Modulation of heat transport in two-dimensional group-III chalcogenides

Wenhui Wan, Ziwei Song, Shan Zhao, Yanfeng Ge and Yong Liu

State Key Laboratory of Metastable Materials Science and Technology & Key Laboratory for Microstructural Material Physics of Hebei Province, School of Science, Yanshan University, Qinhuangdao, 066040, People’s Republic of China
E-mail: ycli@ysu.edu.cn and yongliu@ysu.edu.cn

Received 1 November 2019, revised 18 January 2020
Accepted for publication 10 February 2020
Published 27 February 2020

Abstract
We systematically investigated the modulation of heat transport of experimentally accessible two-dimensional (2D) group-III chalcogenides by first-principles calculations. It was found that intrinsic thermal conductivity ($\kappa$) of chalcogenides MX (M = Ga, In; X = S, Se) were desirable for efficient heat dissipation. Meanwhile, we showed that the long-ranged harmonic and anharmonic interactions played an important role in heat transport of the chalcogenides. The difference of $\kappa$ among the 2D group-III chalcogenides can be well described by the Slack model and can be mainly attributed to phonon group velocity. Based on that, we proposed three methods including strain engineering, size effect and making Janus structures to effectively modulate the $\kappa$ of 2D group-III chalcogenides, with different underlying mechanisms. We found that tensile strain and rough boundary scattering could continuously decrease the $\kappa$ while compressive strain could increase the $\kappa$ of 2D group-III chalcogenides. On the other side, the change of $\kappa$ by producing Janus structures is permanent and dependent on the structural details. These results provide guilds to modulate heat transport properties of 2D group-III chalcogenides for devices application.

Supplementary material for this article is available online

Keywords: group-III chalcogenides, thermal transport, strain, Janus structure

(Some figures may appear in colour only in the online journal)

1. Introduction

Two-dimensional (2D) materials with high carrier mobility ($\mu$) have great potential applications in future electronic, optoelectronic and thermoelectric devices [1–3]. These applications are inevitably related to heat management and heat rectification in devices. A high thermal conductivity ($\kappa$) is requested for fast heat dissipation of nanoscale electronic devices [4]. Contrary to that, nanoscale thermoelectric devices with high conversion efficiency require a high $\mu$ and a low $\kappa$ at the same time [5]. Thus, the understanding and modulation of thermal transport properties of 2D materials with high $\mu$ are of technological importance for relevant device performance.

The well-known graphene [6] and 2D MoS$_2$ [7] suffers from the lack of a natural band gap and the low $\mu$, respectively. Phosphorene has a high $\mu$, but its $\mu$ will degrade at atmosphere condition [8]. Group-III chalcogenides including GaS, GaSe and InSe are hexagonal layered semiconductor and consists of quadruple sublayers (see figure 1(b)) which are held together by van der Waals (vdW) interactions [9]. Group-III chalcogenides have attracted great interest recently due to their superior properties, such as direct band gap, small effective mass, rare p-type electronic behaviors, high charge density, good thermoelectric properties and so on. [10, 11]. Recently, 2D InSe were demonstrated to have a high electron $\mu$(> 10$^3$ cm$^2$/V.s) [12, 13] which is comparable with its...
bulk counterpart [14]. On the other side, the bendable photodetectors based on 2D GaS [15], GaSe [16] and InSe [17] have a ultrahigh photoresponsivity, detectivity and a broadband spectral response on flexible and transparent mica substrates, regardless of repeated bending [9]. Moreover, nanodevices base on 2D InSe and GaSe have demonstrated to have good ambient stability [18, 19].

These advantages have intrigued many works on the electrical and optoelectronic properties of 2D group-III chalcogenides [20–25]. It also call for a systematical investigation to phonon transport properties and its modulation of 2D group-III chalcogenides, which is still limited [26, 27]. Besides, though 2D InS with InSe-like structure has been synthesized, its thermal properties have not been investigated [28]. In this work, we studied the heat transport of monolayer group-III chalcogenides by first-principles calculations, coupled with phonon Boltzmann transport equation (BTE). We first calculated the intrinsic thermal conductivity \( \kappa \) of chalcogenides MX (M = Ga, In; X = S, Se) and found their \( \kappa \) can be well described by the Slack model. Meanwhile, we showed the important role of long-ranged anharmonic interaction in the heat transport of group-III chalcogenides. Based on that, taking monolayer InSe as an example, we displayed three effective approaches to modulate \( \kappa \) of 2D group-III chalcogenides including strain engineering, nanstructuring, and producing Janus structure.

