Elastic and transport properties of topological semimetal ZrTe

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Abstract
Topological semimetals may have substantial applications in electronics, spintronics, and quantum computation. Recently, ZrTe was predicted as a new type of topological semimetal due to the coexistence of Weyl fermions and massless triply degenerate nodal points. In this work, the elastic and transport properties of ZrTe are investigated by combining the first-principles calculations and semiclassical Boltzmann transport theory. Calculated elastic constants prove the mechanical stability of ZrTe, and the bulk modulus, shear modulus, Young’s modulus, and Poisson’s ratio also are calculated. It is found that spin–orbit coupling (SOC) has slightly enhanced effects on the Seebeck coefficient, which along the $a(b)$ and $c$ directions for pristine ZrTe at $300\,\text{K}$ is $46.26\,\mu\text{VK}^{-1}$ and $80.20\,\mu\text{VK}^{-1}$, respectively. By comparing the experimental electrical conductivity of ZrTe ($300\,\text{K}$) with the calculated value, the scattering time is determined as $1.59 \times 10^{-14}\,\text{s}$. The predicted room-temperature electronic thermal conductivity along the $a(b)$ and $c$ directions is $2.37\,\text{Wm}^{-1}\text{K}^{-1}$ and $2.90\,\text{Wm}^{-1}\text{K}^{-1}$, respectively. The room-temperature lattice thermal conductivity is predicted as $17.56\,\text{Wm}^{-1}\text{K}^{-1}$ and $43.08\,\text{Wm}^{-1}\text{K}^{-1}$ along the $a(b)$ and $c$ directions, showing very strong anisotropy. Calculated results show that isotope scattering produces an observable effect on lattice thermal conductivity. To observably reduce lattice thermal conductivity by nanostructures, the characteristic length should be smaller than 70 nm, based on cumulative lattice thermal conductivity with respect to the phonon mean free path (MFP) at $300\,\text{K}$. It is noted that the average room-temperature lattice thermal conductivity of ZrTe is slightly higher than that of isostructural MoP, which is due to larger phonon lifetimes and smaller Grüneisen parameters. Finally, the total thermal conductivity as a function of temperature is predicted for pristine ZrTe. Our works provide valuable information for ZrTe-based nano-electronics devices, and motivate further experimental works to study elastic and transport properties of ZrTe.

1. Introduction

From topological insulator to semimetal, the recent discovery of new types of topological nontrivial phases has sparked intense research interest in condensed matter physics and material science [1–15]. The representative topological semimetals include Dirac semimetals, Weyl semimetals, and nodal line semimetals [3, 7, 14], such as Na$_3$Bi as a classic Dirac Semimetal [7], TaAs as a representative Weyl semimetal [8–11], and ZrSiS as a typical nodal line semimetal [13], which have been confirmed by angle-resolved photoemission spectroscopy (ARPES). In Dirac and Weyl semimetals, four-fold degenerate Dirac points and two-fold degenerate Weyl points can be observed in the momentum space [7, 8, 14, 15], while two bands cross in the form of a periodically continuous line or closed ring for node-line semimetals [3, 13].

Beyond Dirac and Weyl fermions, some new types of topological semimetals are proposed, which are identified by three--, six- or eight-fold band crossings [16]. By the crossing of a double-degeneracy band and a non-degeneracy band, the three-fold degenerate crossing points are predicted in materials with a WC-type structure, such as MoP, WC, and ZrTe [17, 18], and in InAs$_{0.5}$Sb$_{0.5}$ [19]. Then, the ARPES declares the presence of a triply degenerate point in MoP, and pairs of Weyl points coexist with the three-component fermions [2]. Experimentally, the highly metallic characteristics with remarkably low resistivity and high mobility (2 K) has
been found in MoP [20]. The recent ARPES experiments and transport measurements have also shown that WC has a nontrivial topological nature [21, 22]. The experimental results of the magnetoresistance, Hall effect, and quantum Shubnikov–de Haas oscillations on single crystals of ZrTe have been reported, indicating ZrTe with low carrier density, high carrier mobility, small cross-sectional area of the Fermi surface, and light cyclotron effective mass [23].

