Ultrahigh lattice thermal conductivity in topological semimetal TaN caused by a large acoustic-optical gap

San-Dong Guo¹ and Bang-Gui Liu²,³

¹ School of Electronic Engineering, Xi’an University of Posts and Telecommunications, Xi’an 710121, People’s Republic of China
² Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, Chinese Academy of Sciences, Beijing 100190, People’s Republic of China
³ School of Physical Sciences, University of Chinese Academy of Sciences, Beijing 100190, People’s Republic of China

E-mail: sandongyuwang@163.com

Received 2 December 2017, revised 17 January 2018
Accepted for publication 29 January 2018
Published 15 February 2018

Abstract
Topological semimetals may have potential applications such as in topological qubits, spintronics and quantum computations. Efficient heat dissipation is a key factor for the reliability and stability of topological semimetal-based nano-electronics devices, which is closely related to high thermal conductivity. In this work, the elastic properties and lattice thermal conductivity of TaN are investigated using first-principles calculations and the linearized phonon Boltzmann equation within the single-mode relaxation time approximation. According to the calculated bulk modulus, shear modulus and $C_{44}$, TaN can be regarded as a potential incompressible and hard material. The room-temperature lattice thermal conductivity is predicted to be 838.62 W m$^{-1}$ K$^{-1}$ along the $a$ axis and 1080.40 W m$^{-1}$ K$^{-1}$ along the $c$ axis, showing very strong anisotropy. It is found that the lattice thermal conductivity of TaN is several tens of times higher than other topological semimetals, such as TaAs, MoP and ZrTe, which is due to the very longer phonon lifetimes for TaN than other topological semimetals. The very different atomic masses of Ta and N atoms lead to a very large acoustic-optical band gap, and then prohibit the scattering between acoustic and optical phonon modes, which gives rise to very long phonon lifetimes. Calculated results show that isotope scattering has little effect on lattice thermal conductivity, and that phonons with mean free paths larger than 20 (80) µm along the $c$ direction at 300 K have little contribution to the total lattice thermal conductivity. This work implies that TaN-based nano-electronics devices may be more stable and reliable due to efficient heat dissipation, and motivates further experimental works to study lattice thermal conductivity of TaN.

Keywords: lattice thermal conductivity, group velocities, phonon lifetimes

(Some figures may appear in colour only in the online journal)
type of topological semimetal [16]. A band crossing between a doubly degenerate band and a nondegenerate band, namely three-fold degenerate crossing points, has been predicted in TaN, MoP and ZrTe with WC-type structure [17–19], and InAs$_0.5$Sb$_{0.5}$ [20]. Experimentally, MoP has been confirmed to be a topological semimetal with triply degenerate nodal points (TDNPs), coexisting with the pairs of Weyl points [2].

These topological semimetals may have substantial applications in electronics, spintronics and quantum computation [21]. Efficient heat dissipation is a key factor for the reliable performance and stable function of electronic devices based on these topological semimetals, especially for the high-power situations [22]. High lattice thermal conductivity is in favor of high-performance thermal management [23]. The lattice thermal conductivities in TaAs, MoP and ZrTe have been calculated from a first principles calculation, showing obvious anisotropy along the $a$ and $c$ crystal axes [24–27]. However, their lattice thermal conductivities are relatively low, about 17–44 W m$^{-1}$ K$^{-1}$ at 300 K, which is against efficient heat dissipation. Therefore, searching for topological semimetal with high lattice thermal conductivity is very necessary and interesting. Recently, the TaN is proposed as a topological

---

**Figure 1.** (a) The crystal structure of TaN in one unit cell; (b) the Brillouin zone with high-symmetry points.

**Figure 2.** The calculated energy band structures of TaN along high-symmetry paths using GGA + SOC, with thicker bands projected onto N (left) and Ta (right) atoms.

| Name  | $C_{11}$  | $C_{12}$  | $C_{13}$ | $C_{33}$ | $C_{44}$ | $C_{66}$ | $B$   | $G$   | $E_{xx}$ | $E_{zz}$ |
|-------|-----------|-----------|----------|----------|----------|----------|-------|-------|----------|----------|
| TaN   | 566.40    | 128.23    | 62.41    | 706.39   | 215.02   | 219.09   | 260.26| 233.16| 534.04   | 695.17   |
| MoP   | 359.00    | 153.73    | 160.14   | 515.15   | 169.22   | 102.64   | 239.10| 134.96| 274.28   | 415.11   |
| ZrTe  | 140.82    | 58.78     | 88.81    | 201.11   | 110.36   | 41.02    | 102.50| 61.26 | 97.83    | 122.07   |

**Table 1.** The elastic constants $C_{ij}$, bulk ($B$), shear ($G$) and Young’s ($E_{xx}$ and $E_{zz}$) moduli (in GPa) of TaN, MoP and ZrTe.
Figure 3. Phonon dispersion curve of TaN, along with the atom partial density of states (PDOS).