2. Methodology

Based on the phonon BTE, lattice thermal conductivity \( \kappa \) is calculates by [29]

\[
\kappa_{\alpha\beta} = \frac{1}{N\Omega} \sum_{q,i} C_{q,i} v_{q,i}^{\alpha} v_{q,i}^{\beta} T_{q,i},
\]

where \( N \) and \( \Omega \) is the number of \( q \) point and volume of the unit cell, respectively. \( \alpha \) and \( \beta \) are Cartesian indices. \( C_{q,i} \), \( v_{q,i}^{\alpha} \) and \( T_{q,i} \) are the mode specific capacity, phonon group velocity and lifetime of the phonon mode with wavevector \( q \) and branch index \( i \), respectively. The scattering mechanism to estimate phonon lifetime \( T_{q,i} \) includes the anharmonic scattering \((1/\tau_{q,i}^{\text{anh}})\), isotope impurities scattering \((1/\tau_{q,i}^{\text{iso}})\) and boundary roughness scattering \(1/\tau_{q,i}^{\text{br}} = |v_{q,i}|/L \) with \( L \) be the sample size. The computational details are given in the supplementary material is available online at stacks.iop.org/JPhysD/50/185102/mmedia.

3. Results and discussion

3.1. The thermal conductivity of monolayer group-III chalcogenides

Figures 1(a) and (b) display the crystal structure of monolayer group-III chalcogenides, which has the D\(_{3h}\) crystal symmetry. The optimized lattice constants, bond lengths (labeled in figure 1(b)) and thickness of monolayer are listed in table S1 in the supplementary material. 2D group-III chalcogenides are semiconductors [10] and the heat is mainly carried by lattice vibrations. The phonon dispersion of monolayer InS and other materials are displayed in figures 1(c) and S1 to display its lattice stability. The acoustic branches (see red line in figure 1(c)) consist of the in-plane longitudinal (LA) branch, transverse (TA) branch and out-of-plane flexural branch (ZA) branch.

We found that long-ranged harmonic and anharmonic interatomic force constants (2nd and 3rd IFCs) are common features in monolayer group-III chalcogenides. It can be directly reflected by the response of charge density to perturbations of the atomic displacements. Taking InSe as an example, we induced a small distortion (~0.02 Å) to the central Se atoms along the zigzag or armchair direction. As a result, the disturbance of the absolute charge density \(|\Delta\rho|\) is particularly extended along the zigzag direction, as shown in figure 2(a). A clear \(|\Delta\rho|\) at the zone with distance from origin Se atoms less than of 8.19 Å which corresponds to 11th nearest neighbors (NN). Furthermore, the non-negligible \(|\Delta\rho|\) can take place as long as 10 Å (16th NN), as shown in figure 2(a). Similar to our previous work [30], for the 2nd and 3rd IFCs of monolayer group-III chalcogenides, we extracted the normalized trace of 2nd IFCs tensor \(|Tr(2ndIFCs)|\) (see the supplemental material), the maximum component of 3rd IFCs \((\Phi_{ij,k}\text{max})\) and the maximum interatomic distance \(d_{\text{max}}\) between three atoms \((i, j, k)\) [31]. The distribution of the interatomic distance dependence of \(|Tr(2ndIFCs)|\) was shown in figure S2. The non-negligible 2nd IFCs can exist at a distance as long as 10 Å. The distribution of \((\Phi_{ij,k}\text{max})\) with respect to \(d_{\text{max}}\) was shown in figure S3. We identified that the triplets \((\Phi_{ij,k}\text{max})\) are particularly large at the 2nd and 11th NN for all the group-III chalcogenides. Meanwhile, the populations of the 3rd IFCs as the function of \(d_{\text{max}}\) are shown in the inset of figure S3. We found that though the triplets...
the calculation of anharmonic relaxation time $\tau$ where $B$ is a numerical coefficient; factors that affect heat transport of chalcogenides, we adopted acoustic phonons (see figure S5), to understand the physical is about $20\ \text{W/(m}^2\text{K)}$. Temperatures (T), as shown in figure 2.