The electronic structures and topological properties of these exotic materials have been widely investigated, but little research about the thermal transport of these exotic materials have been found. For application in nano-devices, the thermal transport property of a material plays a key role. A high thermal conductivity is in favor of removing the accumulated heat, which can ensure the stability and extend the lifetime of the electronic device. However, a low thermal conductivity benefits thermoelectric applications. Therefore, studies of the thermal transport properties of topological semimetal ZrTe could provide important guidelines for practical applications, such as topological qubits and low-power electronics. Recently, the elastic and thermal transport properties of some representative topological semimetals have been investigated, such as TaAs and MoP [24–27]. The lattice thermal conductivity of both TaAs and MoP shows obvious anisotropy along the $a(b)$ and $c$ crystal axes [24, 25, 27]. High thermoelectric performance of TaAs has been predicted, and the maximum thermoelectric figure of merit $ZT$ is up to 0.63 (900 K) in n-type doping along the $c$ direction [25].

In this work, the elastic and transport properties of three-fold degeneracy topological semimetal ZrTe are investigated by combining the first-principles calculations and semiclassical Boltzmann transport theory. The elastic constants, bulk modulus, shear modulus, Young’s modulus, and Possion’s ratio are predicted with the generalized gradient approximation (GGA). The electronic transport coefficients are also calculated using both GGA and GGA+SOC. It is found that SOC has slight influences on electronic transport coefficients. For pristine ZrTe, the Seebeck coefficient, electrical conductivity, power factor, and electronic thermal conductivity are calculated, which can be verified by future experiments. The lattice thermal conductivity as a function of temperature is predicted within GGA, which shows a distinct anisotropic property along the $a(b)$ and $c$ crystal axes. Similar results can be found in topological semimetals TaAs and MoP [24, 25, 27]. The isotope and size effects on the lattice thermal conductivity are also studied, and phonon mode analysis is also performed to deeply understand the phonon transport of ZrTe. The total lattice thermal conductivity ($\kappa = \kappa_L + \kappa_e$) as a function of temperature is also predicted for pristine ZrTe. This work sheds light on the elastic and transport properties of ZrTe, and could offer valuable guidance for MoP-based nano-electronics devices.

The rest of the paper is organized as follows. In the next section, we give our computational details. In the third section, we present elastic and transport properties of ZrTe. Finally, we give our conclusions in the fourth section.

2. Computational detail

Within the density functional theory (DFT) [28], a full-potential linearized augmented-plane-waves method, using the GGA of Perdew, Burke, and Ernzerhof (GGA–PBE) [29], is employed to investigate electronic structures of ZrTe, as implemented in the WIEN2k code [30]. The SOC is included self-consistently [31–34], which produces observable effects on electronic transport coefficients. The convergence results are determined using 4000 k-points in the first Brillouin zone (BZ) for the self-consistent calculation, making harmonic expansion up to $F_{\text{max}} = 10$ in each of the atomic spheres, and setting $R_{\text{mt}} \times k_{\text{max}} = 8$ for the plane-wave cutoff. The self-consistent calculations are considered to be converged when the integration of the absolute charge–density difference between the input and output electron density is less than 0.0001$e$ per formula unit, where $e$ is the electron charge. Based on calculated energy band structures, transport coefficients of the electron part are calculated through solving Boltzmann transport equations within the constant scattering time approximation (CSTA), as implemented in the BoltzTrap code [35]. To obtain accurate transport coefficients, the parameter LPFAC is set as 10, and 2772 k-points is used in the irreducible BZ for the calculations of energy band structures.

For elastic properties and phonon transport, the first-principles calculations are performed within the projected augmented wave (PAW) method, and the GGA–PBE is adopted as an exchange–correlation energy functional, as implemented in the VASP code [36–38]. A plane-wave basis set is employed with a kinetic energy cutoff of 400 eV, and the electronic stopping criterion is $10^{-8}$ eV. The lattice thermal conductivity of ZrTe is performed by solving the linearized phonon Boltzmann equation with the single mode relaxation time approximation (RTA), as implemented in the Phonopy code [39]. The lattice thermal conductivity can be expressed as

$$\kappa = \frac{1}{NV_0} \sum_{\chi} \kappa_{\chi} = \frac{1}{NV_0} \sum_{\chi} \mathbf{C}_{\chi} \nu_{\chi} \otimes \nu_{\chi} \tau_{\chi},$$

