Effect of the polar distortion on the thermoelectric properties of GeTe

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Abstract

First principle calculations are performed to investigate the effect of polar order strength on the thermoelectric (TE) properties of GeTe alloy in its rhombohedral structure. The variation in the polarization state using various ferroelectric distortions $\lambda$ ($\lambda = 0, 0.5, 1.0, 1.25, 1.5$) allows to change the thermoelectric properties to a large extent. The polar structure with a high polarization mode ($\lambda = 1.5$) tends to show a higher TE efficiency than the cubic structure at high temperatures. Thus, polarization engineering may play a key role in designing efficient thermoelectric devices. In particular, high TE performances could be achieved by growing epitaxial GeTe films that bi-axially compress the directions perpendicular to the polar axis, which may help to tune the Curie temperature.

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1. Introduction

Technological development and population growth lead to an uncontrolled use of fossil fuels. Increasing world pollution and the related greenhouse effect caused some detrimental side effects that need to be urgently tackled. This spurred an ever-increasing effort to find sustainable, renewable and clean energy sources. One solution of these problems has emerged over the few decades based on thermoelectric (TE) devices. These devices are made of two dissimilar materials having different concentrations of holes and electrons [1]. Thermoelectric materials have attracted a lot of attention due to their promising applications as a clean source of energy, which converts waste heat into electricity and vice versa [2-4]. The efficiency of TE materials is characterized by the dimensionless figure of merit \(ZT = (S^2/\kappa_e + \kappa_l)T\), where \(S, \sigma, \kappa_e, \kappa_l\) and \(T\) are the Seebeck coefficient, electrical conductivity, electrical thermal conductivity, lattice thermal conductivity and temperature, respectively [5]. The main goal is to develop materials or designs using state-of-the-art techniques in order to improve \(ZT\) [6]. Through the classification of current thermoelectric materials we can identify specific desired properties based on the figure of merit as follows: \(ZT=1\) inefficient, \(ZT=2\) recover waste heat, \(ZT>4\) able to match a refrigerator [7]. An ideal thermoelectric material with high \(ZT\) either exhibits a high power factor \((S^2\sigma)\) or/and low thermal conductivity \((\kappa_e + \kappa_l = \kappa)\). Unfortunately, most of the materials properties involved vary in a competing manner: a low concentration of free carriers tends to increase the Seebeck coefficient but also results in poor electrical conductivity. Similarly, improving the electrical conductivity causes higher thermal conductivity [8]. Some approaches demonstrate pathways to increase the power factor such as engineering energy degeneracy levels by adopting low dimensional nanostructures, decreasing bipolar effect [9] or reducing the lattice thermal conductivity by nanostructuring [10]. Yet, these approaches remain costly and complicated. Thus finding a good TE material is an
important challenge due to the aforementioned restrictions. Although a variety of materials were studied and investigated for thermoelectric properties, only three of them were marked for mass production, bismuth telluride (Bi$_2$Te$_3$), lead telluride (PbTe), and silicon germanium (SiGe) [11]. For a long time Bi$_2$Te$_3$ had been studied and considered as the best thermoelectric material with ZT=1 and an efficiency ranging from 5 to 7% for most applications at low temperatures. The optimal temperature for Bi$_2$Te$_3$ is about 450 K and the maximum operating temperature is between 550 and 600 K [7]. Another commercial TE material is lead telluride (PbTe), which works at a moderate temperature range of 350–850 K. The maximum achieved ZT value is about 0.8, which is still insufficient for large-scale commercial applications [12]. Lead telluride has been used in many applications such as thermoelectric generators, pacemaker batteries and even space craft vehicles [13]. The use of thermoelectric materials in power generation applications and the subsequent interest in finding more efficient TE materials paved the way for the discovery of silicon germanium (SiGe). The advantage of using SiGe is due to the possibility of forming n-type and p-type materials [14]. This material can operate at a high temperature range (800-1300 K), which is useful for radioisotope thermoelectric generators [15]. Recently, an experimental work reported a ZT of 2.6 at 973 K along the b-axis of bulk SnSe [16]. This groundbreaking work spurred the current interest in IV-VI chalcogenides as promising TE materials, which are capable to work in intermediate temperatures of 600-900 K[17]. One of those IV-VI group compounds is GeTe, which exhibits high-performance thermoelectric properties [18]. In ambient conditions, GeTe has a rhombohedral structure (R3m space group), which is a ferroelectric material [19-22]. This material shows a temperature dependent phase transition to a cubic structure in the range of 600 K–700K depending on the carrier concentration [19-22]. There are contradictory reports about which phase of GeTe is the most suitable for TE applications. For instance, one study reported that the cubic phase of
$p$-doped GeTe is more interesting for TE applications [20], while another study indicates that the rhombohedral phase always shows a higher power factor than that of the cubic phase [23]. It thus appeared to us that there is a need to disentangle the various degrees of freedom (such as polarization) in order to better understand and engineer the TE properties of GeTe. In this paper, we thus report *ab initio* calculations of electronic band structure and thermoelectric properties of bulk GeTe.