Figure 4. Top: the lattice thermal conductivities of infinite (pure and isotope) TaN, ZrTe and MoP as a function of temperature, including the $a$ and $c$ directions. Bottom: the cumulative lattice thermal conductivity (200, 300 and 400 K) of infinite (pure) TaN divided by total lattice thermal conductivity with respect to phonon frequency, along $a$ and $c$ directions.

Figure 5. The mode level phonon group velocities and phonon lifetimes (300 K) of infinite (pure) TaN in the first BZ.
semimetal with TDNPs using first-principles calculation and symmetry analysis [17]. The TDNPs of TaN is protected by crystalline symmetries. Various topological phases can be achieved by breaking the crystalline symmetry.

In this work, the elastic properties of topological semimetal TaN are studied from first-principles calculations, and the phonon transport properties are performed by solving the phonon Boltzmann transport equation. The calculated bulk modulus, shear modulus and $C_{44}$ suggest that TaN is a potential low compressible and hard material. The calculated lattice thermal conductivity is much higher than those of TaAs, MoP and ZrTe [24–27], and the room-temperature lattice thermal conductivity is predicted to be 838.62 (1080.40) $\text{W m}^{-1} \text{K}^{-1}$ along the $a$ ($c$) axis. This can be attributed to the large acoustic-optical frequency gap due to the large mass difference of Ta and N, producing inefficient scattering among acoustic and optical phonon modes. The mass difference factor suggests that WC and WN are potential topological materials with ultrahigh lattice thermal conductivities.

The rest of the paper is organized as follows. In section 2, we shall give our computational details about phonon transport. In section 3, we shall present elastic and phonon transport properties of TaN. Finally, we shall give our discussion and conclusions in section 4.

2. Computational detail

First-principles calculations are carried out within the projected augmented wave method, as implemented in the VASP code [28–30]. The generalized gradient approximation of the Perdew–Burke–Ernzerhof [31] is adopted for the exchange-correlation functional with the plane-wave-cut-off energy of 500 eV. The 2s and 2p electrons of N, and 6s and 5d electrons of Ta are treated as valance ones. The energy convergences are less than $10^{-8}$ eV. The lattice thermal conductivity of TaN is calculated by solving the linearized phonon Boltzmann equation with the single mode relaxation time approximation (RTA), as implemented in the Phonopy code [32]. The lattice thermal conductivity can be expressed as

$$\kappa = \frac{1}{N V_0} \sum_\lambda \kappa_\lambda = \frac{1}{N V_0} \sum_\lambda \sum_\nu \nu_\lambda \tau_\lambda$$

where $\lambda$ is the phonon mode, $N$ is the total number of q-points sampling the Brillouin zone (BZ), $V_0$ is the volume of a unit cell, and $C_\lambda$, $\nu_\lambda$ and $\tau_\lambda$ are the specific heat, phonon velocity and phonon lifetime. The phonon lifetime $\tau_\lambda$ can be attained by the phonon linewidth $2\Gamma_\lambda(\omega_\lambda)$ of the phonon mode $\lambda$:

$$\tau_\lambda = \frac{1}{2\Gamma_\lambda(\omega_\lambda)}.$$  

$\Gamma_\lambda(\omega)$ takes the form analogous to the Fermi golden rule:

$$\Gamma_\lambda(\omega) = \frac{18\pi}{\hbar^2} \sum_{\lambda'\lambda''} |\Phi_{-\lambda\lambda'\lambda''}|^2 \left[ (f'_\lambda + f''_{\lambda'}) [\delta(\omega - \omega'_\lambda - \omega''_{\lambda'} - \omega''_{\lambda''}) - \delta(\omega - \omega'_\lambda + \omega''_{\lambda'})] \right].$$

in which $f_\lambda$ is the phonon equilibrium occupancy and $\Phi_{-\lambda\lambda'\lambda''}$ is the strength of the interaction between the three phonons $\lambda$, $\lambda'$, and $\lambda''$ involved in the scattering.