(1)
where $\lambda$ is the phonon mode, $N$ is the total number of q points sampling the BZ, $V_0$ is the volume of a unit cell, and $C_{\lambda}$, $v_\lambda$, and $\tau_\lambda$ are the specific heat, phonon velocity, and phonon lifetime, respectively. The interatomic force constants (IFCs) are calculated by the finite displacement method. The second-order harmonic IFCs are calculated using a $4 \times 4 \times 4$ supercell containing 128 atoms with k-point meshes of $2 \times 2 \times 2$. Using the harmonic IFCs, phonon dispersion of ZrTe can be attained by the Phonopy package $^{[40]}$. The group velocity and specific heat can be attained from phonon dispersion, which also determines the allowed three-phonon scattering processes. The third-order anharmonic IFCs are calculated using a $3 \times 3 \times 3$ supercell containing 54 atoms with k-point meshes of $3 \times 3 \times 3$, and the total number of displacements is 508. Based on third-order anharmonic IFCs, the phonon lifetimes can be attained from the three-phonon scattering. To compute lattice thermal conductivities, the reciprocal spaces of the primitive cells are sampled using the $20 \times 20 \times 20$ meshes.

3. Main calculated results and analysis

3.1. Elastic properties

The WC-type ZrTe possesses space group $P\bar{6}m2$ (No. 187), with Zr and Te atoms occupying the 1d ($1/3, 2/3, 1/2$) and 1a (0, 0, 0) Wyckoff positions, respectively. The crystal structure and BZ of ZrTe are shown in figure 1. All the results attained in the following are from calculations with experimental lattice constants ($a = b = 3.7707$ Å, $c = 3.8606$ Å). $^{1}$ The most basic physical quantities of elastic properties are elastic constants $C_{ij}$, which can be used to construct elastic physical quantities. The elastic constants are a four-rank tensor. However, the elastic constants are reduced to five independent ones, $C_{11}$, $C_{12}$, $C_{13}$, $C_{33}$, and $C_{44}$, due to the symmetry of the hexagonal crystal, and $C_{66}$ can be obtained by $(C_{11} - C_{12})/2$. The calculated $C_{ij}$ are shown in table 1. To prove mechanical stability of ZrTe, we use the following mechanical stability criterion for the hexagonal materials $^{[41, 42]}$:

$C_{44} > 0$ (2)

$C_{11} > |C_{12}|$ (3)

$(C_{11} + 2C_{12})C_{33} > 2C_{13}^2$. (4)

By simple calculations, these criteria are satisfied for ZrTe, which means no strong tendency to become unstable with increasing pressure.

Voigt’s, Reuss’s, and Hill’s bulk moduli can be attained by the following equations:

$B_V = \frac{1}{9}(2C_{11} + C_{33} + 2C_{12} + 4C_{13})$ (5)

$B_R = (2S_{11} + S_{33} + 2S_{12} + 4S_{13})^{-1}$ (6)

$^{1}$ The experimental lattice constants are attained from the Inorganic Crystal Structure Database (ICSD).
Voigt’s, Reuss’s, and Hill’s shear moduli can be calculated by using these formulas:

\[
B_{11} = \frac{1}{2}(B_V + B_R). \tag{7}
\]

Voigt’s, Reuss’s, and Hill’s shear moduli can be calculated by using these formulas:

\[
G_V = \frac{1}{15}(2C_{11} + C_{33} - C_{12} - 2C_{13} + 6C_{44} + 3C_{66}) \tag{8}
\]

\[
G_R = \left[ \frac{1}{15}(8S_{11} + 4S_{33} - 4S_{12} - 8S_{13} + 6S_{44} + 3S_{66}) \right]^{-1} \tag{9}
\]

\[
G_{11} = \frac{1}{2}(G_V + G_R). \tag{10}
\]

The \( S_{ij} \) values can be obtained by inverting the elastic constants matrix. The calculated Voigt’s, Reuss’s, and Hill’s bulk moduli are 106.17 GPa, 98.82 GPa, and 102.50 GPa, respectively, and their shear moduli are 68.77 GPa, 53.75 GPa, and 61.26 GPa, respectively. Hill’s bulk and shear moduli are listed in Table 1. The \( B \) and \( G \) can be used to measure material behavior as ductile or brittle. If the \( B/G \) ratio value is larger than 1.75, the material behaves as ductile; otherwise, it shows a brittle character. For ZrTe, the calculated \( B/G \) ratio value with Hill’s bulk and shear modulus is 1.67, indicating that the brittle character is dominant. This is different from MoP, where the ductile character is dominant [27].