2. Computational Methods

First-principle electronic structure calculations based on Kohn-Sham density functional theory (DFT) are performed using the Vienna ab initio simulation package (VASP) to obtain the electronic, structural and thermoelectric properties of GeTe alloy. The generalized gradient approximation in the formal Perdew–Burke–Ernzerhof (PBE) parametrization scheme is used to describe the exchange correlation energy of electrons. The kinetic plane wave cut-off was chosen as 520 eV, and the Brillouin zone (BZ) was meshed using a $12 \times 12 \times 12$ $\Gamma$-centered grid. The lattice parameters and ionic positions were optimized using a force convergence criterion of 0.01 eV/Å. Phonon dispersion and second order harmonic interaction force constants are calculated in a $4\times 4 \times 4$ supercell with the Phonopy package [24].

The electronic band structure obtained from first-principles is interpolated on a denser k-mesh of $60\times 60 \times 60$ to calculate the thermoelectric properties using the semi-classical Boltzmann transport theory as implemented in Boltztrap [25].

3. Results and Discussion

This section presents structural, electronic and transport properties of the cubic ($Fm\overline{3}m$) structure of GeTe alloy as well as the rhombohedral ($R\overline{3}m$) structure (at different levels of polarization).
3.1 Structural properties

In this subsection we summarize the structural properties of GeTe. This material has allotropic structures, such as R3m, P1, Cm, and Fm̅3m, where the first three structures may coexist at the room temperature, whereas Fm̅3m exists at temperatures above 680K [26]. The rhombohedral (so-called α – GeTe) structure is known to be the most stable structure in the temperature range 300-600K. This structure is considered as a distorted cubic structure (the so-called β – GeTe), see Fig.1.

Germanium telluride in rhombohedral phase is a ferroelectric material [21]. It is characterized by a polar distortion where the Ge and Te atoms are displaced from their high symmetry position of (0,0,0) and (1/2,1/2,1/2), respectively along the [111] crystallographic direction (see Fig. 1). As a result, their general position in the ferroelectric ground state can be denoted as $r_{Ge} = (0,0,0) + (\delta_{Ge}, \delta_{Ge}, \delta_{Ge})$ and $r_{Te} = (\frac{1}{2}, \frac{1}{2}, \frac{1}{2}) + (\delta_{Te}, \delta_{Te}, \delta_{Te})$, where $\delta_{Ge} = -0.0057136$ and $\delta_{Te} = 0.026713$ are the distortions in the ground state. We studied the effect of changing the polarization on the thermoelectric properties by varying the amplitude of the ferroelectric distortion. Specifically, we studied structures with the Ge and Te atoms fixed at the positions $r_{Ge} = (0,0,0) + \lambda(\delta_{Ge}, \delta_{Ge}, \delta_{Ge})$ and $r_{Te} = (\frac{1}{2}, \frac{1}{2}, \frac{1}{2}) + \lambda(\delta_{Te}, \delta_{Te}, \delta_{Te})$, where $\lambda = 1$ and $\lambda = 0$ represents the rhombohedral polar ground state and the rhombohedral non-polar state, respectively. The interaxial angle ($\alpha$) was kept the same as that of the rhombohedral polar ground state structure.

