1. Introduction

Since the successful synthesis of graphene [1], 2D materials have attracted increasing attention due to potential applications in electronics, spintronics and optoelectronics [2–10]. Thermal management is a significant factor for these applications [11]. To efficiently dissipate heat in electronic devices, a high thermal conductivity is required, while a low lattice thermal conductivity is beneficial to thermoelectric applications, to achieve good thermoelectric performance [12, 13]. Diverse anisotropy of phonon transport in group IV–VI monolayer is predicted by solving the Boltzmann transport equation [14]. Phonon transport properties of group-IV and -VA element monolayers have been performed theoretically [15–17]. The \( \kappa_L \) of transition metal dichalcogenide (TMD) and Janus TMD monolayers have been systematically studied by phonon Boltzmann transport equation approach [18, 19]. Strain effects on thermal transports of Sb monolayer [20], group-IV monolayers [21] and 2D penta-structures materials [22] have also been studied, showing diverse strain dependence, such as monotonously increasing or decreasing and up-and-down behaviors with increasing tensile strain.

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Abstract

Due to potential applications in nano- and opto-electronics, two-dimensional (2D) materials have attracted tremendous interest. Their thermal transport properties are closely related to the performance of 2D materials-based devices. Here, the phonon transports of monolayer GeC with a perfect planar hexagonal honeycomb structure are investigated by solving the linearized phonon Boltzmann equation within the single-mode relaxation time approximation (RTA). Without inclusion of Born effective charges \( Z^* \) and dielectric constants \( \varepsilon \), the lattice thermal conductivity \( \kappa_L \) decreases almost linearly above 350 K, deviating from the usual \( \kappa_L \sim 1/T \) law. The underlying mechanism is because the contribution to \( \kappa_L \) from high-frequency optical phonon modes increases with increasing temperature, and the contribution exceeds one from acoustic branches at high temperature. These can be understood by huge phonon band gap caused by large difference in atom mass between Ge and C atoms, which produces important effects on scattering process involving high-frequency optical phonon. When considering \( Z^* \) and \( \varepsilon \), the phonon group velocities and phonon lifetimes of high-frequency optical phonon modes are obviously reduced with respect to ones without \( Z^* \) and \( \varepsilon \). The reduced group velocities and phonon lifetimes give rise to small contribution to \( \kappa_L \) from high-frequency optical phonon modes, which produces the the traditional \( \kappa_L \sim 1/T \) relation in monolayer GeC. Our works highlight the importance of \( Z^* \) and \( \varepsilon \) to investigate phonon transports of monolayer GeC, and motivate further theoretical or experimental efforts to investigate thermal transports of other 2D materials.

Keywords: lattice thermal conductivity, monolayer, Born effective charge

(Some figures may appear in colour only in the online journal)
For most bulk and 2D materials, the temperature-dependent $\kappa_L$ follows the relation of $\kappa_L \sim 1/T$. Recently, anomalously temperature-dependent $\kappa_L$ of monolayer ZnO and GaN is predicted by a first-principles study [23, 24], which is due to the huge phonon band gap in their phonon dispersions. The predicted room-temperature $\kappa_L$ of monolayer ZnO and GaN is 4.5 W m$^{-1}$ K$^{-1}$ with the thickness of 3.04 Å and 14.93 W m$^{-1}$ K$^{-1}$ with the thickness of 3.74 Å, respectively. The SiC monolayer has the same perfect planar hexagonal honeycomb structure with ZnO and GaN, but the $\kappa_L$ of SiC monolayer follows the conventional 1/T law [25], which may be due to small phonon band gap. For GeC monolayer with the same structure, a large phonon band gap can be observed due to a large difference in atom mass between Ge and C atoms [26]. The similar anomalous temperature dependence of $\kappa_L$ may also exist in monolayer GeC. In this work, based on first-principles calculations, the phonon transport properties of monolayer GeC are investigated by solving the linearized phonon Boltzmann equation. When neglecting $Z'$ and $\varepsilon$, the $\kappa_L$ deviates from the usual $\kappa_L \sim 1/T$ law. The $\kappa_L$ above 200 K is much higher than the expected $\kappa_L$ predicted from the general $\kappa_L \sim 1/T$ law. The large deviation stems from the high-frequency optical phonon modes, whose contribution to $\kappa_L$ increases with increasing temperature, and eventually dominates $\kappa_L$. With inclusion of $Z'$ and $\varepsilon$, the phonon group velocities and phonon lifetimes of high-frequency optical phonon modes are obviously reduced, which gives rise to small contribution to $\kappa_L$ from high-frequency optical phonon modes, producing the the traditional $\kappa_L \sim 1/T$ relation in monolayer GeC. In many polar materials, the non-analytical corrections have little effects on their lattice thermal conductivities [14, 18, 19, 22, 27]. Therefore, the non-analytical corrections have been neglected in many calculations. Here, we emphasize the importance of the non-analytical corrections to calculate lattice thermal conductivity of GeC monolayer.