The second- and third-order interatomic force constants (IFCs) are calculated by the supercell approach with finite atomic displacement of 0.03 Å. For second-order harmonic IFCs, a $4 \times 4 \times 4$ supercell containing 128 atoms is used with k-point meshes of $2 \times 2 \times 2$. For second-order harmonic IFCs, a $3 \times 3 \times 3$ supercell containing 54 atoms is used with k-point meshes of $3 \times 3 \times 3$. Based on cubic and second-order anharmonic IFCs, the three-phonon scattering rate can be attained and, further, the phonon lifetimes can be calculated. 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

TaN shows WC-type crystal structure with space group $P6m2$ (no. 187), and the crystal structure is shown in figure 1, along with the first BZ. MoP and ZrTe have the same crystal structure as TaN. Ta and N atoms occupy the 1d $(1/3, 2/3, 1/2)$ and $1a$ $(0, 0, 0)$ Wyckoff positions, respectively. Experimentally, it can be synthesized at high pressure within a proper high temperature range. The experimental lattice constants ($a = b = 2.9333$ Å, $c = 2.8844$ Å) [34] are used to investigate the elastic properties and lattice thermal conductivity of TaN. Firstly, the energy band structures of TaN with thicker bands projected onto N and Ta atoms are plotted in figure 1. It can be seen that there are two TDNPs along the $\Gamma$–A direction with Ta-d character. Our calculated energy band structures agree well with a previous report [17]. For MoP and ZrTe, there are Weyl nodes besides TDNPs in the first BZ [2, 18].

Figure 6. At 200, 300 and 400 K, the cumulative lattice thermal conductivity divided by total lattice thermal conductivity with respect to the phonon mean free path (MFP) along the $a$ and $c$ directions.
Based on the experimental crystal structure, the elastic constants $C_{ij}$ of the TaN are calculated, which are listed in Table 1, along with ones of MoP and ZrTe. The elastic constants satisfy the following mechanical stability criteria [35, 36]

\[ C_{44} > 0 \]  
\[ C_{11} > \lvert C_{12} \rvert \]

(4)

\[ (C_{11} + 2C_{12})C_{33} > 2C_{11}^2. \]

(5)

This indicates that the system of TaN is mechanically stable. Based on calculated elastic constants, the bulk, shear and Young’s modulus can be obtained by Voigt–Reuss–Hill approximations. The Voigt–Reuss–Hill bulk modulus can be calculated by the following equations:

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

(7)

\[ B_R = (2S_{11} + S_{33} + 2S_{12} + 4S_{13})^{-1} \]

(8)

\[ B_H = \frac{1}{2} (B_V + B_R). \]

(9)

The Voigt–Reuss–Hill shear modulus can be attained by using these formulas:

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

(10)

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

(11)

\[ G_H = \frac{1}{2} (G_V + G_R). \]

(12)

The Young’s modulus $E_{ii}$ can be computed by the relationship:

\[ E_{ii} = \frac{1}{S_{ii}}. \]

(13)

The $S_{ij}$ are the elastic compliance constants. The related data are tabulated in Table 1, together with ones of MoP and ZrTe. The $B/G$ can be used to measure material behavior as ductile ($B/G > 1.75$) or brittle ($B/G < 1.75$). For TaN, the calculated $B/G$ ratio value is 1.12, indicating that the brittle character is dominant. The bulk modulus or shear modulus can measure the hardness of materials [37]. The materials with higher bulk or shear modulus may be harder materials. The magnitude of the shear modulus $C_{44}$ may be a better hardness predictor for transition-metal carbonitrides [38, 39]. Based on these criteria, TaN may be an incompressible and hard material. Experimental studies on structural and mechanical properties of TaN are strongly recommended.