The calculated lattice parameters for the ground state rhombohedral structure of GeTe ($\lambda = 1$) are $a = 4.41 \text{ Å}$ and $\alpha = 57.28^\circ$, see Table I. From this table one can see that the calculated lattice parameter of the rhombohedral GeTe agrees with previous DFT calculations within a percentage difference of 2% [12-14]. It is also in fair agreement with the experimental findings.
using X-ray diffraction (XRD) and Raman analyses within 3-4% [26]. The calculated interaxial angle is found to differ from previous calculations by 1% and from the experimental results by 2-3% [12-14], see Table I. The lattice parameters for the cubic primitive cell of GeTe are $a = 4.25\, \text{Å}$ and $\alpha = 60^\circ$. The calculated interaxial angle is as exact as reported previous calculations, whereas the lattice parameter differs by 0.23-1% [26,27].

| System | Work | $a$ (Å) | Interaxial angle ($^\circ$) | $E_g$ (eV) |
|--------|------|--------|-----------------|-----------|
| $R3m$  | Present | 4.41   | 57.28            | 0.55      |
|        | Other   | 4.32$^a$ -4.41$^b$ | 57.7$^c$-58.08$^b$ | 0.70$^b$-0.80$^d$ |
|        | Experiment | 4.24-4.27$^d$ | 58.62-58.97$^d$ | 0.55$^e$ |
| $Fm\bar{3}m$ | Present | 4.25   | 60               | 0.35      |
|        | Other   | 4.18$^d$ -4.26$^f$ | 60$^d$          | 0.34$^d$ |

$^a$Reference [23].

$^b$Reference [28].

$^c$Reference [21].

$^d$Reference [26].

$^e$Reference [29].

$^f$Reference [27].
**3.2 The electronic structure**

This subsection presents the band structure and the density of states of rhombohedral and cubic structures of GeTe. The band gap is determined as the difference between the valence band maximum (VBM) and the conduction band minimum (CBM). Figure 2 (a) presents the band structure and the density of states of the rhombohedral structure at $\lambda=1$. This structure exhibits an indirect band gap of 0.55 eV (VBM is at the $\Sigma$ point between $P$ and $\Gamma$ and CBM is at $L$), which is thus of the same nature as the reported experimental band gap [29]. By imposing a polar distortion $\lambda = 0$ (i.e. non-polar state) the band gap is significantly reduced to 0.165 eV. Interestingly, it decreases further to 0.005 eV when $\lambda = 0.3$ (i.e. polarization approximately reduced by 70% with respect to the ground state) after which the band gap increases steadily up to 0.558 eV for $\lambda = 0.7$ (polarization reduced by 30%), see Fig. S1. However, the changes in the band gap are not significant for higher ferroelectric distortions ($\lambda \geq 0.7$). In contrast, a direct band gap of 0.35 eV is obtained for the cubic GeTe structure, see Fig. 3 (a), in agreement with previous calculations (0.34 eV) [26].
The total and projected density of states TDOS and PDOS, are presented in Fig. 2 (b) and Fig. 3 (b) for rhombohedral and cubic phases, respectively. The Te p-orbitals dominate the valence bands, while the conduction bands are dominated by Ge p-orbitals. The density of states plots of both structures have sharp peaks near the conduction band minima and valence band maxima, which is promises to lead to higher Seebeck coefficient values near the band gaps. However, the rhombohedral phase shows higher peaks in the density of states, which indicates higher Seebeck coefficient values than those of the cubic phase.

![Diagram](image-url)

**Fig.2:** (a) The electronic band structure and (b) density of states of the ground state rhombohedral GeTe.
3.3 Thermoelectric properties

