Nonmonotonic strain dependence of lattice thermal conductivity in monolayer SiC: a first-principles study

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An increasing number of two-dimensional (2D) materials have already been achieved experimentally or predicted theoretically, which have potential applications in nano- and opto-electronics. Various applications for electronic devices are closely related to their thermal transport properties. In this work, the strain dependence of phonon transport in monolayer SiC with a perfect planar hexagonal honeycomb structure is investigated by solving the linearized phonon Boltzmann equation. It is found that room-temperature lattice thermal conductivity ($\kappa_L$) of monolayer SiC is two orders of magnitude lower than that of graphene. The low $\kappa_L$ is due to small group velocities and short phonon lifetimes, which can also be explained by polarized covalent bond due to large charge transfer from Si to C atoms. In considered strain range, it is proved that the SiC monolayer is mechanically and dynamically stable. With increased tensile strain, the $\kappa_L$ of SiC monolayer shows an unusual nonmonotonic up-and-down behavior, which is due to the competition between the change of phonon group velocities and phonon lifetimes of low frequency phonon modes. At low strains (<8%), the phonon lifetimes enhancement induces the increased $\kappa_L$, while at high strains (>8%) the reduction of group velocities as well as the decrease of the phonon lifetimes are the major mechanism responsible for decreased $\kappa_L$. Our work further enrich studies on phonon transports of 2D materials with a perfect planar hexagonal honeycomb structure, and motivate further experimental studies.

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I. INTRODUCTION

Due to their fascinating physical and chemical properties, 2D materials have attracted increasing attention since the successful synthesis of graphene\(^1\). In comparison with the gapless graphene, semiconducting transition-metal dichalcogenide (TMD)\(^2\), group IV-VI\(^3\), group-VA\(^4,5\), group-IV\(^6\), GaN\(^7\) and ZnO\(^8\) monolayers have intrinsic energy band gaps. Thermal management is very important for next generation of electronics and optoelectronic devices based on these 2D materials\(^9\), which has been hot spot in the field of materials. The thermal transports of many 2D materials have been studied from a combination of first-principles calculations and the linearized phonon Boltzmann equation\(^10-15\). The phonon transports of 2D orthorhombic group IV-VI compounds (GeS, GeSe, SnS and SnSe) have been systematically investigated, and they show diverse anisotropic properties along the zigzag and armchair directions\(^10\). Phonon transport properties of 2D group-IV materials have been performed, and although the $\kappa_L$ decreases monotonically from graphene to silicene to germanene, unexpected higher $\kappa_L$ is observed in stanene\(^11\). The thermal transports of group-VA elements (As, Sb, Bi) monolayers with graphene-like buckled structure have been studied, including both electron and phonon parts\(^12\). The phonon transports of TMD MX$_2$ (M=Mo, W, Zr and Hf; X=S and Se) monolayers have been systematically investigated\(^13\). The $\kappa_L$ of 2H-type TMD monolayers are generally higher than those of 1T-type ones due to the larger acoustic-optical frequency gap\(^15\). Strain effects on $\kappa_L$ have also been carried out in various kinds of 2D materials, such Sb and AsP monolayer\(^16,17\), 2D group-IV\(^18\), 2D MoTe$_2$\(^19\) and 2D penta-structures materials\(^20\). The $\kappa_L$ shows diverse strain dependence, such as monotonously increasing, up-and-down and monotonously decreasing behaviors with increasing strain.

Like graphene, ZnO and GaN monolayers possess a perfect planar hexagonal honeycomb structural configuration, and their $\kappa_L$ have been investigated from a first-principles study\(^21,22\). The room-temperature $\kappa_L$ of monolayer ZnO is 4.5 Wm$^{-1}$K$^{-1}$ with the thickness of 3.04 Å, and it’s lattice thermal conductivity shows anomalous temperature dependence\(^21\). The $\kappa_L$ of monolayer GaN (300 K) is 14.93 Wm$^{-1}$K$^{-1}$ with the thickness of 3.74 Å, and the low $\kappa_L$ can be explained by the special sp orbital hybridization mediated by the Ga-d orbital\(^22\).