Figure 2. (a) The absolute change of charge density $|\Delta \rho|$ (in unit of $10^{-5}\ \text{e/Å}^3$) due to the small displacement (0.02 Å) of the central Se atom along the zigzag direction. The red arrow and circle represents the distance of the 11th- and 16th-nearest neighbors with respect to the central Se atoms, respectively. (b) Lattice thermal conductivity of monolayer group-III chalcogenides at 300 K as a function of the $d_{max}$ which is in unit of nearest neighbors (NN).

$(\Phi_{\alpha\beta\gamma}^{i,j,k})_{\alpha\beta\gamma}$ at 14th NN are small, it has a particularly large population. The distribution of 3rd IFCs is consistent with the aforementioned distribution of $|\Delta \rho|$. The convergence test of the $\kappa$ of monolayer group-III chalcogenides shows that $\kappa$ happens a clear change (see figure 2(b)) when we include the 3rd IFCs within the $d_{max}$ of 11th neighbors and 14th neighbors in the calculation of anharmonic relaxation time $\tau_{q_{\alpha\beta\gamma}}$. That can be understood from the aforementioned large size and large population of 3rd IFCs at these distances. The $\kappa$ can reach convergence at $d_{max}$ of 16th NN (see figure 2(b)), consistent with previous perturbation of charge density due to the atomic displacements.

The intrinsic $\kappa$ of monolayer group-III chalcogenides without boundary scattering are calculated at different temperatures (T), as shown in figure 1(d). It corresponds $1/\kappa_{q_{\alpha\beta\gamma}} = 1/a_{q_{\alpha\beta\gamma}} + 1/b_{q_{\alpha\beta\gamma}}$ according to the Matthiessen rule. The overall $\kappa$ is in the decreasing order of GaS, GaSe, InS and InSe. At T = 300 K, the $\kappa$ of monolayer GaS, GaSe, InS and InSe is estimated to be 111.0, 83.10, 58.9 and 44.9 W/(m·K), which is compatible with the previous work [27]. The $\kappa$ of monolayer group-III chalcogenides are comparable with that of conventional bulk Ge (65 W/(m·K) [32]) and GaAs (45 W/(m·K) [32]), and larger than $\kappa$ of phosphorene which is about 20 W/(m·K) along zigzag direction [33, 34]. Therefore, the intrinsic $\kappa$ of 2D group-III chalcogenides are desirable for efficient heat dissipation.

As the $\kappa$ of 2D group-III chalcogenides are dominated by acoustic phonons (see figure S5), to understand the physical factors that affect heat transport of chalcogenides, we adopted the Slack model which gives $\kappa$ as [35],

$$\kappa = B \cdot \frac{\bar{m} \theta_D^3 n \delta}{\gamma^2 T}, \tag{2}$$

where $B$ is a numerical coefficient; $\bar{m}$ is the average atomic mass; $n$ is the number of atoms in the unit cell; $\delta$ gives the volume per atom; $\theta_D$ and $\gamma$ is the acoustic Debye temperature and Grüneisen parameter, respectively. The simulation details are given in the supplementary material. The results are shown in table 1.

As shown in table 1, the acoustic Debye temperature $\theta_D$ increases from monolayer InSe to GaS. A larger acoustic $\theta_D$ reflects a larger bandwidth of acoustic branches and more dispersive acoustic phonon bands (see figure S1), which should lead to larger acoustic phonon group velocities $v_{q_{\alpha\beta\gamma}}$. Actually, the overall order of calculated $v_{q_{\alpha\beta\gamma}}$ of acoustic phonons from high to low is in the sequence of GaS, GaSe, InS and InSe (see figure S4(a)), which agrees with the order of $\theta_D$.

The behavior of $\theta_D$ can be qualitatively understood by another simple diatomic chain model which contains two types of atoms per unit cell [36]. In this model, the mass of heavy atom and bonding stiffness have a negative and positive effect on the acoustic $v_{q_{\alpha\beta\gamma}}$ and $\theta_D$, respectively. In 2D group-III chalcogenides, the bonding stiffness can be described by 2D elastic module $C_{2D}$ [37]. From GaS to InSe, the mass of the heavy atom and $C_{2D}$ are in the increasing and decreasing order, respectively (see table 1), which lead to the aforementioned order of acoustic $\theta_D$ and $v_{q_{\alpha\beta\gamma}}$.