The Young’s modulus \( E_{ii} \) can be calculated by the relationship

\[
E_{ii} = 1/S_{ii}. \tag{11}
\]

The numerical calculated values are \( E_{xx} = E_{yy} = 97.83 \) GPa and \( E_{zz} = 122.07 \) GPa, respectively. The Poisson’s ratios \( \nu_{ij} \) can be calculated by

\[
\nu_{ij} = -S_{ij}/S_{ii}. \tag{12}
\]

The calculated results are \( \nu_{xy} = \nu_{yx} = 0.19, \nu_{xz} = \nu_{zx} = 0.36, \) and \( \nu_{yz} = \nu_{zy} = 0.45. \) The characteristics of chemical bonds can be reflected by the Poisson’s ratio. For covalent materials, the \( \nu \) is low with a typical value of 0.10; for ionic materials it has a high typical value of 0.25 [43]. Based on \( \nu \) values of ZrTe, ionic bonding is dominant.

### 3.2. Electronic transport

The energy band structures of ZrTe along high-symmetry paths are shown in Figure 2 using both GGA and GGA + SOC. Our calculated results agree well with previous theoretical ones [17]. It is found that the six-fold degenerated nodal point splits into the two triply degenerate nodal points (TDNPs) along the \( \Gamma \)–\( A \) direction when the SOC is included [17]. However, the six pairs of Weyl nodes appear around the K point in its first BZ [17]. Based on calculated energy band structures, the electronic transport coefficients of ZrTe can be attained using the CSTA Boltzmann theory. Although the calculated electrical conductivity depends on scattering time \( \tau \) using CSTA, the Seebeck coefficient is independent of scattering time, directly compared with experimental results. At room temperature, the Seebeck coefficient \( S \), electrical conductivity with respect to scattering time \( \sigma/\tau \), power factor with respect to scattering time \( S^2\sigma/\tau \), and electronic thermal conductivity with respect to scattering time \( \kappa_e/\tau \) along the \( a(b) \) and \( c \) directions as a function of doping level using both GGA and GGA + SOC are plotted in Figure 3. Within the framework of the rigid band approach, the n- or p-type doping can be

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**Figure 2.** The calculated energy band structures of ZrTe along high-symmetry paths with GGA (left) and GGA + SOC (right).
simulated by simply shifting the Fermi level into conduction or valence bands, which is effective at the low doping level \[44-46\].

Calculated results show that SOC has a slightly enhanced effect on n- and p-type Seebeck coefficients (absolute value) along both \(a(b)\) and \(c\) directions at the low doping level. It is found that the Seebeck coefficients are relatively strongly anisotropic along \(a(b)\) and \(c\) directions. The calculated \(S\) along \(a(b)\) and \(c\) directions for pristine ZrTe is 46.26 \(\mu\text{VK}^{-1}\) and 80.20 \(\mu\text{VK}^{-1}\), respectively, which can be further verified by the experiment.

When the Fermi level is at the Weyl nodes, the Seebeck coefficient will vanish \[47\], which has been proved in Weyl semimetal TaAs by combining the first-principles calculations and semiclassical Boltzmann transport theory \[25\]. According to figure 3, the Seebeck coefficient vanishes near the Weyl nodes and TDNPs of ZrTe. When the Seebeck coefficient (300 K) vanishes, the doping level along \(a(b)\) and \(c\) directions is about \(-0.0065\) and \(-0.0124\), respectively. It is found that n-type doping has a more excellent Seebeck coefficient than p-type doping. The band inversion around the K point results in many local extrema above the Fermi level, which can enhance the density of electronic states, giving rise to enhanced Seebeck coefficients. For \(\sigma/\tau\), the slightly reduced influence caused by SOC can be observed along both \(a(b)\) and \(c\) directions. The electronic thermal conductivity \(\kappa_e\) relates to the electrical conductivity \(\sigma\) via the Wiedemann–Franz law:

\[
\kappa_e = \frac{L}{\tau}\sigma T
\]  