Recently, atomic resolution scanning transmission electron microscopy observations provide direct experimental indication of a two-dimensional form of silicon carbide, and the ground state of 2D SiC is indeed completely pla-

![FIG. 1. (Color online) The top and side views of monolayer SiC, and the frame surrounded by a black box is unit cell. The blue and red balls represent Si and C atoms, respectively.](image-url)
nar by extensive simulations. Similar to ZnO and GaN monolayers, 2D-SiC adopts a perfect planar hexagonal honeycomb structure with the gap of 2.58 eV using GGA.

In this work, strain-dependent phonon transport properties of SiC monolayer are studied by solving the linearized phonon Boltzmann equation based on first-principles calculations. The calculated room-temperature sheet thermal conductance of SiC monolayer is 301.66 WK$^{-1}$, which is substantially lower than that of graphene (about 12884 WK$^{-1}$). The mode level phonon group velocities and phonon lifetimes are used to investigate the mechanism underlying the lower $\kappa_L$ of monolayer SiC compared with graphene. The strongly polarized Si-C bond, caused by large charge transfer between Si and C atoms, induces large phonon anharmonicity, and gives rise to the intrinsic low $\kappa_L$ of monolayer SiC. As the strain increases, the $\kappa_L$ of Si monolayer shows a nonmonotonic up-and-down behavior, which can be understood by the competition between the change of phonon group velocities and phonon lifetimes of low frequency phonon modes.

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 strain-dependent phonon transport of monolayer SiC. Finally, we shall give our conclusions in the fourth section.

II. COMPUTATIONAL DETAIL

First-principles calculations are carried out using the projected augmented wave (PAW) method, and the exchange-correlation functional of generalized gradient approximation of the Perdew-Burke-Ernzerhof (GGA-PBE) is adopted, as implemented in the VASP code. A plane-wave basis set is employed with kinetic energy cutoff of 700 eV, and the 2$^\text{nd}$ ($3^\text{rd}$) and $2p$ ($3p$) orbitals of C(Si) atoms are treated as valance ones. The unit cell of monolayer SiC is built with the vacuum region of larger length of unit cell along z direction to avoid spurious interaction. The electronic stopping criterion is $10^{-8}$ eV. The $\kappa_L$ of monolayer SiC is calculated by solving linearized phonon Boltzmann equation with the single mode relaxation time approximation (RTA), as implemented in the Phono3py code. The $\kappa_L$ can be expressed as:

$$\kappa = \frac{1}{N V_0} \sum_{\lambda} \kappa_{\lambda} = \frac{1}{N V_0} \sum_{\lambda} C_{\lambda} \nu_{\lambda} \otimes \nu_{\lambda} \tau_{\lambda}$$  \hspace{1cm} (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 $\lambda$:

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

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

$$\Gamma_{\lambda}(\omega) = \frac{18\pi}{\hbar^2} \sum_{\lambda'\lambda''} |\Phi_{-\lambda\lambda'} \Phi_{\lambda''}|^2 [(f_{\lambda} + f_{\lambda''} + 1)\delta(\omega - \omega_{\lambda}) - (f_{\lambda} - f_{\lambda''})|\delta(\omega - \omega_{\lambda} + \omega_{\lambda''}) - \delta(\omega - \omega_{\lambda} + \omega_{\lambda''})]|$$  \hspace{1cm} (3)

in which $f_{\lambda}$ and $\Phi_{-\lambda\lambda'\lambda''}$ 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 IFCs are calculated using a $5 \times 5 \times 1$ supercell containing 50 atoms with k-point meshes of $3 \times 3 \times 1$. Using the harmonic IFCs, phonon dispersion of monolayer SiC can be attained, as implemented in Phonopy package. The phonon dispersion determines the allowed three-phonon scattering processes, and further the group velocity and specific heat can be attained. The third-order anharmonic IFCs are calculated using a $4 \times 4 \times 1$ supercells containing 32 atoms with k-point meshes of $4 \times 4 \times 1$. Based on third-order anharmonic IFCs, the three-phonon scattering rate can be calculated, and further the phonon lifetimes can be attained. To compute $\kappa_L$, the reciprocal spaces of the primitive cells are sampled using the $120 \times 120 \times 1$ meshes.