The Grüneisen parameter $\gamma$, however, is in the increasing sequence of InS, InSe, GaSe and GaS, which is almost opposite to order of $\theta_D$. Substituting these results into equation (2), the ratio of room-temperature $\kappa$ of monolayer GaS, GaSe, InS and InSe is 1.98:1.64:1.32:1, consistent with that obtained by phonon BTE which is 2.47:1.85:1.31:1. The deviation arises from the neglecting the contribution of low-frequency optical branches (labeled by blue in figure 1(c)) to $\kappa$ in the Slack model whereas those phonon modes make a non-negligible contribution to $\kappa$ of chalcogenides (see figure S5). Thus, the $\theta_D$ in equation (2) ultimately overtake the $\gamma^2$ and other factors, dominating the overall behaviour of $\kappa$ of 2D group-III chalcogenides.

From the other side, we also performed a detailed analysis of mode contribution $\kappa_{q_{\alpha\beta\gamma}}$ to total $\kappa$. The $\kappa_{q_{\alpha\beta\gamma}}$ is given by $\kappa_{q_{\alpha\beta\gamma}} = C_{q_{\alpha\beta\gamma}} v_{q_{\alpha\beta\gamma}}^2 \tau_{q_{\alpha\beta\gamma}}$, where $C_{q_{\alpha\beta\gamma}}$, $v_{q_{\alpha\beta\gamma}}$ and $\tau_{q_{\alpha\beta\gamma}}$ are specific heat per unit volume, group velocities and lifetimes of phonon mode with momentum $q$ and branch index $\alpha\beta\gamma$, respectively. $\tau_{q_{\alpha\beta\gamma}}$ is determined by both the Grüneisen parameter $\gamma_{q_{\alpha\beta\gamma}}$ and phase space for phonon anharmonic scattering $(P_{\gamma_{q_{\alpha\beta\gamma}}})$ [38]. In the low-frequency zone, however, there is a competition between $\gamma_{q_{\alpha\beta\gamma}}$ and $(P_{\gamma_{q_{\alpha\beta\gamma}}})$. This makes the $\tau_{q_{\alpha\beta\gamma}}$ of low-frequency phonons in different chalcogenides have almost the same order of magnitude (see figures S4(b)–(d)). Meanwhile, $C_{q_{\alpha\beta\gamma}}$ approaches the classic value $k_B$ at a temperature higher than $\theta_D$. Thus, the difference of $\kappa$ among chalcogenides is mainly determined by phonon group velocity, which is consistent with previous analysis by the Slack model.

| $\text{Compound}$ | $C_{2D}$ (Jm$^{-2}$) | $\theta_D$ (K) | $\gamma$ |
|-------------------|---------------------|----------------|--------|
| GaS | 50.90 | 81.32 | 136.5 | 0.63 |
| GaSe | 74.34 | 69.46 | 105.9 | 0.58 |
| InS | 73.45 | 56.50 | 90.1 | 0.45 |
| InSe | 96.89 | 49.21 | 76.3 | 0.51 |

Table 1. The average atomic mass $\bar{m}$ in atomic mass unit (amu), 2D effective elastic module $C_{2D}$ (Jm$^{-2}$), Debye temperature $\theta_D$ (K) and Grüneisen parameter $\gamma$ of monolayer group-III chalcogenides.
Figure 3. (a) The phonon dispersion of monolayer InSe at tensile of $\varepsilon = 0\%$ and 4\% tensile strain. (b) Strain dependence of normalized $\kappa$ and Grüneisen parameter $\gamma$ with respect to that of strain-free monolayer InSe according to Slack model. The ref pentagram represents the $\kappa$ gotten through the phonon BTE equation.

3.2. The methods to modulate the lattice conductivity

Thermal engineering of 2D material is significant to improve the transport properties and expand its application perspective. Considering group-III chalcogenides share common features in structural symmetry, IFCs and thermal transport model, in the following, we only considered feasible methods to modulate the $\kappa$ of 2D InSe, the conclusion will be universal in other group-III chalcogenides.