where \(L\) is the Lorenz number. Thus, there are similar dependencies of doping level and SOC between \(\kappa_e/\tau\) and \(\sigma/\tau\). The \(\tau\) is attained by comparing the experimental electrical conductivity \[23\] of ZrTe with the calculated value of \(\sigma/\tau\) at room temperature, and the \(\tau\) is found to be \(1.59 \times 10^{-14}\) s. For pristine ZrTe, the electronic thermal conductivity along the \(a(b)\) and \(c\) directions is 2.37 Wm\(^{-1}\)K\(^{-1}\) and 2.90 Wm\(^{-1}\)K\(^{-1}\), respectively. Using the calculated \(\tau\), the electrical resistivity of pristine ZrTe along the \(a(b)\) and \(c\) directions is \(5.26 \times 10^{-6}\) \(\Omega\)m and \(3.66 \times 10^{-6}\) \(\Omega\)m, respectively. An enhanced SOC effect on the power factor can be observed along both \(a(b)\) and \(c\) directions, which is due to improved \(S\) caused by SOC. For pristine ZrTe, the power factor along the \(a(b)\) and \(c\) directions is 3.82 \(\mu\text{Wcm}^{-1}\text{K}^{-2}\) and 17.33 \(\mu\text{Wcm}^{-1}\text{K}^{-2}\), respectively, showing obvious anisotropy.

Next, we obtain the scattering time \(\tau\) at different temperatures by \(\tau \propto T^{-1}\) \[48\]. For pristine ZrTe, the Seebeck coefficient \(S\), electrical resistivity \(\rho\), and electronic thermal conductivity \(\kappa_e\) as a function of temperature with GGA+SOC are plotted as in figure 4. It is found that the Seebeck coefficient and electrical resistivity along both \(a(b)\) and \(c\) directions firstly increase with increasing temperature, and then decrease. It is noted that the
Seebeck coefficient along the c direction changes from positive values to negative ones when the temperature is larger than 870 K. At high temperature, the electrical resistivity along both a(b) and c directions almost coincides. With increasing temperature, the electronic thermal conductivity increases along both a(b) and c directions, showing weak anisotropy.

### 3.3. Phonon transport

Based on the harmonic IFCs, the phonon dispersion of ZrTe can be attained along high-symmetry paths, which along with atom partial density of states (DOS) are shown in figure 5. Due to each primitive cell containing two atoms, there are six vibrational branches consisting of three acoustic and optical ones, respectively. No imaginary frequencies in the phonon dispersion indicate the thermodynamic stability of ZrTe. The ZrTe belongs to the P6/m2¯ space group whose point group is D3h. Then, the BZ-center optical phonon modes of this crystal can be decomposed as

$$\Gamma = A_2 + 2E.$$ (14)

The $A_2$ and $E$ modes are infrared-active, and the $E$ mode is also Raman-active. The phonon frequencies of $A_2$ and $E$ are shown in table 2. It can be clearly seen that there is a well-separated acoustic-optical gap of 0.15 THz at the A point (0, 0, π/2) on the boundary of the BZ. The top phonon band of the gap at the A point is doubly degenerate, while the bottom phonon band is a singlet state. A similar phonon gap can also be found in MoP [27], which is larger than the one of ZrTe. However, the isoelectronic ZrSe shows no acoustic-optical gap, and

![Table 2](image-url)

Table 2. Theoretical optical phonon frequencies (THz) at the Γ point; acoustic-optical gap (THz); lattice thermal conductance (WmK⁻¹).

| Mode | Frequency (THz) | Gap (THz) | $\kappa_a$ (WmK⁻¹) | $\kappa_c$ (WmK⁻¹) |
|------|----------------|-----------|---------------------|---------------------|
| $A_2$ | 6.21           | 6.07      | 6.07                | 0.15                |
| $E_1$ | 6.07           |           | 17.56               | 43.08               |

Seebeck coefficient along the c direction changes from positive values to negative ones when the temperature is larger than 870 K. At high temperature, the electrical resistivity along both a(b) and c directions almost coincides. With increasing temperature, the electronic thermal conductivity increases along both a(b) and c directions, showing weak anisotropy.
the presence of the TDNPs of phonon has been predicted [49]. From atom partial DOS, contribution to the acoustic (optical) phonon branches mainly comes from Te (Zr) atoms.