For 2D material, the calculated $\kappa_L$ depends on the length of unit cell along z direction. The $\kappa_L$ 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. In this work, the length of unit cell (18 Å) along z direction is used as the thickness of monolayer SiC. To make a fair comparison between various 2D monolayers, the thermal sheet conductance can be used, defined as $\kappa_L \times d$.  

![FIG. 2. (Color online)Phonon band structures of monolayer SiC with the corresponding density of states (DOS), and the atom partial DOS (PDOS) are also shown. The red dots represent ZO branch.](image-url)
III. MAIN CALCULATED RESULTS AND ANALYSIS

Like graphene, monolayer ZnO and monolayer GaN, monolayer SiC possesses a perfect planar hexagonal honeycomb structure, which can be constructed by substituting one C atom in the unit cell of graphene with Si atom. The space symmetry group is P6\textit{m}2 for monolayer SiC, being lower than that of graphene (P6\textit{m}3\textit{m}3\textit{m}), which is because monolayer SiC contains two kinds of atoms in the unit cell. The schematic crystal structure is shown in Figure 1, and the optimized lattice parameter is 3.104 Å. It is worth noting that the bulk SiC possesses buckled structure for SiC layer, being different from planar structure for monolayer SiC, which may be due to the variation of orbital hybridization from sp\textsuperscript{3} to sp\textsuperscript{2}.

Based on the harmonic IFCs, the phonon dispersion of monolayer SiC is obtained along high-symmetry path, which along with total and partial density of states (DOS) are plotted in Figure 2. The phonon dispersion gives no imaginary frequencies, which indicates the thermodynamic stability of monolayer SiC. Due to two atoms per unit cell, the phonon dispersion of monolayer SiC includes 3 acoustic and 3 optical phonon branches. The two highest phonon branches are the in-plane transverse optical (TO) and in-plane longitudinal optical (LO) branches. It is clearly seen that there is a phonon band gap of 7.47 THz, separating TO and 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. The phonon band gap may be caused by different atomic masses of C and Si atoms. Based on the highest acoustic frequency, the Debye temperature can be attained by $\theta_B = \hbar \nu_m/k_B$, where $\hbar$ is the Planck constant, and $k_B$ is the Boltzmann constant. The calculated value is about 935 K, which is lower than that of graphene (1977 K). The ZO branch crosses with the TA and LA branches, and there is a phonon band gap of 0.89 THz between ZA and ZO branches. Similar crosses can also be found in ZnO and GaN monolayers, but a phonon band gap is absent between ZA and ZO branches for monolayer GaN. The TA and LA branches are linear near the $\Gamma$ point, while the ZA branch deviates from linearity near the $\Gamma$ point, which can be found in many 2D materials. The partial DOS indicates that TO and LO branches are mainly contributed by the vibrations of C atoms. According to Figure 3, TA and LA branches are mainly from Si vibrations, while ZA and ZO branches are contributed by the vibrations of C and Si atoms.

The intrinsic $\kappa_L$ of monolayer SiC is calculated by solving the linearized phonon Boltzmann equation within single-mode RTA method. The phonon-isotope scattering is calculated based on the formula proposed by Shinichiro Tamura. For boundary scattering, $v_g/L$ is just used as the scattering rate, where $v_g$ is the group velocity and $L$ is the boundary mean free path (MFP). The lattice thermal conductivities of infinite (Pure and Isotope) and finite-size (3, 0.3, 0.1, 0.08 and 0.03 μm) monolayer SiC as a function of temperature; Bottom: cumulative lattice thermal conductivity of infinite (Pure) monolayer SiC with respect to phonon mean free path at room temperature, and the derivatives. The horizontal blue line represents room-temperature lattice thermal conductivity.
FIG. 5. The mode level phonon group velocities, phonon lifetimes (300K) and Grüneisen parameters of infinite (Pure) monolayer SiC in the first BZ.

FIG. 6. (Color online) The charge density distributions of monolayer SiC (unit: |e|/bohr^3).