3.2.1. Strain engineering. Experimentally, strain engineering can be utilized to manipulate the heat transport of 2D materials [39]. We defined the strain as $\varepsilon = (a_i - a_0)/a_0 \times 100\%$, where $a_i$ and $a_0$ is the lattice constants of monolayer InSe with and without strain, respectively. When applying tensile strain, both $d_{ac}$ and $d_{wa}$ are enlarged and the bonding are weakened. The phonon dispersion curves downshift except the Slack mode [40] rather than IFCs calculations. For strain-free monolayer InSe, it gives $\gamma = 0.53$ which agrees with $\gamma = 0.50$ obtained by calculation of 2nd and 3rd IFCs. The frequency of phonon and force constants are known to have a negative and positive correlation with $\gamma$ [41], leading to complex behavior of $\gamma$ with respect to strain $\varepsilon$. In monolayer InSe, we found that $\gamma$ increases as tensile $\varepsilon$ increase (see figure 3(b)). Thus, the decrease of $\theta_D$ and increase of $\gamma$ lead to the decrease of $\kappa$ of monolayer InSe under tensile strain according to Slack model [35]. That is similar to many bulk materials [42] and other 2D materials such as MoS$_2$ [43]. On the other side, the compressive strain will decrease the $\kappa$ of 2D InSe. We have also calculated the $\kappa$ of monolayer InSe under tensile strain of $\varepsilon = 2.0\%$ and $\varepsilon = 4.0\%$ through more exact phonon BTE equation (see figure 3(b)). It was found that $\kappa$ was reduced by 11\% and 18\% with respect to $\kappa$ at strain-free case, which is consistent with the estimation by Slack model.

3.2.2. Size effects. Considering the limited sample size (L), the size effects is another method to modulate $\kappa$. Here we consider the boundary scattering in the range of diffusive thermal transport, which corresponds $1/\tau_{\text{q}a} = 1/\tau_{\text{a}\text{a}} + 1/\tau_{\text{q}\text{a}} + 1/\tau_{\text{b}a}$. The result of monolayer group-III chalcogenides are displayed in figure S6. At room temperature, the phonon mean free path (MFP) of monolayer group-III chalcogenides is about $10^4$ nm, which is mainly determined by the MFP of ZA and LA phonons. The $\kappa$ can be decreased by 90\% as the L decrease down to 10 nm (see figure S6), indicating that nanostructuring might be an effective method to reduce the $\kappa$ of 2D group-III chalcogenide, consistent to previous work [26].

3.2.3. Janus structures. Recently, a new Janus-type structure, monolayer MoSSe, has been synthesized through the replacement of the S atoms at one side of monolayer MoS$_2$ by Se atoms or Se atoms of monolayer MoSe$_2$ by S atoms [44]. The $\kappa$ of monolayer MoSSe is between that of monolayer MoS$_2$ and MoSe$_2$ [45]. Motivated by that, the effort has been denoted into the electronic [46], piezoelectric [47] and valleytronics [48] properties of Janus structures based on 2D group-III chalcogenide. In a previous work, we have shown that monolayer InS$_2$Se has a higher $\kappa$ but a lower $\mu$ than monolayer InSe [30]. On the other side, monolayer InSeTe has a higher $\mu$ but a lower $\kappa$ than InSe. Here, we considered another 2D Janus structure InGaSe$_2$. The cohesive energy of monolayer InGaSe$_2$ is -3.43 eV/atom, larger than InSe (-3.34 eV/atom) and smaller than GaSe (-3.58 eV/atom). Meanwhile, Indium atoms of monolayer InSe are also on the surface, so Janus InGaSe$_2$ may could be formed by replacing the In atoms of one side of InSe by Ga atoms. The phonon dispersion ensures its structural stability (see figure S1(e)).