The rest of the paper is organized as follows. In the next section, we shall give our computational details about phonon transport. In the third section, we shall present phonon transport of monolayer GeC. Finally, we shall give our discussion and conclusions in the fourth section.

2. Computational detail

All first-principles calculations are carried out based on the density functional theory (DFT) using the projected augmented wave (PAW) method, and the generalized gradient approximation of the Perdew–Burke–Ernzerhof (GGA-PBE) is adopted as exchange-correlation energy functional, as implemented in the Vienna $ab$ initio simulation package (VASP) [28–31]. A plane-wave basis set is employed with kinetic energy cutoff of 700 eV, and the 2s2p (4s4p) orbitals of C (Ge) atoms are treated as valance ones. To avoid spurious interaction, the unit cell of monolayer GeC is built with the vacuum region of 18 Å along the out-of-plane direction. The energy convergence threshold is set as $10^{-8}$ eV.

The $\kappa_L$ of monolayer GeC is calculated by solving linearized phonon Boltzmann equation with the single mode RTA, as implemented in the Phono3py code [32]. The $\kappa_L$ can be expressed as:

$$\kappa_L = \frac{1}{N V_0} \sum \kappa_\lambda = \frac{1}{N V_0} \sum \lambda C_{\lambda} \nu_{\lambda} \otimes \nu_{\lambda} \tau_\lambda$$

(1)

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

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

(2)

The $\Gamma(\omega)$ takes the form analogous to the Fermi golden rule:

$$\Gamma(\omega) = \frac{18\pi}{h^2} \sum_{\lambda' \lambda''} |\Phi_{-\lambda' \lambda''}|^2 [(f^{' \prime}_\lambda + f^{'' \prime}_\lambda + 1)\delta(\omega - \omega'_\lambda - \omega''_\lambda)

+ (f^{' \prime}_\lambda - f^{'' \prime}_\lambda)\delta(\omega - \omega'_\lambda - \omega''_\lambda)]$$

(3)

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

The interatomic force constants (IFCs) are calculated by the finite displacement method. The second-order harmonic (third-order anharmonic) IFCs are calculated using a 5 × 5 × 1 (4 × 4 × 1) supercell containing 50 (32) atoms with k-point meshes of 4 × 4 × 1. Using the harmonic IFCs, phonon dispersion of monolayer GeC can be attained, using Phonopy package [33]. To compute lattice thermal conductivities, the reciprocal spaces of the primitive cells are sampled using the 100 × 100 × 1 meshes. For 2D material, the calculated lattice thermal conductivity depends on the length of unit cell used in the calculations along $z$ direction [34]. The lattice thermal conductivity should be normalized by multiplying $L_z/d$, in which $L_z$ is the length of unit cell along $z$ direction and $d$ is the thickness of 2D material, but the $d$ is not well defined like graphene. In this work, the length of unit cell (18 Å) along $z$ direction is used as the thickness of monolayer GeC. To make a fair comparison between various 2D monolayers, the thermal sheet conductance can be used, defined as $\kappa_L \times d$.