The Seebeck coefficient \( (S) \) characterizes the ability to produce a voltage from the temperature gradient existing in a material. Figure 4 presents the Seebeck coefficient \( S \) as a function of the chemical potential \( \mu \) (which is plotted with respect to the Fermi energy, \( E_f \)), for the most stable structure \( (\lambda = 1) \), at different temperatures below the transition temperature. This figure shows that the Seebeck coefficient decreases as the temperature increases for chemical potentials close to the Fermi energy (approximately for \( \mu \) laying within the bandgap). This is due to concurrent excitation of intrinsic free holes and electrons across the bandgap, which contributes
oppositely to the Seebeck coefficient (the so-called bipolar effect) [30]. Therefore, the highest Seebeck coefficient values are found at low temperatures. For instance, at 300 K, maximum values of 1055 μV/K and 986 μV/K are found for p- and n-type doping, respectively. The values of the Seebeck coefficient increase rapidly near the Fermi energy, which indicates that the highest values can be obtained for low carrier concentrations of the n- and p-type doping. This behavior is related to the fact that the Seebeck coefficient is proportional to $T \frac{\partial \ln(N(E))}{\partial E}$ [31], where $N(E)$ being the electronic density of states and $T$ the temperature. The large slope of the DOS near the band edges in Fig. 2(b) is thus responsible for the large enhancement of the Seebeck coefficient for $\mu$ values close to the band edges, as well as the temperature dependency of the Seebeck coefficient.

![Fig.4: The Seebeck coefficient as a function of the chemical potential deviation from the Fermi level for the ground state rhombohedral structure ($\lambda = 1$), at 300 K, 400 K, 500 K, and 600 K.](image-url)
Fig. 5: The Seebeck coefficient as a function of the chemical potential deviation from Fermi level for the rhombohedral structure at 0.0, 0.5, 1.0, and 1.25 polarizations in addition to the cubic structure at (a) 300 K and (b) 600 K.

Calculations using various ferroelectric distortions $\lambda$ ($\lambda = 0, 0.5, 1.0, 1.25, 1.5$) at fixed cell geometry are performed to understand the effect of the electrical polarization on the thermoelectric properties. The Seebeck coefficient at different polarization levels is presented in Fig. 5 at two temperatures of 300 K and 600 K. From these figures, it appears clear that the Seebeck coefficient is greatly reduced when the polarization is reduced. For vanishing polarization ($\lambda = 0$), the extrema of the Seebeck coefficient are reduced by an order of magnitude as compared to the polar ground state ($\lambda = 1$). For 0.5 polarization the Seebeck coefficient shows a maximum at 647 $\mu$V/K for $p$-doping and 620 $\mu$V/K for $n$-doping near the Fermi level at 300 K. By increasing the polarization from 0.5 to 1.0, the maximum value of the Seebeck coefficient at 300 K increases to 1055 $\mu$V/K for $p$-type doping and 986 $\mu$V/K for $n$-type doping. Interestingly, there is a slight decrease in the Seebeck coefficient peaks for polarization levels beyond 1.0. It is obvious from Figs. 5 (a) and (b) that the Seebeck coefficient decreases when the temperature increases, as
discussed before. The peak value of $S$ at 600 K for the polarization level of 0.5 is 349 μV/K and 374 μV/K for $p$-type and $n$-type doping, respectively. Fig. 6 summarizes the effect of the polar distortion on the Seebeck coefficient (at 300 K). This figure shows a steady increase in the Seebeck coefficient until the polarization state reaches that of the ground state. Beyond that point, the Seebeck coefficient reaches a plateau.

Fig. 6: Seebeck picks as a function of polarization level in 300K.

The Seebeck coefficient is also calculated for the cubic structure without polarization, see Fig. 5. In this case, the peaks of the Seebeck coefficient are 531 μV/K and 613 μV/K for $p$-type and $n$-type doping, respectively, which are much higher than those of the non-polar ($\lambda = 0$) rhombohedral structure at 300K. However, these values remain smaller by 4% as compared to the rhombohedral polar ground state structure. By increasing the temperature of the cubic structure to 600 K, the Seebeck coefficient peak values decrease to 373 μV/K and 364 μV/K for $p$-type and $n$-type doping, respectively.