TABLE I. Born effective charges $Z^*$ of Si and C atoms and the dielectric constants ($\varepsilon$) of monolayer SiC. They along other directions are zero except $xx$, $yy$ and $zz$ directions.

| Direction | $Z^*$ (C) | $Z^*$ (Si) | $\varepsilon$ |
|-----------|-----------|-----------|-------------|
| $xx$      | -3.674    | 3.674     | 2.531       |
| $yy$      | -3.674    | 3.674     | 2.531       |
| $zz$      | -0.271    | 0.271     | 1.180       |

and finite-size (3, 0.3, 0.1, 0.08 and 0.03 μm) monolayer SiC as a function of temperature are plotted in Figure 4. The room-temperature $\kappa_L$ of infinite (Pure) monolayer SiC is 16.76 Wm^{-1}K^{-1} with the thickness of 18 Å, and the corresponding thermal sheet conductance is 301.66 WK^{-1}, which is two orders of magnitude lower than that for graphene (about 12884 WK^{-1})^{24}. It is clearly seen that the isotope scattering has little effect on the lattice thermal conductivity of monolayer SiC, which may be due to the strong phonon-phonon scattering. With the sample size decreasing, the lattice thermal conductivity decreases due to enhanced boundary scattering. For the 3 and 0.3 μm cases, the change is very small with respect to infinite case. The $\kappa_L$ for the 0.03 μm case is reduced to about half of that for infinite case at room temperature.

To further understand the size dependence, the cumulative $\kappa_L$ along with the derivatives with respect to MFP (300 K) are plotted in Figure 4. With MFP increasing, the cumulative $\kappa_L$ approaches maximum. Phonons with MFP larger than 0.15 μm have very little contribution to the $\kappa_L$. Phonons with MFP smaller than 0.03 μm contribute around 50% to the $\kappa_L$.

To understand deeply phonon transport of monolayer SiC, the mode level phonon group velocities and lifetimes are shown in Figure 5. The largest group velocity for TA and LA branches near Γ point is 8.74 kms^{-1} and 14.80 kms^{-1}, which are lower than those of graphene^{22}. Moreover, the overall phonon group velocities of monolayer SiC are smaller than those of graphene.
FIG. 8. (Color online) The elastic constants $C_{ij}$, Young’s moduli $Y$ and shear modulus $G$ vs strain for SiC monolayer.

which partially leads to lower $\kappa_L$ for monolayer SiC than graphene. The phonon lifetimes can be calculated from three-phonon scattering rate by third-order anharmonic IFCs. It is found that ZA branch has relatively large phonon lifetimes. Due to the reflectional symmetry of monolayer SiC, the scattering channels involving odd numbers of ZA modes are largely suppressed, which leads to the low scattering rate of ZA, and then induces large phonon lifetimes. The lifetimes of TO and LO phonon branches are much larger than those below the gap, which can be explained by the weak phonon-phonon scattering caused by the large phonon gap. The overall phonon lifetimes of monolayer SiC are much smaller than those of graphene.\(^\text{22}\) The strong coupling of ZO branch with acoustic branches is very important to increase the scattering rate of the phonon modes below the gap by providing additional channels for the acoustic phonon scattering, which can reduce phonon lifetimes of monolayer SiC. The short phonon lifetimes together with small group velocities result in much lower $\kappa_L$ for monolayer SiC than graphene.

Mode Grüneisen parameters can be attained by third order anharmonic IFCs, which can reflect the strength of anharmonic interactions, determining the intrinsic phonon-phonon scattering. The larger $\gamma$ leads to lower $\kappa_L$ due to strong anharmonicity. The mode level phonon Grüneisen parameters of infinite (Pure) monolayer SiC in the first BZ are plotted in Figure 5. For LA, TO and LO branches, the $\gamma$ is fully positive. For TA phonon modes, it shows both negative and partial positive $\gamma$. The $\gamma$ is fully negative for ZA and ZO branches, where the large negative $\gamma$ of ZA branches shares the general feature of 2D materials due to the membrane effect.\(^\text{32}\) Although the ZA branch of monolayer SiC has larger $\gamma$ than that of some 2D materials, the scattering of ZA is largely suppressed due to the symmetry-based selection rule.