3. Main calculated results and analysis

Monolayer GeC prefers a perfect planar hexagonal honeycomb structure, and similar monolayer structure can be found in graphene, ZnO, GaN and SiC [23, 24, 26]. The monolayer GeC can be built by replacing one atom in the unit cell of graphene with Ge atom, and the space symmetry group is P6M2, being lower than that of graphene (P6/M MM). Figure 1 shows the schematic crystal structure of monolayer GeC, and the optimized lattice parameter within GGA-PBE is 3.26 Å. Firstly, the elastic properties of monolayer GeC are studied, and two independent elastic constants $C_{11}(=C_{22})$ and $C_{12}$ due to $D_{3d}$ symmetry can be calculated, and the $C_{66} = (C_{11} - C_{12})/2$. For $C_{11}$, $C_{12}$ and $C_{66}$, the calculated value is 159.42 Nm$^{-1}$, 51.62 Nm$^{-1}$ and 53.90 Nm$^{-1}$, respectively. These $C_{ij}$ satisfy
the Born criteria of mechanical stability. Based on calculated $C_{ij}$, the 2D Youngs moduli $Y_{2D}$ and shear modulus $G_{2D}$ of monolayer GeC [35] are 142.71 Nm$^{-1}$ and 53.90 Nm$^{-1}$, which are lower than ones of graphene and SiC monolayer [25, 35]. The GeC monolayer is more flexible than graphene and SiC monolayer due to smaller $Y_{2D}$.

The calculated phonon dispersion of monolayer GeC along high-symmetry path and total and partial density of states (DOS) are shown in figure 2. No imaginary frequencies are observed in the phonon dispersion, indicating the thermodynamic stability of monolayer GeC. There are 6 phonon branches due to 2 atoms per unit cell, including 3 acoustic and 3 optical phonon branches. A phonon band gap of 13.52 THz is observed, which separates in-plane transverse optical (TO) and the in-plane longitudinal optical (LO) branches from out-of-plane optical (ZO), in-plane longitudinal acoustic (LA), in-plane transverse acoustic (TA) and out-of-plane acoustic (ZA) branches. It is noted that the phonon band gap is larger than width of acoustic branches (11.61 THz), which has important effects on phonon transport. The large gap can be explained by the Ge atom being much heavier than C atom. It is clearly seen that the ZO branch crosses with the TA and LA branches, which has significant effect on the phonon scattering process. The similar phonon dispersion can also be found in SiC, ZnO and GaN monolayers [23–26]. However, for monolayer SiC, a phonon band gap of 7.47 THz is very smaller than width of acoustic branches (19.48 THz). Based on the elastic theory, the ZA phonon branch should have quadratic dispersion with the sheet being free of stress [36, 37]. The quadratic ZA branch near the Γ point can be observed for monolayer GeC. However, the TA and LA branches are linear near the Γ point. The partial DOS indicates that optical branches are mainly contributed by the vibrations of C atoms, while acoustic branches are contributed by the vibrations of Ge atoms.

By solving the linearized phonon Boltzmann equation within single-mode RTA method, the intrinsic $\kappa_L$ of monolayer GeC is calculated, which is plotted in figure 3 as a function of temperature. The room-temperature $\kappa_L$ of monolayer GeC is 15.43 W m$^{-1}$ K$^{-1}$ with the thickness of 18 Å, and the corresponding thermal sheet conductance is 277.74 W K$^{-1}$, being two orders of magnitude lower than that of graphene (about 12 884 W K$^{-1}$) [34]. To understand the mechanism underlying the low $\kappa_L$ of monolayer GeC, the mode level Grüneisen parameters of monolayer GeC are shown in figure 4. It is found that the $\gamma$ of TO and LO branches is fully positive. For the phonon modes below the gap, both negative and partial positive $\gamma$ can be observed, and ZA branch shows very large negative $\gamma$. The $\kappa_L$ of monolayer GeC as a function of temperature with $|Z_1|$ along $xx$ and $yy$ directions artificially changing from 0 to 5.72 (the calculated $|Z_1|$ for 3.72); The $\kappa_L \sim 1/T$ relation is plotted for comparison.
However, due to the symmetry-based selection rule, the scattering of ZA branch is largely suppressed. The large $\gamma$ means strong phonon anharmonicity, which can produce the strong phonon-phonon scattering, leading to the low $\kappa_L$ of monolayer GeC. To have an explicit view on the phonon anharmonicity from another aspect, the potential energy well of monolayer GeC, defined as potential energy change due to the change of lattice constant ($E_{a/\alpha}$ is lattice constant), is shown in the inset of figure 4. It is found that the potential well of monolayer GeC is asymmetric with respect to compressive and tensile strains, which is a direct evidence of the phonon anharmonicity. A three order polynomial curve can be used to fit the potential energy well, and the fitted parameter for the cubic term is $-395$ eV, and the large cubic term is consistent with the $\gamma$.