We now turn our attention to the electronic properties (namely the electrical conductivity) of GeTe. The semi-classical Boltzmann transport theory of electrical conductivity $\sigma$ depends linearly on a relaxation time $\tau$. This dependency can be expressed as:
\[ \sigma = \frac{ne^2m^*}{\tau}, \]  

(1)

where \( n \) is the free carrier concentration, \( e \) is the charge carrier, and \( m^* \) is the free carrier effective mass. Due to phonon defect and boundary scattering it is difficult to determine the relaxation time in bulk materials [32,33]. Thus, a constant relaxation time is adopted to calculate \( \sigma \). Figure 7 presents the \( \sigma/\tau \) ratio as a function of the deviation of the chemical potential (\( \mu \)) from the Fermi-level (\( E_F \)) at different temperatures (300 – 600 K), in the polar ground state structure (\( \lambda = 1 \)). From this figure, one can see that the electrical conductivity \( \sigma \) is almost independent of temperature. The figure shows that there is a positive correlation between the electrical conductivity and chemical potential since a larger chemical potential corresponds to a higher electron concentration (and smaller to higher hole concentration). By comparing Figures 4 and 7, one can see that the electrical conductivity is very small when the Seebeck coefficient reaches its peak value and vice versa. There thus exists a particular Fermi level \( \mu \) and a particular doping concentration that optimizes the power factor ZT to accommodate for those two competing effects.

**Fig.7:** The electrical conductivity as a function of deviation of the chemical potential from Fermi level in 300 K, 400 K, 500 K, and 600 K

The electrical conductivity is also studied at different levels of polarization as depicted in Fig. 8. This figure shows that the electrical conductivity decreases whenever the polarization increases. Note that
the highest electrical conductivity is achieved for the rhombohedral distortion without polarization ($\lambda = 0$); meanwhile, the non-polar cubic structure has the same order of magnitude as the polar rhombohedral ground state ($\lambda = 1$). It is even a slightly better conductor for chemical potentials near the valence band edge.

![Graph](image)

**Fig. 8:** The electrical conductivity as a function of the deviation in chemical potential from Fermi level in 0.0 polarization, 0.5 polarization, 1.0 polarization, 1.25 polarization, 1.5 polarization, and Cubic GeTe in (a) 300 K and (b) 600 K.

The electrical conductivity ($\sigma$) and electronic thermal conductivity ($\kappa_e$) are directly proportional according to Weidemann-Franz law ($\kappa_e = L\sigma T$) [34]. The electronic thermal conductivity is thus, not surprisingly, following similar trends as the electrical conductivity for different levels of polarization, see Figs. S2 and S3 in the supplementary material. The electronic thermal conductivity ($\kappa_e/\tau$) increases as the temperature increases. Consistently with the electrical conductivity data, the electronic thermal conductivity of cubic GeTe near the band gap is also higher than that of the rhombohedral structure at polarization levels of 1.0, 1.25, and 1.5 (see Fig. S1 in the supplementary material).
Although all transport properties were separately described, we are now trying to mend all the previously mentioned notions in a single descriptor, the so-called figure of merit $ZT$. However, this quantity depends on the relaxation time, which is very difficult to be calculated accurately from first-principle calculations. We thus introduce another quantity $ZT_e$, which can be understood as an electronic figure of merit that is related to $ZT$ as follows:

$$ZT = \frac{S^2 \sigma T}{\kappa_e} \frac{\kappa_e}{\kappa_e + \kappa_{latt}} = ZT_e \frac{\kappa_e}{\kappa_e + \kappa_{latt}}$$  \hspace{1cm} (2)

In addition, low polarization states ($\lambda = 0.5$ and 0), as well as the cubic structure, show some imaginary phonon frequencies (optical soft-modes characteristic of the ferroelectric instability, See Fig. S5), which prevent the proper calculation of the lattice thermal conductivity, $\kappa_{latt}$. Hence, $ZT_e$ is a more proper descriptor here for the thermoelectric properties when comparing materials with different or no polarization. Figure 9 presents the $ZT_e$ values for the rhombohedral structure with different levels of polarization in addition to the cubic structure at 300 K and 600 K. From these figures, one can see that $ZT_e$ decreases significantly as the polarization level decreases for $\lambda \leq 1$. However, the change in $ZT_e$ maxima is marginal in the case of $\lambda \geq 1$. Regarding the cubic structure, the $ZT_e$ peaks are comparable to those of the rhombohedral structure at $\lambda = 0.5$. In addition, Fig.9 shows that the $ZT_e$ values decrease by increasing the temperature. The behavior of $ZT_e$ in the rhombohedral structure at different temperatures is provided in Fig. S4.
Fig. 9: $ZT_e$ as a function of the chemical potential deviation from Fermi level in 0.0 polarization, (b) 0.5 polarization, 1.0 polarization, 1.25 polarization, 1.5 polarization and Cubic GeTe in (a, b, c) 300 K and (d, e, f) 600 K.