The charge density can be used to describe the distribution of electrons in real space, which is plotted Figure 6 for monolayer SiC. It is clearly seen that the charge density increases from Si atom to C atom, which means that charge transfer is produced between Si and C atoms when the Si-C bond is formed. The charge transfer from Si to C atom induces the strongly polarized covalent bond. For graphene, there is no charge transfer due to the same atom types to form bond. The strongly polarized covalent bond can give rise to larger phonon anharmonicity, and induces stronger intrinsic phonon-phonon scattering, which leads to lower $\kappa_L$ of monolayer SiC with respect to graphene.

The dielectric constants $\varepsilon$ and Born effective charges $Z^*$ effects on lattice thermal conductivity are considered, as given in Table I. The strongly polarized covalent bond can also be characterized by large $Z^*$ and $\varepsilon$. The LO-TO splitting at the Brillouin zone center is produced by long-range electrostatic Coulomb interactions, which can be clearly seen in Figure 7. It is noted that the $\kappa_L$ only has a slight change with or without $\varepsilon$ and $Z^*$. It is because LO and TO branches have little contribution to total $\kappa_L$.

Strain can effectively tune $\kappa_L$ in many 2D materials.\(^\text{16-20}\) The biaxial strain can be described by defining $\varepsilon = (a - a_0)/a_0$, in which $a_0$ is the unstrain lattice constant. Firstly, the strain dependence of elastic constants $C_{ij}$, Young’s moduli $Y$ and shear modulus $G$
FIG. 10. (Color online) The phonon dispersion curves of SiC monolayer with strain from 0% to 14%.

FIG. 11. (Color online) The phonon gap $G$, the width of ZO mode $W$, and the difference of maximum frequency between LA and ZO modes $D$ vs strain for SiC monolayer.

in SiC monolayer are plotted in Figure 8. They all monotonically decrease from 0% to 14% strain. In considered strain range, all the obtained elastic constants are positive, confirming the mechanical stability in strained SiC monolayer. The $Y$ of the unstrained SiC monolayer is lower than those of h-BN and graphene, but higher than one of MoS$_2$. In the strain range of 0% - 14%, the $\kappa_L$ of SiC monolayer as a function of temperature are plotted in Figure 9, together with $\kappa_L$ vs strain at the temperature of 200, 250, 300 and 400 K. The $\kappa_L$ shows a nonmonotonic trend with increased strain, and first increases from 16.75 Wm$^{-1}$K$^{-1}$ (unstrained) to 99.15 Wm$^{-1}$K$^{-1}$ (at 8% strain) then decreases to 75.61 Wm$^{-1}$K$^{-1}$ (at 14% strain). Similar up-and-down behavior is also found in penta-SiC$_2$, $\beta$-AsP and bilayer graphene. The room-temperature $\kappa_L$ at 8% strain is about 5.9 times that of the unstrained case.

To identify the underlying mechanism of strain-dependent up-and-down behavior of $\kappa_L$ in SiC monolayer, the phonon dispersions of SiC monolayer with 0%-14% strain are plotted Figure 10. It is clearly seen that there are no imaginary frequencies in considered strain range, indicating that strained SiC monolayer is dynamically stable. With increasing strain, the dispersions of both TA and LA modes are softened, producing the reduced phonon group velocities. The dispersion of ZA mode near $\Gamma$ point is stiffened, indicating the improved phonon group velocities. It is noted that the change of ZA mode at small strain is more obvious than one at large strain. These can also be observed in penta-graphene, AsP and MoTe$_2$. With strain increasing, the quadratic nature of ZA mode near the $\Gamma$ point disappears, which can also be found in AsP and MoTe$_2$. Due to less strongly interacting between atoms with increased strain, the dispersions of optical branches overall move toward low frequency. The phonon gap $G$, the width of ZO mode $W$, and the difference of maximum frequency between LA and ZO modes $D$ as a function of strain are plotted in Figure 11. It is clearly seen that they all decrease with increased strain, which can produce important effects on phonon transports of SiC monolayer. The large phonon gap hinders acoustic+acoustic$\rightarrow$optical (aao) scattering due to the energy conservation, which can enhance $\kappa_L$. The reduced $G$ with increased strain can give negative contribution to $\kappa_L$. The reduced $W$ and $D$ have positive contribution to $\kappa_L$ due to reduced scattering channels for acoustic phonon.