![Figure 7. The mode level phonon Grüneisen parameters ($\gamma$) of TaN in the first BZ.](image-url)

Based on the harmonic IFC matrix, the phonon dispersion and atom partial density of states (DOS) of TaN are plotted in Figure 3. No imaginary frequencies are observed in the phonon dispersion of TaN, indicating the thermodynamic stability of TaN. Two atoms per unit cell lead to three acoustic and three optical phonon branches. In contrast to MoP and ZrTe, a significant difference is observed. It is clearly seen that there is a phonon band gap of 6.05 THz at the A point (0, 0, π/2) between acoustic and optical branches, which is much larger than those of MoP (0.68 THz) and ZrTe (0.15 THz) [24, 25]. The large phonon band gap is due to very different atomic masses of Ta and N atoms [40, 41]. A mass difference factor, defined as $\delta = (M_{\text{max}} - M_{\text{min}})/M_{\text{min}}$, is used to measure the different strength, and the corresponding values are 11.92 for TaN, 2.10 for MoP and 0.40 for ZrTe. According to the atom partial DOS (PDOS), the vibrations of Ta (N) atoms almost completely dominate acoustic (optical) branches. These are familiar from the diatomic linear chain model, where acoustic (optical) branches are mainly contributed by the vibrations of the larger (smaller) mass.

From harmonic and anharmonic IFCs, the intrinsic lattice thermal conductivity of TaN can be calculated by solving the linearized phonon Boltzmann equation within the single-mode RTA method. Based on the formula proposed by Tamura [42], the phonon–isotope scattering can be included. Along the $a$ and $c$ directions, the lattice thermal conductivities of pure and isotopic TaN as a function of temperature are shown in Figure 4, together with ones of ZrTe and MoP for comparison. Similar to ZrTe and MoP, the lattice thermal conductivity of TaN shows obvious anisotropy. It is clearly seen that the $c$-axis lattice thermal conductivity is higher than the $a$-axis one. The room-temperature lattice thermal conductivity of...
pure (isotopic) TaN along the $a$ and $c$ axis is 838.62 (814.96) W m$^{-1}$ K$^{-1}$ and 1080.40 (1044.06) W m$^{-1}$ K$^{-1}$, respectively. The room temperature ‘isotope effect’ is given by $P = (\kappa_{\text{pure}}/\kappa_{\text{iso}} - 1)$, which is 2.90% along the $a$ axis, and 3.48% along the $c$ axis. These values mean that phonon–isotope scattering has little effect on lattice thermal conductivity. Due to the enhancement of phonon–phonon scattering, the isotopic effect on lattice thermal conductivity gradually becomes weak with increasing temperature. An anisotropy factor \[ \eta = (\kappa_{cc} - \kappa_{aa})/\kappa_{aa} \] [26], defined as \[ A = C_{44}/C_{66} \] [43]. The calculated $A$ for TaN (0.98) is much closer to 1 than those of MoP (1.65) and ZrTe (2.69). It is noted that the lattice thermal conductivity of TaN along the $a$ (or $c$) direction is around 45 (31) times higher than that of MoP, and about 48 (25) times higher than one of ZrTe. The relation between lattice thermal conductivity and Young’s modulus is $\kappa_L \sim \sqrt{E}$ [44]. It is found that the order of lattice thermal conductivity along the $a$ and $c$ directions is consistent with that of Young’s modulus. At 200, 300 and 400 K, the cumulative lattice thermal conductivities divided by total lattice thermal conductivity with respect to frequency along the $a$ and $c$ directions are shown in figure 4. The cumulative thermal conductivity is defined by:

$$\kappa^c(\omega) = \int_{0}^{\omega} \sum_{\lambda} \kappa_{\lambda} \delta(\omega_{\lambda} - \omega') d\omega'.$$

(14)

It is clearly seen that the lattice thermal conductivity is mainly made up of the acoustic phonon branches for the three considered temperatures. It is noted that the cumulative lattice thermal conductivities divided by total lattice thermal conductivity with respect to frequency has weak temperature dependence. The slope along the $a$ direction is larger than that along the $c$ direction, which means that low frequency phonons have a larger contribution to the total lattice thermal conductivity for the $a$ direction than for the $c$ direction.

To gain more insight into the high lattice thermal conductivity of TaN, we show the mode level phonon group velocities and lifetimes in figure 5. In the long-wavelength limit, the largest phonon group velocity of TA1, TA2 and LA branches is 3.91 km s$^{-1}$, 4.12 km s$^{-1}$ and 6.89 km s$^{-1}$, respectively. These are larger than those of ZrTe [25], but smaller than those of MoP [24]. It is clearly seen that most of the group velocities of acoustic branches are higher than those of optical branches. It is found that most of phonon lifetimes of TaN are much longer than those of MoP and ZrTe [24, 25], which leads to much higher lattice thermal conductivity for TaN than for MoP or ZrTe. Unexpectedly, the phonon lifetimes near 6 or 17 THz become very large. This can be understood by very large frequency gap between the acoustic and optical phonon branches. The frequency gap (6.05 THz) is close to the range of acoustic phonons (8.64 THz). While heat is transmitted primarily by the acoustic branches, the optical branches provide important scattering channels for the acoustic modes, particularly through acoustic $+$ acoustic $\rightarrow$ optical scattering. Because of the requirement on energy conservation for phonon–phonon scattering, the annihilation process of two acoustic phonon modes into one optical one becomes ineffective (such an annihilation process is not totally prohibited) caused by large acoustic-optical gap. As a result, a weak phonon–phonon scattering rate is produced, and then results in long phonon lifetimes, giving rise to a much high lattice thermal conductivity. The very high thermal conductivity is
found in BAs [40] and AlSb [45], which is also due to a large frequency gap.