The intrinsic lattice thermal conductivity of ZrTe can be attained from harmonic and anharmonic IFCs by solving the linearized phonon Boltzmann equation within the single mode RTA method. The phonon–isotope scattering is also considered, according to the formula proposed by Shin-ichiro Tamura [51]. The lattice thermal conductivities of pure and isotopic ZrTe along the $a(b)$ and $c$ directions as a function of temperature are shown in figure 6. In the considered temperature region, the intrinsic enhancement of phonon–phonon scattering with increasing temperature leads to the decreased lattice thermal conductivity of ZrTe, which typically results as $1/T$. From figure 6, it is clearly seen that the lattice thermal conductivity of ZrTe shows obvious anisotropy, where the lattice thermal conductivity along the $c$ direction is much higher than that along the $a(b)$ direction. A similar result can be found in MoP [27], but is different from that in TaAs [24]. At room temperature, the lattice thermal conductivities of pure (isotopic) ZrTe along the $a(b)$ and $c$ directions are 17.56 (16.13) $\text{Wm}^{-1}\text{K}^{-1}$ and 43.08 (37.82) $\text{Wm}^{-1}\text{K}^{-1}$, respectively, which of pure ZrTe are shown in table 2. To measure the anisotropic strength, an anisotropy factor [24] is defined as $\eta = (\kappa_{1}(cc) - \kappa_{1}(aa))/\kappa_{1}(aa)$, and the calculated value is 145.3%, which is larger than that of MoP, implying stronger anisotropy. The lattice thermal conductivity is connected to Young’s modulus by the simple relation $\kappa_{1} \sim \sqrt{E}$ [50]. Calculated results show that the orders of Young’s modulus and lattice thermal conductivity along the $a(b)$ and $c$ directions are identical. It is found that phonon–isotope scattering along the $c$ direction produces larger effects on lattice thermal conductivity than those along the $a(b)$ direction. With increasing temperature, the isotropic effect on lattice thermal conductivity gradually decreases, which is due to improvement of phonon–phonon scattering.

At room temperature, the cumulative lattice thermal conductivities with respect to frequency along with the derivatives along $a(b)$ and $c$ directions are plotted in figure 7. The cumulative thermal conductivity is defined by

$$\kappa(\omega) = \int_{0}^{\omega} \sum_{\mathbf{k}\mathbf{\delta}} \delta(\omega_{\mathbf{k}} - \omega') d\omega'.$$

It is clearly seen that the acoustic phonon branches dominate lattice thermal conductivity, up to 96.49% along the $a(b)$ direction and 91.12% along the $c$ direction. It is found that the optical contribution along the $c$ direction is larger than that along the $a(b)$ direction. Furthermore, the relative contributions of six phonon branches to the total lattice thermal conductivity along the $a(b)$ and $c$ directions at 300 K are plotted in figure 7. Along both $a(b)$ and $c$ directions, the longitudinal acoustic (LA) phonon mode has a larger contribution than any of the two transverse acoustic (TA1 or TA2) phonon modes. It is evident that optical branches along the $c$ direction have obvious contribution.

The phonon transport of ZrTe can be further understood with the help of the mode-level phonon group velocities and lifetimes, which are plotted in figure 8. The largest phonon group velocity of TA1, TA2, and LA branches in the long-wavelength limit is 2.23 kms$^{-1}$, 3.86 kms$^{-1}$, and 4.40 kms$^{-1}$, respectively. In the low-frequency region, most group velocities of TA2 and TA1 branches are lower than those of the LA branch, which leads to the main contribution to lattice thermal conductivity being from the LA branch. It is found that most group velocities and phonon lifetimes of both groups of acoustic branches are larger than those of optical branches, which leads to the dominant contribution from acoustic branches to the total lattice thermal conductivity. The Grüneisen parameters ($\gamma$) can reflect the strength of anharmonic interactions, determining the intrinsic phonon–phonon scattering. Here, the Grüneisen parameters are directly calculated by third-order anharmonic IFCs. The mode-level Grüneisen parameters of pure ZrTe are shown in figure 8. The larger $\gamma$ leads to lower phonon lifetimes due to stronger anharmonicity, giving rise to lower lattice thermal conductivity. It is clearly seen that mode-level phonon lifetimes and Grüneisen parameters show the opposite trend. For all
branches, the $\gamma$ is fully positive. The average Grüneisen parameter is 1.52, indicating relatively strong anharmonic phonon scattering.