Compared to the continuously modulation of $\kappa$ by tensile strain and rough boundary scattering, the change of due to Janus structures can keep permanent but depends on the structures details. The phonon group velocity $v_{\text{q},a}$ of monolayer GaInSe$_2$ is larger than InSe, due to smaller atomic mass (see figure 4(a)). GaInSe$_2$ occurs a breaking of mirror symmetry compared to InSe. This will lead to asymmetric chemical bonding and charge density distribution along the z-direction, which will increase bond anharmonicity [49, 50]. Figures 4(c,d) show the square of mode Grüneisen parameter $\gamma_{\text{q},a}^2$ and weighted phase space $W_{\text{q},a}$, which represents the anharmonicity strength and the number of channels available for phonon scattering, respectively [29, 51]. Both $\gamma_{\text{q},a}^2$ and $W_{\text{q},a}$ of monolayer GaInSe$_2$ is larger than InSe, lead to stronger phonon scattering and smaller $\tau_{\text{q},a}$ of phonon modes than that of monolayer InSe at energy zone $\omega > 25$ cm$^{-1}$. As a result, GaInSe$_2$ has overall higher $\gamma_{\text{q},a}$ and lower $\tau_{\text{q},a}$ than InSe. The competition between $v_{\text{q},a}$ and $\tau_{\text{q},a}$ leads to that monolayer GaInSe$_2$ has a $\kappa$ comparable to that of monolayer InSe (see figure 1(d)).

On the other side, the electron mobility $\mu$ of monolayer GaInSe$_2$ was calculated based on the deformation potential theory [52]. The calculation procedure has been explained in previous work [30]. The calculated parameters involved in
InSe and GaInSe

E

ation potential

GaInSe with small

At a tensile strain of 3.4%, the

mainly composed of 5s orbital of Ga atom as well as Se-

orbital analysis indicates that In-5

layer GaInSe (see table. S1). The electron effective mass

m

ac

lus

C

µ

are shown in table 2. The 2D effectively elastic modulus

C_{2D} (J/m^2), deformation potential constant E_i

(eV) and room-temperature µ (cm^2/Vs) of monolayer

InSe and GaInSe.

Table 2. The electron effective mass m^* (1/m_0) along x and y axis, 2D elastic module C_{2D} (J/m^2), deformation potential constant E_i (eV) and room-temperature µ (cm^2/Vs) of monolayer InSe and GaInSe.

| Type          | m^*_x/m_0 | m^*_y/m_0 | C_{2D}  | |E_i| | µ_x |
|---------------|-----------|-----------|---------|---|---|-----|
| InSe          | 0.181     | 0.182     | 49.21   | 5.815 | 943.3 | |
| GaInSe        | 0.160     | 0.160     | 56.76   | 6.537 | 1107.4 | |

μ are shown in table 2. The 2D effectively elastic modulus C_{2D} of monolayer GaInSe is larger than that of monolayer InSe. That is consistent with that shorter bonding length d_{se} and d_{cx} of monolayer GaInSe than monolayer InSe (see table. S1). The electron effective mass m^* of monolayer GaInSe is smaller than that of monolayer InSe. The orbital analysis indicates that In-5s orbitals dominate the electronic states at conduction band minimum (CBM) of monolayer InSe. In contrast, the CBM of monolayer GaInSe is mainly composed of 5s orbital of Ga atom as well as Se-p_z orbital (see figure 5(a)), due to electric potential difference arising from the charge transferring from In atoms to Ga atoms. The Ga side of monolayer GaInSe experiences a tensile strain about 3.4% compared to that of monolayer GaSe, seen from the lattice constant in table S1. The m^* of GaSe will decrease as the increase of tensile strain (see figure 5(b)). At a tensile strain of 3.4%, the m^* is 0.144 m_0, consistent with small m^* of GaInSe (see table 2). Thus, monolayer GaInSe has a smaller m^*, a larger C_{2D} and a larger deformation potential E_i, leading to a higher μ than that of InSe. Meanwhile, considering its κ is comparable to monolayer InSe, Janus monolayer GaInSe is superior to monolayer InSe, monolayer InSe and monolayer InSeTe in the electronic applications.

4. Conclusion

Based on the first-principles calculations, we investigated the modulation of lattice thermal conductivity of monolayer group-III chalcogenides. The room-temperature thermal conductivity of monolayer GaS, InS, GaSe and InSe is 111.0, 83.10, 58.9 and 44.9 W/(mK), respectively, which is desirable for heat dissipation of relevant devices. The heat transport of group-III chalcogenides can be well described by Slack mode and are dominated by phonon group velocity. Both acoustic branches and low-frequency optical branches have contribution to thermal transport of group-III chalcogenides. Based on that, we proposed three feasible methods to modulate the κ. We found that the κ of 2D group-III chalcogenides could be continuously decreased by tensile strain and rough boundary scattering but be increased by compressive strain. The change of κ due to Janus structures is permanent which depends on the structures details. Taking 2D InSe as an example, among the various Janus structure we found that the Janus monolayer GaInSe could keep a comparable κ and a higher electron mobility than that of monolayer InSe. Our work helps to understand of the thermal transport of 2D group-III chalcogenides and provides a guide for the thermal management in the devices based on these materials.

