 \times 10^{20}$ cm⁻³ in CdSe-free sample to 2.02×10^{20} cm⁻³ in 5% CdSe-alloyed sample, while the effective mass (m^*) undergoes a remarkable enhancement from 2.3 m_0 in CdSe-free sample to 5.0 m_0 in 5% CdSe-alloyed sample, as depicted in Figure 1d. To delve into the origin of the rapidly elevated Seebeck coefficient, Figure 1e exhibits the Pisarenko curves of CdSe-alloyed samples based on the single parabolic band model. The m^* enhances as rising CdSe fraction at both 303 and 673 K, while $n_{\rm H}$ -dependent carrier mobility shows the opposite trend in Figure 1f. The effective mass is tightly relevant with band structure, which can be evaluated by the following equation

$$m^* = (N_v)^{2/3} m_b^* \tag{1}$$

where N_V denotes the number of degenerate valleys and m_b^* denotes a single-valley effective mass. As can be seen from formula (1), there are two mechanisms to increase m^* : i) enlarging the band degeneracy (N_V) including band convergence and activation of multiple bands near Fermi level and ii) increasing a single band effective mass m_b^* such as band flattening and DOS distortion.^[8,16,36,41] Alloying CdSe has negligible influence on carrier density at lower temperatures in this work, excluding the possibility of multiple bands activation. Therefore, we speculate that the increased m^* derives from the band structure evolution upon CdSe alloying, which leads to the increased Seebeck coefficient.

The weighted mobility (μ W) can well estimate the elevated carrier transport properties in terms of electronic band structure, which correlates with the effective mass (m^*) and carrier mobility ($\mu_{\rm H}$).^[50,51] And the calculative details are listed in Supporting Information. As displayed in **Figure 2a**, the overall weighted mobility of CdSe-alloyed samples is superior to that of the CdSe-free sample in the entire working temperature, which contributes to the superior power factor in CdSe-alloyed samples. Notably, the visibly enhanced weighted mobility is a manifestation of band structure evolution in this work. The higher effective mass can attain the larger *S*, but degrade the $\mu_{\rm H}$. It is essential to balance the $\mu_{\rm H}$ and m^* for optimizing the electrical

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Figure 1. Electrical transport properties of Ge_{0.9}Sb_{0.1}Te-*x*%CdSe (x = 0, 1, 2, 3, 4, and 5): a) σ , b) S, c) PF, and d) $n_{\rm H}$ and m^* at ambient temperature. Pisarenko relationship of $n_{\rm H}$ dependent e) S at 300 and 700 K and f) $\mu_{\rm H}$ at 300 and 700 K.

transport properties. To comprehensive assess the role of CdSe alloying on carrier transport characteristics of GeTe, we make comparisons with other *M*-alloyed GeTe thermoelectrics at room temperature (M = MnTe,^[43] PbTe,^[44] CdTe,^[36] FeTe₂,^[45] GeSe,^[46] In₂Te₃,^[34] AgSbTe₂^[47]), as depicted in Figure 2c. Obviously, the m^* and μ_H can be well equilibrated upon CdSe alloying, finally resulting in the maximum μ W of ~199 cm² V⁻¹ s⁻¹ and optimum PF at room temperature, as depicted in Figure 2c. Compared with other alloying, CdSe-alloyed GeTe is predominant in GeTe-based thermoelectric materials with similar carrier density as illustrated in Figure 2d.^[35,37,39,48,49] It strongly confirms the importance of weighted mobility as one of the key parameters in electrical transport properties to consider band engineering effects.

Considering the special behavior of electrical conductivity, high-temperature Hall measurements were conducted to investigate the relationship between $n_{\rm H}$ and temperature. As illustrated in Figure 2b, the $n_{\rm H}$ of CdSe-alloyed samples first

undergoes a slight fluctuation and then starts to enhance at 600 K, which is absent in the CdSe-free sample. The sharply increased carrier density after CdSe alloying indicates a special charge transport mechanism. Density functional theory (DFT) theoretical calculations are implemented, as illustrated in Figure S3 in the Supporting Information. In Figure S3b in the Supporting Information, it is found that an impurity level is introduced by Cd alloying. The Cd-induced level can be regarded as a carrier supplier which releases holes with increasing temperature, leading to the rapid elevation of $n_{\rm H}$ at high temperature.^[36] The boosting $n_{\rm H}$ over the entire test temperature range could ensure an excellent power factor.^[51]

2.2. Electronic Band Structures in Ge0.9Sb0.1Te with Alloying CdSe

To verify our speculation and further comprehend the impact of alloying CdSe on charge transport mechanism, we