The size dependence of the lattice thermal conductivity of TaN can be reflected by the cumulative lattice thermal conductivity with respect to the mean free path (MFP), which shows how phonons with different MFPs contribute to the thermal conductivity. The MFP cumulative lattice thermal conductivity is defined as:

\[ \kappa^c(l) = \int_0^l \sum_\lambda \kappa_\lambda \delta(l_\lambda - l') dl' \]  
\[ l_\lambda = |l_\lambda| = |v_\lambda \otimes \tau_\lambda| \]  

At 200, 300 and 400 K, the cumulative lattice thermal conductivity divided by the total lattice thermal conductivity with respect to the MFP along the a and c directions is shown in figure 6. It is clearly seen that the cumulative lattice thermal conductivity of TaN along both the a and c axes approaches saturation value with the MFP increasing. With the increasing temperature, the critical MFP gradually decreases. At 300K, phonons with MFPs larger than 20 (84) μm along the a (c) direction have little contribution to the total lattice thermal conductivity. At room temperature, phonons with MFPs smaller than 1 (2) μm along the a (c) direction contribute around half to the total lattice thermal conductivity. These results mean that the lattice thermal conductivity along the c direction is tuned more easily than that along the a direction.

4. Discussions and conclusion

MoP, ZrTe and TaN have the same crystal structure, and their lattice thermal conductivities show obvious anisotropy along the a and c directions, where the lattice thermal conductivity along the c direction is larger than that along the a direction. However, a much higher lattice thermal conductivity of TaN is observed than those of MoP and ZrTe. Traditionally, a low Debye temperature \( T_D \) indicates low lattice thermal conductivity. All phonon modes are excited with the temperature above \( T_D \), which can give rise to strong three-phonon scattering, and then suppress lattice thermal conductivity. When the temperature is below \( T_D \), some phonon modes begin to be frozen out [46]. The Debye temperature can be obtained from the average sound velocity using the following equation [47]:

\[ T_D = \left( \frac{3N}{4\pi V_0} \right)^{1/3} \frac{hV_L}{k_B} \]  

where \( N \) denotes the number of atoms in the primitive unit cell, \( V_0 \) denotes the unit cell volume, and \( h \) and \( k_B \) denote the Planck and Boltzmann constants. The average sound speed \( v_\lambda \) can be calculated from the longitudinal and transversal sound velocities, \( v_L \) and \( v_T \):

\[ v_\lambda = \left[ \frac{1}{3} \left( \frac{1}{v_L^2} + \frac{2}{v_T^2} \right) \right]^{-1/3} \]  

The longitudinal and transversal sound velocities, \( v_L \) and \( v_T \), are related to the bulk, shear modulus and the density of the material, \( B, G \) and \( \rho \)

\[ v_L = \sqrt{(B + 4G/3)/\rho} \]  
\[ v_T = \sqrt{G/\rho} \]  