Fig. 10: Temperature-dependent thermoelectric properties in different levels of polarization and cubic structure: a) Seebeck coefficient b) electrical conductivity in terms of relaxation time c) electronic thermal conductivity in terms of relaxation time d) electronic thermoelectric figure of merit.

Figure 10 shows the temperature dependent thermoelectric properties in the temperature range of 50 K to 1500 K for rhombohedral GeTe with different levels of polarization as well as for
the cubic structure. Different levels of carrier concentrations were considered ranging from $1 \times 10^{20}$ to $9 \times 10^{21} \text{cm}^{-3}$. For the sake of comparison with previous theoretical and experimental results [23,35], transport properties are calculated at the carrier concentration of $7 \times 10^{20} \text{cm}^{-3}$. The calculated Seebeck coefficient at this doping level at 300 K is found to be 73 $\mu\text{V/K}$, which agrees with a previous theoretical work (68 $\mu\text{V/K}$) [22] and the reported experimental value (80 $\mu\text{V/K}$) [23,35]. Figure 10 shows that the rhombohedral polar ground state ($\lambda = 1$) has the highest Seebeck coefficient in the temperature range from 75 K up to around 250 K. It appears that increasing the polarization could increase the Seebeck coefficient at high temperatures (Fig. 10 a), provided one was able to stabilize such a phase. Indeed, the figure shows that the highest Seebeck coefficient reaches 244 $\mu\text{V/K}$ at 1500 K for the rhombohedral structure at $\lambda = 1.5$ (which would be well above the Curie temperature). The cubic structure has a smaller Seebeck coefficient values than the rhombohedral ground state at all temperatures. This behavior can be attributed to the lower band gap of the cubic structure than that of the rhombohedral ground state. Figure 10 (b) shows the electrical conductivity within the constant relaxation time approximation as a function of temperature. By increasing the polarization, the conductivity decreases. By increasing the temperature, the conductivity decreases to less than $0.5 \times 10^{20} \Omega^{-1}\text{m}^{-1}\text{s}$ for cubic and rhombohedral GeTe with polarization states $\lambda \geq 1$. However, the electrical conductivity shows a constant behavior at most temperatures only for $\lambda = 1.5$ of the rhombohedral structure. Figure 10 (c) shows a nonlinear increase in the electronic thermal conductivity $\kappa_e/\tau$ as a function of temperature for different polarization levels. Figure 10 (d) shows a subsequent increase in $ZT_e$ as the polarization level increases. The rhombohedral structure shows higher $ZT_e$ values than the cubic structure even at temperatures higher than the transition temperature. The polar structure at $\lambda = 1.5$ shows higher $ZT_e$ values than the cubic structure at
high temperatures. Therefore, it becomes clear that by stabilizing a structure with a large polarization at high temperatures would be desirable to obtain more efficient TE materials. Potential pathways towards that would be to use solid solutions with a high Curie temperature polar material or use strain engineering. In the latter case, growing epitaxial films that bi-axially compress the directions perpendicular to the polar axis may help to tune the Curie temperature of GeTe in order to achieve high TE performances.

4. Conclusion

The structural electronic, and thermoelectric properties of rhombohedral GeTe with different levels of polarization and Cubic GeTe are investigated using density functional theory combined with Boltzmann transport theory. The rhombohedral structure at $\lambda = 1$ is the ground state structure, which has an indirect band gap of 0.55 eV, while the cubic structure has a direct band gap of 0.35 eV. The rhombohedral structure shows better thermoelectric behavior in high polarization levels than the cubic phase even at temperatures above transition temperatures. This indicates that stabilizing large polarization at high temperatures in polar thermoelectric materials may help to enhance their thermoelectric properties.

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