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Figure 2. Electrical transport properties analysis of $Ge_{0.9}Sb_{0.1}Te-x\%CdSe$ (x = 0, 1, 2, 3, 4, and 5): a) temperature-dependent weighted mobility and b) temperature-dependent carrier density. c) Comparison of weighted mobility and PF (the inset) in *M*-alloyed GeTe thermoelectrics at 300 K (M = MnTe,^[43] PbTe,^[44] CdTe,^[36] FeTe₂,^[45] GeSe,^[46] In₂Te₃,^[34] AgSbTe₂^[47]) as function of carrier density. d) Comparison of the peak PF among GeTe based thermoelectric materials with similar carrier density.^[35,37,39,48,49]

performed SR-XRD and then obtain variable temperature band structures based on DFT calculations, as depicted in Figures S4 and S5 in the Supporting Information. The roomtemperature electronic band structures of Ge0.9Sb0.1Te and Ge0.9Sb01Te-2%CdSe are calculated in Figure 3a, which were obtained from atomic position refinements based on SR-XRD. It can be seen that multivalence bands (VBs) in *p*-type GeTe contribute to electrical transports.^[28,31] The energy offset (ΔE) between the heavy and light VBs descends from 0.06 eV in Ge0.9Sb0.1Te to 0.04 eV in Ge0.9Sb0.1Te-2%CdSe, which demonstrates that the heavy VB is more facilitately involved in electrical transport as shown in Figure 3c. The band convergence brings about the enlarged band degeneracy, leading to the significant enhancement of effective mass upon CdSe alloying. Meanwhile, the DOS of Ge27Te27, Ge26CdTe27, and Ge₂₆CdTe₂₆Se are displayed in Figure 3b, respectively. Notably, the energy of DOS highly increases after Cd and Se alloving as depicted in the inset of Figure 3b, acting to forcefully increase effective mass, which is named DOS distortion as observed in PbTe and SnTe.^[8,9] Therefore, the remarkable increase in effective mass derives from the band convergence and DOS distortion with the evolution of multiple VBs by CdSe alloying, as illustrated in Figure 3c. Particularly, the DOS plots show that a peak of the impurity level appears near the conduction band in Ge₂₆CdTe₂₇ and Ge₂₆CdTe₂₆Se due to the hybridization of Cd. The results are fully consistent with our DFT theoretical calculations.

Figure 4a,b exhibits the electronic band structures of Ge_{0.9}Sb_{0.1}Te-2%CdSe at 473 and 523 K, respectively. The schematic of the dynamic evolution of multivalence bands and crystal structure with rising temperature in GeTe-CdSe before phase transition are depicted in Figure 4c. As increasing temperature, the heavy VB undergoes an energy convergence with the light VB. The energy offset between heavy and light VBs further decreases to 0.024 eV at 473 K and experiences an energy alignment at 523 K before phase transformation. As illustrated in Figure 4d,e, Brillouin zones of the rhombohedral-structured Ge0.9Sb0.1Te-2%CdSe at 473 and 523 K are calculated, respectively. Obviously, the Brillouin zones of Ge0.9Sb0.1Te-2%CdSe gradually change from Figure 4d to Figure 4e with promoting the convergence of the two VBs, which enlarges the band degeneracy. With increasing temperature, the interaction of multiple valence bands contributes to the elevated effective mass, thus improving the Seebeck coefficient of Ge0.9Sb0.1Te-CdSe. The modification of valence bands upon CdSe alloying well elucidates the optimized electrical transport properties.

2.3. Thermal Transport Properties in $Ge_{0.9}Sb_{0.1}Te$ with Alloying CdSe

The overall total thermal conductivity (κ_{tot}) of CdSe-alloyed Ge_{0.9}Sb_{0.1}Te is lower than that of the CdSe-free sample in





Figure 3. a) Valence band structures of $Ge_{0.9}Sb_{0.1}Te$ and $Ge_{0.9}Sb_{0.1}Te-2\%CdSe$. b) Density of states (DOS) of $Ge_{27}Te_{27}$, $Ge_{26}CdTe_{27}$, $Ge_{27}Te_{26}Se$, and $Ge_{26}CdTe_{26}Se$. c) Schematic of dynamic evolution of multivalence bands and DOS in GeTe with CdSe and without CdSe.

the entire temperature region and shows a downward trend with increasing CdSe fraction. The κ_{tot} sharply descends from 1.60 W m⁻¹ K⁻¹ for Ge_{0.9}Sb_{0.1}Te to 1.04 W m⁻¹ K⁻¹ in Ge_{0.9}Sb_{0.1}Te-5%CdSe, which is almost 35% decrement compared with that of the CdSe-free sample at ambient temperature (**Figure 5**a). The electronic thermal conductivity (κ_{ele}) of all samples is calculated with the Wiedemann–Franz relationship as displayed in Figure 5c,^[52] which increases with rising temperature. The lattice thermal conductivity (κ_{iat}) is obtained by subtracting κ_{ele} from κ_{tot} , as depicted in Figure 5b. The ambient-temperature κ_{lat} undergoes a significant decrement with increasing CdSe content from 1.21 W m⁻¹ K⁻¹ in CdSe-free samples to 0.86 W m⁻¹ K⁻¹ in Ge_{0.9}Sb_{0.1}Te-5%CdSe. The minimum κ_{lat} of ~0.62 W m⁻¹ K⁻¹ is achieved in Ge_{0.9}Sb_{0.1}Te-5%CdSe at 773 K.