The longitudinal, transversal and average sound speeds, and the Debye temperatures of TaN, MoP and ZrTe are listed in table 2. Assumed from Debye temperature, the lattice thermal conductivity of TaN should be lower than that of MoP, and should be slightly higher than that of ZrTe. In contrast to this straightforward prediction, the calculated lattice thermal conductivity of TaN is dozens of times higher than those of MoP or ZrTe. Based on the formula proposed by Slack [48], four factors, including the average atomic mass, interatomic bonding, crystal structure and anharmonicity, determine the lattice thermal conductivity. A high Debye temperature can be produced by low average atomic mass and strong interatomic bonding, leading to a high thermal conductivity. Mode Grüneisen parameters \( \gamma \) can measure the strength of anharmonic interactions, determining the intrinsic phonon–phonon scattering. The larger \( \gamma \) gives rise to stronger anharmonic phonon scattering, leading to lower lattice thermal conductivity. The mode level Grüneisen parameters of TaN are plotted in figure 7. The average Grüneisen parameter is 1.60, which is close to 1.57 of MoP [24] and 1.52 of ZrTe [25]. Therefore, other factors should be found to explain the very high lattice thermal conductivity in TaN. Although TaN, MoP and ZrTe have similar outlines of phonon dispersion (see figure 8) a significant difference is found. A very large frequency gap (6.05 THz) between the optical and acoustic phonon branches in TaN is observed, while the gap is only 0.68 THz for MoP and 0.15 THz for ZrTe. The large thermal conductivity of TaN is due to the large acoustic-optical frequency gap caused by the large mass difference of Ta and N, which can lead to inefficient scattering among acoustic and optical phonon modes. The frequency gap between the acoustic and optical phonons, the a-axis and c-axis and the average lattice thermal conductivities (\( \kappa_\lambda = (\kappa_{aa} + \kappa_{bb} + \kappa_{cc})/3 \)) of TaN, MoP and ZrTe are listed in table 2. Therefore, the extremely large frequency gap has a dramatic effect on the lattice thermal conductivities of materials. Recently, many materials with WC-type crystal structure have been predicted as topological metal candidates [6]. The mass difference factor \( \delta \) for these topological metals is plotted in...
The large $\delta$ can lead to large acoustic–optical gap, inducing large lattice thermal conductivity by restricting acoustic + acoustic $\rightarrow$ optical scattering. It is clearly seen that $\delta$ of WC and WN are larger than 10, being close to the one of TaN. So, WC and WN may be potential candidates with ultrahigh lattice thermal conductivity. The mechanical stability of TaN is very important for ultrahigh lattice thermal conductivities. If the soft phonon modes in optical branches were observed in TaN, the acoustic-optical frequency gap would be reduced, which would lead to efficient scattering among acoustic and optical phonon modes, producing low lattice thermal conductivity. It is concluded that the high shear modulus $G$ may be key for ultrahigh lattice thermal conductivity in TaN.

In summary, the elastic and phonon transport properties of TaN are investigated by combining the first-principles calculations and semiclassical Boltzmann transport theory. Based on elastic tensor components $C_{ij}$, the mechanical stability of TaN is confirmed by mechanical stability criteria. The bulk modulus, shear modulus, Young’s modulus, the longitudinal sound speed, transversal sound speed and Debye temperature are also attained, according to the calculated $C_{ij}$. It is predicted that TaN may be a potential low compressible and hard material, based on calculated bulk modulus, shear modulus, and $C_{44}$. It is found that TaN has ultrahigh lattice thermal conductivity, showing an obvious anisotropy along the $a$ and $c$ crystal axes. The extremely large frequency gap in TaN strongly restricts acoustic + acoustic $\rightarrow$ optical scattering through the energy conservation, which leads to ultrahigh lattice thermal conductivity in TaN. Calculated results show that isotope scattering has little effect on the lattice thermal conductivity of TaN, and phonons with MFPs larger than 20 (80) $\mu$m along $a$ ($c$) direction have little contribution to the total lattice thermal conductivity. Our work sheds light on the elastic and phonon transport properties of TaN, and helps to seek ultrahigh lattice thermal conductivity in topological semimetals using a large frequency gap, such as in WC and WN.

Acknowledgments

This work is supported by the National Natural Science Foundation of China (Grant No. 11404391). We are grateful to the Advanced Analysis and Computation Center of CUMT for the award of CPU hours to accomplish this work.

ORCID iDs

San-Dong Guo https://orcid.org/0000-0002-4894-1585
Bang-Gui Liu https://orcid.org/0000-0002-6030-6680