Acknowledgments

This work was supported by National Natural Science Foundation of China (Nos. 11904312 and 11904313), the Project of Hebei Educational Department, China (Nos. ZD2018015 and QN2018012), the Advanced Postdoctoral Programs of Hebei Province (No.B2017003004) and the Natural Science Foundation of Hebei Province (No. A2019203507). The numerical calculations in this paper have been done on the supercomputing system in the High Performance Computing Center of Yanshan University.

ORCID iDs

Wenhui Wan https://orcid.org/0000-0002-6824-0495
Yong Liu https://orcid.org/0000-0002-5435-9217
References

[1] Liao L et al 2010 High-speed graphene transistors with a self-aligned nanowire gate Nature 467 305–8
[2] Liu H Neal A T Zhu Z Luo Z Xu X Tománek D and Ye P D 2014 Phosphorene: an unexplored 2D semiconductor with a high hole mobility ACS Nano 8 4033–41
[3] Zhang X, Zhao X, Wu D, Jing Y, and Zhou Z 2015 High and anisotropic carrier mobility in experimentally possible Ti$_2$CO$_3$ (MXene) monolayers and nanoribbons Nanoscale 7 16020–5
[4] Zou J and Balandin A 2001 Phonon heat conduction in a semiconductor nanowire J. Appl. Phys. 89 2932–8
[5] Hochbaum A I, Chen R, Delgado R D, Liang W, Garnett E C, Najarian M, Majumdar A, and Yang P 2008 Enhanced thermoelectric performance of rough silicon nanowires Nature 451 163–7
[6] Geim A K 2009 Graphene: status and prospects Science 324 1530–4
[7] Baugher B W, Churchill H O, Yang Y, and Jarillo-Herrero P 2013 Intrinsic electronic transport properties of high-quality monolayer and bilayer MoS$_2$ Nano Lett. 13 4212–16
[8] Wang G, Slough W J, Pandey R, and Karnan S P 2016 Degradation of phosphorene in air: understanding at atomic level 2D Materials 3 025011
[9] Huang W, Gan L, Li H, Ma Y, and Zhai T 2016 2D layered Bhowmick S and Shenoy V B 2006 Effect of strain on Dey P, Paul J, Glikin N, Kovalyuk Z, Kudrynskyi Z, 6 Cao T, Li Z, and Louie S G 2015 Tunable magnetism and Zhao Q 092107 Fabian J and Allen P B 1997 Thermal expansion and 7991–8 26 114513 335702 Wan W, Zhao S, Yanfeng G, and Liu Y 2019 Phonon and 305–8 3815–19 Yang S, Li Y, Wang X, Huo N, Xia J-B, Li S-S, and Li J 2017 Engineering the electronic 1885–8 223–7 Xu K, Yin L, Huang Y, Shifa T A, Chu J, Wang F, Cheng R, 29 5708–17 Jin H, Li J, Dai Y, and Wei Y 2017 Engineering the electronic and optoelectronic properties of InX (X = S, Se, Te) monolayers via strain Phys. Chem. Chem. Phys. 19 4855–60 15 Debibichi L, Eriksson O, and Lebegue S 2015 Two-dimensional indium selenides compounds: An ab initio study J. Phys. Chem. Lett. 6 3086–103 21 Nissimoguador A S, Ma J, Chen Y, and Li W 2017 Thermal transport in monolayer InSe J. Phys.: Condens. Matter 29 335702 Pandey T, Parker D S, and Lindsay L 2017 Ab initio phonon transport in monolayer InSe, GaSe, GaS, and alloys Nanotechnology 28 455706 Hollingsworth J A, Poojary D M, Clearfield A, and Bultro W E 2000 Catalyzed growth of a metastable InS crystal structure as colloidal crystals J. Am. Chem. Soc. 122 3562–3 Wu Li, Carrete Jús, Katcho N A, and Mingo N 2014 ShengBTE: A solver of the boltzmann transport equation for phonons Comput. Phys. Commun. 