For the most bulk and 2D materials, the temperature-dependent $\kappa_L$ follows $\kappa_L \sim 1/T^\alpha$ relationship with $\alpha$ changing from 0.85 to 1.05 [23]. It is very strange that the $\kappa_L$ of monolayer GeC shows an anomalous linear temperature dependence above about 350 K, which is obviously different from usual picture $\kappa_L \sim 1/T$ relationship. The $\kappa_L \sim 1/T$ relation is also shown in figure 3 for comparison. To understand the anomalous temperature dependence of $\kappa_L$ of monolayer GeC, the ratio between accumulated and total $\kappa_L$ with respect to frequency at 100, 200, 300, 400 and 600 K are plotted in figure 5. It is clearly seen that, with the temperature increasing, the contribution from LO and TO branches increases. When the temperatures are lower than 300 K, the contribution of phonon modes below the phonon gap is larger than 50%. However, for temperatures higher than 300 K, the LO and TO branches dominate the $\kappa_L$ with the contribution larger than 50%. If acoustic phonon branches dominate $\kappa_L$, the temperature-dependent $\kappa_L$ would follow $\kappa_L \sim 1/T$ relationship, which can be found for most materials [23]. So, the anomalous linear temperature dependence of $\kappa_L$ of monolayer GeC is due to dominant contribution from LO and TO branches, when the temperature is larger than 300 K. Anomalously temperature-dependent $\kappa_L$ has been predicted in monolayer ZnO and GaN by Hu et al [23].

Table 1. The $Z'$ of C and Ge atoms and $\varepsilon$ of monolayer GeC. Except for $xx$, $yy$ and $zz$ directions, the $Z'$ and $\varepsilon$ along other directions are zero.

| Direction | $Z'(C)$ | $Z'(Ge)$ | $\varepsilon$ |
|-----------|---------|----------|--------------|
| $xx$      | -3.72   | 3.72     | 2.90         |
| $yy$      | -3.72   | 3.72     | 2.90         |
| $zz$      | -0.25   | 0.25     | 1.18         |

To understand the mechanism underlying the sudden change of $\kappa_L$, the mode level phonon group velocities and phonon lifetimes (300 K) of monolayer GeC with or without $\varepsilon$ and $Z'$ are plotted in figure 7. The group velocities and phonon...
lifetimes of phonon modes below the gap have little difference between with and without $\epsilon$ and $Z'$. However, for LO and TO branches, the group velocities and phonon lifetimes with $\epsilon$ and $Z'$ are smaller than ones without $\epsilon$ and $Z'$, which dramatically reduces contribution to $\kappa_L$ from LO and TO branches, and then the normal $\kappa_L \sim 1/T$ relationship is observed in GeC monolayer.