In a solid solution compound, the significant decrement of κ_{lat} is considered to be caused by the point defects from the strain and mass field fluctuations via elements alloying.^[53] To further confirm the effects of these point defects on the decreased κ_{lat} , the phonon transport is investigated using the Callaway model.^[54] The calculated distortion parameters (Γ) are illustrated in Figure 5e, which is estimated by $\Gamma = \Gamma_{\rm M} + \Gamma_{\rm S}$, where $\Gamma_{\rm M}$ denotes mass fluctuation scattering parameter and $\Gamma_{\rm S}$ denotes strain field fluctuation scattering parameter. It can be seen that the values of $\Gamma_{\rm S}$ is rather high than that of $\Gamma_{\rm M}$. Therefore, strain field fluctuation dominates the phonon scattering compared to mass fluctuation. However, the calculated κ_{lat} based on Callaway mode is relatively higher than the experimental data, as illustrated in Figure 5d. The apparent gap between calculated and experimental data demonstrates the existence of other phonon scatter sources. Essentially, the sound speed of acoustic phonons is a macroscopic expression of chemical bonds.^[43] As depicted in Figure 5f, the average sound velocity (ν_a), transverse velocity (ν_t), and the longitudinal velocity (ν_l) all descend with increasing CdSe content. The results imply that CdSe alloying softens the chemical bonds of CdSe-alloyed samples, which could contribute to further reducing the lattice thermal conductivity.^[55]

2.4. Microstructures in Ge0.1Sb0.9Te with Alloying CdSe

To delve into the potential phonon scattering sources upon CdSe alloying, we implement aberration-corrected STEM. As depicted in Figure S7a in the Supporting Information, the low-magnification image exhibits numerous herringbone stripes with nanoscale in $Ge_{0.9}Sb_{0.1}Te-2\%CdSe$, which is a typical microstructure of $GeTe.^{[31,43]}$ And its corresponding STEM HAADF (high angle annular dark field) and ABF (annular bright field) images present Van der Waals gaps which derive from the absence of Ge atoms to form Ge vacancies. The



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Figure 4. Valence band structures of $Ge_{0.9}Sb_{0.1}$ Te- 2%CdSe at a) 473 K and b) 523 K. c) Schematic of the dynamic evolution of multiple VBs and crystal structure with rising temperature in GeTe-2%CdSe before phase transition. d) Rhombohedral structure Brillouin zones of $Ge_{0.9}Sb_{0.1}$ Te-2%CdSe at d) 473 K and e) 523 K.

Van der Waals gaps due to Ge vacancies are also the form of phonon scattering source.^[36] Notably, we also observe nanoscale precipitates in the Ge0.9Sb0.1Te-2%CdSe, as illustrated in Figure 6a. STEM-energy dispersive X-ray spectroscopy (EDS) is conducted to figure out the constituent of the inclusions. The elemental mappings reveal that the second phase can be identified as the CdSe phase, as displayed in Figure 6b–f. In high-magnification STEM ABF imaging mode, the CdSe inclusion with irregular particle shapes is tens of nanometers in size, as shown in Figure 6g. Geometric phase analysis (GPA) is performed to attain the strain distribution in the CdSe precipitate. As illustrated in Figure 6h,i, high ε_{xx} (horizontal axis) strain center appears in the middle area of the nanoprecipitate and the interface between the nanoprecipitate and matrix, while high ε_{vv} (vertical axis) exists at the midzone of the nanoprecipitate. The CdSe phase incorporation with nanoscale plays a significant role in scattering phonon, leading to the rapidly decreased κ_{lat} .