To further understand the size dependence of lattice thermal conductivity of ZrTe, the cumulative lattice thermal conductivity divided by the total lattice thermal conductivity with respect to MFP ($300 \text{ K}$) along the $a(b)$ and $c$ directions is plotted in figure 9. The MFP cumulative lattice thermal conductivity is given by the following:

$$\kappa^c(l) = \sum_{\lambda} \kappa_{\lambda} \delta(l - l') dl'$$

(16)

$$l_{\lambda} = |l_{\lambda}| = |\nu_{\lambda} \otimes \tau_{\lambda}|.$$  

(17)

This can reflect the contribution to total lattice thermal conductivity from individual phonon modes with different MFPs, namely, it shows how phonons with different MFPs make contributions to the thermal conductivity. It is clearly seen that the total lattice thermal conductivity along both $a(b)$ and $c$ directions approaches one with increasing MFP. The contribution from phonons with an MFP larger than 0.60 $\mu$m is very little. Phonons with an MFP smaller than 0.13 (0.07) $\mu$m along the $a(b)$ direction and 0.07 (0.05) $\mu$m along the $c$ direction contribute around 80% (60%) to the lattice thermal conductivity. It is found that phonons dominating the lattice thermal conductivity along the $a(b)$ direction have longer MFPs than those along the $c$ direction.
Based on the calculated electronic and lattice thermal conductivity, the total thermal conductivity can be attained, which is plotted in figure 10. It is clearly seen that $\kappa$ firstly decreases with increasing temperature, and then increases. This is because the lattice part dominates thermal conductivity at low temperature, while the electronic part is predominant at high temperature. The minimum $\kappa$ along the $a(b)$ and $c$ directions is 13.98 W m$^{-1}$K$^{-1}$ and 23.15 W m$^{-1}$K$^{-1}$, respectively, and the corresponding temperatures are 650 K and 1000 K, respectively. The room-temperature $\kappa$ is 19.94 W m$^{-1}$K$^{-1}$ and 45.98 W m$^{-1}$K$^{-1}$, respectively. These results are useful for the thermal management of ZrTe-based electronics devices.

4. Conclusion

The elastic properties and phonon transport of the isostructural topological semimetal MoP has been investigated by the same method as in [27]. It is found that the bulk modulus, shear modulus, and Young’s modulus of ZrTe are smaller than those of MoP, which means that ZrTe deforms easily with applied external force. The lattice thermal conductivity of ZrTe (17.56 W m$^{-1}$K$^{-1}$) along the $a(b)$ direction is very close to that of MoP (18.41 W m$^{-1}$K$^{-1}$), while the lattice thermal conductivity of ZrTe (43.08 W m$^{-1}$K$^{-1}$) along the $c$ direction is larger than that of MoP (34.71 W m$^{-1}$K$^{-1}$). It is noted that the average lattice thermal conductivity

$$\kappa_{\text{av}}(a b) = \frac{\kappa_{\text{av}}(a a) + \kappa_{\text{av}}(b b) + \kappa_{\text{av}}(c c)}{3}$$

of ZrTe is slightly higher than that of MoP. This is because ZrTe has larger phonon lifetimes and smaller Grüneisen parameters than MoP, which gives rise to a higher lattice thermal conductivity for ZrTe than MoP. Phonon transport of another classic topological semimetal, TaAs, has been investigated [24]. ZrTe, MoP, and TaAs all show obvious anisotropic lattice thermal conductivity along the $a(b)$ and $c$ directions. However, for TaAs, the lattice thermal conductivity along the $a(b)$ direction is larger than one along the $c$ direction, while the lattice thermal conductivity of ZrTe or MoP along the $a(b)$ direction is smaller than that along the $c$ direction.

In summary, the elastic and transport properties of ZrTe are shown by the first-principles calculations and semiclassical Boltzmann transport theory. The elastic tensor components $C_{ij}$ for ZrTe are presented, which confirm the mechanical stability of the structure. The bulk modulus, shear modulus, Young’s modulus, and...
Poisson’s ratio are also attained by calculating $C_{ij}$. The electronic transport coefficients are also calculated within the CSTA Boltzmann theory. For pristine ZrTe, the Seebeck coefficient, electrical resistivity, and electronic thermal conductivity will be of use for comparison with future experimental measurements. The lattice thermal conductivity of ZrTe shows an obvious anisotropy along the $a(b)$ and c crystal axis. It is found that isotope scattering has an observable effect on the lattice thermal conductivity, and phonons with an MFP larger than 0.60 $\mu$m have little contribution to the total lattice thermal conductivity. The higher lattice thermal conductivity of ZrTe than MoP can be explained by larger phonon lifetimes and smaller Grüneisen parameters. The total thermal conductivity is also attained for pristine ZrTe. Our works shed light on the elastic and transport properties of ZrTe, and will motivate further experimental studies of these properties in topological semimetal ZrTe.

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