4. Discussion and conclusion

It is interesting to compare phonon transports of monolayer GeC with ones of SiC and GeSi monolayers. The monolayer SiC has also a perfect planar hexagonal honeycomb structure, but monolayer GeSi has a buckled structure due to the decrease in the overlap between the $p_z$ orbitals [26]. The phonon band structures and $\kappa_L$ of monolayer GeC, SiC and GeSi without $\epsilon$ and $Z'$ are plotted in figure 8. The $\epsilon$ and $Z'$ produce little effects on $\kappa_L$ of monolayer SiC and GeSi, so only the $\kappa_L$ of monolayer GeC with $\epsilon$ and $Z'$ is shown in figure 8. It is clearly seen that anomalous temperature dependence of $\kappa_L$ is absent in monolayer SiC and GeSi. These can be understood by their phonon dispersions. There is a huge phonon band gap of 13.52 THz (larger than width of acoustic branches [11.61 THz]) in monolayer GeC, which can weaken the scattering between acoustic and high frequency optical phonon modes, producing very large phonon lifetimes of LO and TO branches. For monolayer SiC, a phonon band gap of 7.47 THz is observed (smaller than width of acoustic branches [19.48 THz]), and the LO and TO modes can effectively scattered with acoustic modes, leading to short phonon lifetimes of LO and TO branches. In monolayer GeSi, there is a very large gap of 7.17 THz (larger than width of acoustic branches [3.81 THz]) between LO/TO and acoustic branches, but ZO branch is in the gap, which provide effective scattering channels for LO and TO branches, giving rise to short

Figure 6. Phonon band structures of monolayer GeC with $|Z'|$ along $xx$ and $yy$ directions artificially changing from 0 to 5.72.

Figure 7. The mode level phonon group velocities and phonon lifetimes (300 K) of monolayer GeC in the first BZ with or without $\epsilon$ and $Z'$.

Figure 8. Left: phonon band structures of monolayer GeC, SiC and GeSi without $\epsilon$ and $Z'$; Right: the $\kappa_L$ of monolayer GeC (without and with $\epsilon$ and $Z'$), SiC and GeSi.
phonon lifetimes. When considering $\varepsilon$ and $Z'$, the order of $\kappa_L$ is GeSi < GeC < SiC, which is consistent with their atomic mass.

For ZnO monolayer [23], one can observe the opposite effect, namely, it is the inclusion of the non-analytical corrections in the calculation which deviates more the thermal conductivity from the $\kappa_L \sim 1/T$ relationship. For SiC monolayer [25], the non-analytical corrections are shown to have an effect on the LO–TO splitting similar to the GeC monolayer, leading to a reduction in the LO group velocity, however they have a negligible effect on the lattice thermal conductivity. For SiC monolayer, a phonon band gap of 7.47 THz is observed (smaller than width of acoustic branches [19.48 THz]), and the LO and TO modes can be effectively scattered with acoustic modes, leading to short phonon lifetimes of LO and TO branches. For GeC monolayer, there is a huge phonon band gap of 13.52 THz leading to short phonon lifetimes of LO and TO branches. For ZnO monolayer, the inclusion of the non-analytical corrections reduce phonon lifetimes of LO and TO branches, while the phonon band gap of ZnO monolayer is smaller than width of acoustic branches. The non-analytical corrections produce phonon lifetimes of LO and TO branches of GeC, and the non-analytical corrections should enhance phonon lifetimes of LO and TO branches of ZnO. Therefore, for ZnO monolayer, the inclusion of the non-analytical corrections in the calculation deviates more the thermal conductivity from the $\kappa_L \sim 1/T$ relationship.

In summary, the phonon transports of monolayer GeC are investigated by the first-principles calculations and semiclassical Boltzmann transport theory. When neglecting $\varepsilon$ and $Z'$, monolayer GeC possesses anomalously linear temperature dependent $\kappa_L$, which is different from the commonly established $\kappa_L \sim 1/T$ relationship. The large deviation is because the contribution to $\kappa_L$ from LO and TO branches increases with increasing temperature, and eventually dominates the $\kappa_L$ with $T$ being larger than 300 K. However, considering $\varepsilon$ and $Z'$, the common $\kappa_L \sim 1/T$ relationship is observed by reduced group velocities and phonon lifetimes of LO and TO branches. This work presents a comprehensive understanding of the phonon transports of monolayer GeC, and sheds light on further studies of phonon transports of other 2D materials.

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