2.5. Quality Factor and Figure of Merit ZT in $Ge_{0.9}Sb_{0.1}Te$ with Alloying CdSe

To comprehensively assess the function of CdSe in $Ge_{0.9}Sb_{0.1}$ Te-*x*%CdSe samples, the quality factor (*B*) is calculated by the following relationship^[56]

$$B = 9 \frac{\mu_{\rm W}}{\kappa_{\rm lat}} \left(\frac{T}{300}\right)^{5/2}$$
(2)

where *T* denotes the absolute temperature. As depicted in **Figure** 7a, a significant improvement of quality factor is attained in the entire temperature range upon CdSe alloying, especially in high temperature range. Due to the rather high μ W and the remarkably decreased κ_{iat} , an increment of nearly 53% is attained in the GeTe-2%CdSe at 673 K compared to that of Ge_{0.9}Sb_{0.1}Te. As illustrated in Figure 7b, the weighted mobility and the reciprocal of lattice thermal conductivity

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Figure 5. Thermal transport properties of $Ge_{0.9}Sb_{0.1}Te$ -x%CdSe (x = 0, 1, 2, 3, 4, and 5): a) κ_{iat} , c) κ_{ele} , d) the comparison of ambient temperature κ_{iat} between the calculated values based on the Callaway model and the experimental data, e) Γ_S and Γ_M , and f) sound velocities as a function of CdSe content.

of GeTe-*x*%CdSe in this work are superior to those of other *H*-alloyed (H = GeSe,^[46] In₂Te₃,^[34] MnTe,^[43] PbTe,^[44] FeTe₂,^[45] CrTe,^[49] AgSbTe₂,^[47] Bi₂Te₃,^[48]) GeTe thermoelectrics.

Combing the optimized charge and phonon transport properties, the peak *ZT* could reach 2.3 at 673 K through modifying multiple valence bands and incorporating all-sale defects into the Ge_{0.9}Sb_{0.1}Te matrix. This further leads to an ultrahigh $ZT_{ave} \approx 1.46$ at 303–773 K, which is superior to these reported GeTe samples, such as $ZT_{ave} \approx 1.21$ in GeTe-SnTe,^[30] $ZT_{ave} \approx 1.20$ in GeTe-PbSe,^[57] $ZT_{ave} \approx 1.20$ in GeTe-GeSe,^[46] $ZT_{ave} \approx 1.24$ in GeTe-Bi₂Te₃,^[48] $ZT_{ave} \approx 1.20$ in GeTe-CrTe,^[49] $ZT_{ave} \approx 1.04$ in GeTe-Cu₂Te,^[40] and $ZT_{ave} \approx 1.25$ in GeTe-FeTe₂.^[45] Importantly, the excellent thermoelectric properties obtained in this work exhibit superior thermal stability and reliability, which is verified by cycle testing (heating–cooling), as illustrated in Figure S8 in the Supporting Information.

3. Conclusions

In this work, we found that the complex TE parameters of GeTe can be optimized through introducing a simple CdSe compound. The weighted mobility of GeTe can be significantly enhanced through realizing electronic band convergence and DOS distortion, thus resulting in outstanding high electrical transport properties. Meanwhile, along with manipulating electronic bands, strongly scattering phonons caused by the introduction of all-scale defects via CdSe alloying also leads to a very low thermal conductivity. With the integration of the optimized electrical and thermal properties, an ultrahigh *ZT* of 2.3 at 673 K and a *ZT*_{ave} of 1.46 at 303–773 K are obtained in Ge_{0.9}Sb_{0.1}Te-2%CdSe. This work sheds light on boosting thermoelectric performance via synergistic band and nanostructure engineering.



Figure 6. Microstructures observation in Ge_{0.9}Sb_{0.1}Te-2%CdSe sample: a) low-magnification STEM HAADF image; b–f) EDS mappings of Ge, Sb, Te, Cd, and Se; g) high-magnification STEM HAADF image. GPA analysis mappings from g) along h) horizontal (ε_{xx}) and i) vertical (ε_{yy}) directions of CdSe nanoprecipitate.



Figure 7. TE performance of $Ge_{0.9}Sb_{0.1}Te-x\%CdSe$ (x = 0, 1, 2, 3, 4, 5): a) the comparison of μ W and $1/\kappa_{lat}$ between this work and reported (GeTe-GeSe,^[46] GeTe-In₂Te₃,^[34] GeTe-PbTe,^[44] GeTe-MnTe,^[43] GeTe-FeTe₂,^[45] GeTe-CrTe,^[49] GeTe-AgSbTe₂,^[47] and GeTe-Bi₂Te₃,^[48]); b) quality factor; c) ZT values; d) ZT_{ave} compared with previous reported data (GeTe-SnTe,^[30] GeTe-PbSe,^[56] GeTe-GeSe,^[46] GeTe-Bi₂Te₃,^[48] GeTe-CrTe,^[49] GeTe-Cu₂Te,^[40] and GeTe-FeTe₂.^[45]).

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Supporting Information

Supporting Information is available from the Wiley Online Library or from the author.

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Conflict of Interest

The authors declare no conflict of interest.

Data Availability Statement

The data that support the findings of this study are available in the supplementary material of this article.

Keywords

band convergence, CdSe alloying, DOS distortion, effective mass, GeTe, nanoprecipitates, thermoelectric materials

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