185 1747–58 Wang W, Zhao S, Yanfeng G, and Liu Y 2019 Phonon and electron transport in janus monolayers based on InSe J. Phys.: Condens. Matter 31 435501 Li C W, Hong J, May A F, Bansal D, Chi S, Hong T, Ehlers G, and Delaire O 2015 Orbitally driven giant phonon anharmonicity in SnSe Nat. Phys. 11 1063–9 Morelli D T and Slack G A 2006 High Thermal Conductivity Materials (New York: Springer) Luo Z, Maassen J, Deng Y, Du Y, Garrelts R P, Lundstrom M S, Ye Peide D, and Xu X 2015 Anisotropic in-plane thermal conductivity observed in few-layer black phosphorus Nat. Commun. 6 8572 Qin G, Zhang X, Yue S-Y, Qin Z, Wang H, Han Y, and Ming H 2016 Resonant bonding driven giant phonon anharmonicity and low thermal conductivity of phosphorene Phys. Rev. B 94 165445 Slack G 1973 Nonmetallic crystals with high thermal conductivity J. Phys. Chem. Solids 34 321–35 Ziman J M 1960 Electrons and Phonons: Theory of Transport Phenomena in Solids (International Series of Monographs on Physics) (Oxford: Clarendon) Sun C, Xiang H, Xu B, Xia Y, Yin J, and Liu Z 2016 Ab initio study of carrier mobility of few-layer InSe Appl. Phys. Express 9 035203 Lindsay L and Brodico D 2008 Three-phonon phase space and lattice thermal conductivity in semiconductors J. Phys.: Condens. Matter 20 165209 Meng X et al 2019 Thermal conductivity enhancement in MoS$_2$ under extreme strain. Phys. Rev. Lett. 122 155901 Togo A and Tanaka I 2015 First principles phonon calculations in materials science Scr. Mater. 108 1–5 Fabian J and Allen P B 1997 Thermal expansion and grüneisen parameters of amorphous silicon: A realistic model calculation Phys. Rev. Lett. 79 1885–8 Bhowmick S and Stenoy V B 2006 Effect of strain on the thermal conductivity of solids J. Chem. Phys. 125 164513 Zhu L, Zhang T, Sun Z, Li J, Chen G, and Yang S A 2015 Thermal conductivity of biaxial-strained MoS$_2$: sensitive strain dependence and size-dependent reduction rate Nanotechnology 26 465707
[44] Li R, Cheng Y, and Huang W 2018 Recent progress of Janus 2D transition metal chalcogenides: From theory to experiments Small 14 1802091
[45] Guo S-D 2018 Phonon transport in Janus monolayer mosse: a first-principles study Phys. Chem. Chem. Phys. 20 7236–42
[46] Kandemir A and Sahin H 2018 Janus single layers of In2SSe: A first-principles study Phys. Rev. B 97 155410
[47] Guo Y, Zhou S, Bai Y, and Zhao J 2017 Enhanced piezoelectric effect in Janus group-III chalcogenide monolayers Appl. Phys. Lett. 110 163102
[48] Peng R, Yandong M, Zhang S, Huang B, and Dai Y 2018 Valley polarization in Janus single-layer MoSSe via magnetic doping J. Phys. Chem. Lett. 9 3612–17
[49] Zhang A-X, Liu J-T, Guo S-D, and Li H-C 2017 Strain effects on phonon transport in antimonene investigated using a first-principles study Phys. Chem. Chem. Phys. 19 14520–6
[50] Wu X, Varshney V, Lee J, Zhang T, Wohlwend J L, Roy A K, and Luo T 2016 Hydrogenation of penta-graphene leads to unexpected large improvement in thermal conductivity Nano Lett. 16 3925–35
[51] Li W and Mingo N 2015 Ultralow lattice thermal conductivity of the fully filled skutterudite YbFe4Sb12 due to the flat avoided-crossing filler modes Phys. Rev. B 91 144304
[52] Bardeen J and Shockley W 1950 Deformation potentials and mobilities in non-polar crystals Phys. Rev. 80 72–80