Due to dominant contribution to $\kappa_L$ from modes below
and Figure 13. With increased MFP, the ratio is. Due to stiffened ZA is identical with increases with increased strain, and then decreases, which close to one for all strains. The critical MFP firstly in-

FIG. 12. (Color online) The phonon mode group velocities of SiC monolayer with strain 0% (Black), 8% (Red) and 14% (Blue) in the first BZ for modes below the phonon gap.

the phonon gap, we only show these phonon mode group velocities and phonon lifetimes with 0%, 8% and 14% strains in Figure 12 and Figure 13. Due to stiffened ZA dispersion, group velocities of ZA mode increase in low frequency region with increased strain. Near the Γ point, the group velocity of ZA mode increases from 0.94 kms\(^{-1}\) (0%) to 4.30 kms\(^{-1}\) (6%) to 5.15 kms\(^{-1}\) (10%). In high frequency region, most of group velocities of ZA mode increase from 0% to 8% strain, and have little change from 8% to 14% strain. Due to softened phonon dispersions, the reduced phonon group velocities of LA and TA branches are found with strain increasing. The phonon group velocities of ZO branch decrease with increased strain due to reduced W. The reduction of most phonon group velocities have negative contribution to \(\kappa_L\) with increased strain. It is clearly seen that most of phonon lifetimes of SiC monolayer firstly increase, and then decrease. The strain dependence of phonon lifetimes is consistent with that of \(\kappa_L\). The opposite effects on phonon lifetimes caused by the reduce of between \(G\) and \(W/D\) lead to unusual strain dependence of phonon lifetimes. Through considering synthetically strain dependence of phonon group velocities and phonon lifetimes, at low strains (<8%), the phonon lifetimes enhancement is responsible for increased \(\kappa_L\), while at high strains (>8%) the reduction of group velocities and phonon lifetimes results in decreased \(\kappa_L\).

The ratio between cumulative and total lattice thermal conductivity of SiC monolayer with 0%, 4%, 8%, 12% and 14% strains as a function of phonon MFP are shown in Figure 14. With increased MFP, the ratio is close to one for all strains. The critical MFP firstly increases with increased strain, and then decreases, which is identical with \(\kappa_L\). The critical MFP changes from 0.27 \(\mu m\) (unstrained) to 17.87 \(\mu m\) (at 8% strain), then drop to 7.45 \(\mu m\) (at 14% strain). The critical MFP at 8% strain is 66 times larger than unstrain that, demonstrating that strain can produce very strong size effects for \(\kappa_L\) of SiC monolayer. Similar results can also be found in antimonene, AsP monolayer, silicene, germanene and stanene\(^{16,17,36}\).

IV. CONCLUSION

In summary, the first-principles calculations are performed to predict the \(\kappa_L\) of SiC monolayer under strain. The calculated room-temperature \(\kappa_L\) of monolayer SiC is substantially lower than that of graphene. The underlying mechanism for the low \(\kappa_L\) of monolayer SiC can be understood by the mode level phonon group velocities and lifetimes. We further perform analysis from the view of charge density distribution. Significantly different from that in graphene, there is very large charge transfer between Si and C atoms, forming the strongly polarized covalent Si-C bond. The strongly polarized Si-C bond gives rise to the low \(\kappa_L\) of monolayer SiC by inducing large phonon anharmonicity. Within 14% tensile strain, the \(\kappa_L\) of SiC monolayer first increases, and then decreases. The maximum \(\kappa_L\) is at 8% tensile strain, which is about 5.9 times that of the unstrained case. This trend of \(\kappa_L\) with increased strain is mainly
the cumulative lattice thermal conductivity divided by total lattice thermal conductivity with respect to phonon MFP at room temperature. Similar strain-dependent $\kappa_L$ may also be found in GaN and ZnO monolayers with the same perfect planar hexagonal honeycomb structure. Our works will motivate further experimental studies, and studies of phonon transports of other 2D materials with a perfect planar hexagonal honeycomb structure.

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