References

[1] Lutchyn R M, Sau J D and Sarma S D 2010 Phys. Rev. Lett. 105 077001
[2] Lv B Q et al 2017 Nature 546 627
[3] Fang C, Weng H M, Dai X and Fang Z 2016 Chin. Phys. B 25 117106
[4] Zhang H J, Liu C X, Qi X L, Dai X, Fang Z and Zhang S C 2009 Nat. Phys. 5 438
[5] Hasan M Z and Kane C L 2010 Rev. Mod. Phys. 82 3045
[6] Lv B Q et al 2015 Phys. Rev. X 5 031013
[7] Qi X L and Zhang S C 2011 Rev. Mod. Phys. 83 1057
[8] Yang L X et al 2015 Nat. Phys. 11 728
[9] Xu S Y et al 2015 Nat. Phys. 11 748
[10] Xu S Y et al 2015 Sci. Adv. 10 e1501902
[11] Wang Z J, Sun Y, Chen X Q, Franchini C, Xu G, Weng H M, Dai X and Fang Z 2012 Phys. Rev. B 85 195320
[12] Liu Z K et al 2014 Science 343 864
[13] Huang S M et al 2015 Nat. Commun. 6 7373
[14] Xu S Y et al 2015 Science 349 613
[15] Schoop L M, Ali M N, Stra C, Topp A, Varykhalov A, Marchenko D, Duppel V, Parkin S S P, Lotsch B V and Ast C R 2016 Nat. Commun. 7 11696
[16] Bradlyn B, Cano J, Wang Z, Vergniory M G, Felser C, Cava R J and Bernevig B A 2016 Science 353 aa5037
[17] Weng H, Fang C, Fang Z and Dai X 2016 Phys. Rev. B 93 241202
[18] Weng H, Fang C, Fang Z and Dai X 2016 Phys. Rev. B 94 165201
[19] Zhu Z M, Winkler G W, Wu Q S, Li J and Soluyanov A A 2016 Phys. Rev. X 6 031003
[20] Winkler G W, Wu Q S, Troyer M, Krogstrup P and Soluyanov A A 2016 Phys. Rev. Lett. 117 076403
[21] Li Z, Chen H, Jin S, Gan D, Wang W, Guo L and Chen X 2016 Cryst. Growth Des. 16 1172
[22] Han N et al 2013 Nat. Commun. 4 1452
[23] Qin G Z, Qin Z Z, Wang H M and Hu M 2017 Phys. Rev. B 95 195146
[24] Guo S D 2017 J. Phys.: Condens. Matter 29 435704
[25] Guo S D, Wang Y H and Lu W L 2017 New J. Phys. 19 113044
[26] Ouyang T, Xiao H P, Tang C, Hu M and Zhong J X 2016 Phys. Chem. Chem. Phys. 18 16709
[27] Peng B, Zhang H, Shao H Z, Lu H L, Zhang D W and Zhua H 2016 Nano Energy 30 225
[28] Kresse G 1995 J. Non-Cryst. Solids 193 222
[29] Kresse G and Furthm J 1996 Comput. Mater. Sci. 6 15
[30] Kresse G and Joubert D 1999 Phys. Rev. B 59 1758
[31] Perdew J P, Burke K and Ernzerhof M 1996 Phys. Rev. Lett. 77 3865
[32] Togo A, Chaput L and Tanaka I 2015 Phys. Rev. B 91 094306
[33] Togo A, Oba F and Tanaka I 2008 Phys. Rev. B 78 134106
[34] Friedrich A, Morganroth W, Bayarjargal L, Juarez-Arellano E A, Winkler B and Koppikov Z 2013 High Press. Res. 33 633
[35] Ledbetter H M 1977 J. Phys. Chem. Ref. Data 6 1181
[36] Wu Z J, Zhao E J, Xiang H P, Hao X F, Liu X J and Meng J 2007 Phys. Rev. B 76 054415
[37] Teter M 1998 MRS Bull. 23 22
[38] Jhi S H, Ihm J, Louie S G and Cohen M L 1999 Nature 399 132
[39] Wu Z G, Chen X J, Struzhkin V V and Cohen R E 2005 Phys. Rev. B 71 214103
[40] Lindsay L, Broidio D A and Reinecke T L 2013 Phys. Rev. Lett. 111 025901
[41] Gu X and Yang R 2014 Appl. Phys. Lett. 105 131903
[42] Tamura S I 1983 Phys. Rev. B 27 858
[43] Wang J Y and Zhou Y C 2004 Phys. Rev. B 69 144108
[44] Kim W 2015 J. Mater. Chem. C 3 10336
[45] Lindsay L, Broidio D and Reinecke T 2013 Phys. Rev. B 87 165201
[46] Nakashima T and Umakoshi Y 1992 Phil. Mag. Lett. 66 317
[47] Ravindran P, Fast L, Kozhavay P A, Johnnsson B, Wills J and Eriksson O 1998 J. Appl. Phys. 84 4891
[48] Slack G A 1973 J. Phys. Chem. Solids 34 321