A comparative study of the thermoelectric performance of graphene-like BX (X = P, As, Sb) monolayers

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Abstract

The electronic and phonon transport properties of graphene-like boron phosphide (BP), boron arsenide (BAs), and boron antimonide (BSb) monolayers are investigated using first-principles calculations combined with the Boltzmann theory. By considering both the phonon–phonon and electron–phonon scatterings, we demonstrate that the strong bond anharmonicity in the BAs and BSb monolayers can dramatically suppress the phonon relaxation time but hardly affect that of electron. As a consequence, both systems exhibit comparable power factors with that of the BP monolayer but much lower lattice thermal conductivities. Accordingly, a maximum ZT value above 3.0 can be realized in both BAs and BSb monolayers at optimized carrier concentration. Interestingly, very similar p- and n-type thermoelectric performance is observed in the BSb monolayer along the zigzag direction, which is of vital importance in the fabrication of thermoelectric modules with comparable efficiencies.

Keywords: thermoelectric performance, first-principles, Boltzmann theory, electron-phonon coupling

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1. Introduction

Thermoelectric materials, which can harvest waste heat and directly convert it into electricity, have attracted much attention since most of the energy produced from fossil fuels is lost as waste heat [1, 2]. Materials designed for thermoelectric applications should have suitable band gap, high carrier mobility, and low thermal conductivity. However, the complex intercorrelation among these properties makes it rather difficult to enhance the conversion efficiency. So far, various strategies have been adopted to optimize the thermoelectric performance including band engineering [3], hierarchical architecturing [4], and seeking new potential materials such as Li2TlBi [5] and TaFeSb-based compounds [6]. In particular, Hicks and Dresselhaus [7, 8] theoretically suggested that low-dimensional structures may achieve high thermoelectric performance compared with their bulk counterparts. Experimentally, Venkatasubramanian et al [9] prepared the Bi2Te3/Sb2Te3 superlattice thin film, which exhibits large p-type figure-of-merit (ZT value) of 2.4 at 300 K. These pioneering works have attracted great interest in the thermoelectric performance of low-dimensional and nanostructured systems [10–18].

As the best-known low-dimensional materials, the graphene [19–21] is however not suitable for thermoelectric applications due to the gapless energy band. To open a gap in the graphene, several methods such as hydrogenation [22] and fluorination [23] have been suggested. On the other hand, Sahin et al [24] theoretically predicted that the graphene-like III–V binary compounds exhibit intrinsic band gaps. Subsequently, the successful isolation of hexagonal boron nitride (h-BN) [25] has attracted much interest. For example,
Dean et al. [26] found that the h-BN is an appealing substrate dielectric for application in graphene-based devices. Owing to the exceptional thermal and chemical stabilities, the ultrathin h-BN films can serve as excellent oxidation-resistant coatings even at high temperature [27]. Besides, Kong et al. [28] showed the potential applications of h-BN as barrier materials in vertical heterostructures. However, further utilization as thermoelectric materials is hindered by the large band gap of h-BN [24], which could hardly exhibit electron transport even after adsorbing metal ions [29]. On the other hand, it is found that the boron phosphide (BP), boron arsenide (BAs), and boron antimonide (BSb) monolayers all exhibit direct band gaps of about 1.0 eV [24], which are very desirable as thermoelectric materials. In fact, previous first-principles calculations on the hexagonal BP monolayer found that it simultaneously possesses a moderate band gap and low effective mass [30, 31]. Nevertheless, investigations on the transport properties of these graphene-like III–V binary systems are less known, and a complete understanding is thus quite necessary.

In this work, we give a comparative study of the phonon, electronic and thermo-electric transport properties of the hexagonal BP, BAs and BSb monolayers. Compared with that of the BP, we find that the strong bond anharmonicity in both the BAs and BSb systems lead to obviously lower lattice thermal conductivities and thus much higher thermoelectric figure-of-merit (ZT > 3.0). Equally importantly, almost identical p- and n-type ZT of ~2.5 can be realized in the BSb monolayer, which is quite desirable in the manufacture of advanced thermoelectric devices.

2. Computational methods

For the phonon transport, the interatomic force constants (IFCs) of the BX (X = P, As, Sb) monolayer are obtained by density functional theory (DFT) and the finite displacement method, as coded in the Vienna *ab initio* simulation package (VASP) [32] and the PHONOPY program [33], respectively. A 5 × 5 × 1 supercell with Γ point is employed to calculate the second- and third-order IFCs. The eighth nearest neighbors are considered for the anharmonic IFC calculations, which correspond to a cutoff distance of 5.2 Å, 5.8 Å, and 6.5 Å for the BP, BAs, and BSb systems, respectively. The lattice thermal conductivity (κl) is computed by solving the phonon Boltzmann transport equation, as implemented in the so-called ShengBTE package [34]. A fine 100 × 100 × 1 q-mesh combined with the scalebroad of 0.1 for Gaussian smearing is adopted to ensure the convergence.

The band structures of the BX monolayers are calculated within the framework of DFT, which is implemented in the QUANTUM ESPRESSO package [35] with the core-valence interaction described by the norm-conserving scalar-relativistic pseudopotentials [36]. The hybrid density functional in the form of Heyd–Scuseria–Ernzerhof (HSE) [37] is adopted to obtain accurate results, which has been successfully used to predict the band gap of the graphene-like BN monolayer [38]. The electronic transport coefficients, including the Seebeck coefficient (S), the electrical conductivity (σ), and the electronic thermal conductivity (κe), can be derived from the Boltzmann transport theory [39]. By fully considering the electron–phonon coupling (EPC), the k-dependent carrier relaxation time (τc) is calculated using the density functional perturbation theory (DFPT) [40] and the Wannier interpolation techniques [41], which is coded in the electron–phonon Wannier (EPW) package [42]. To obtain converged results, the EPC calculations have been performed by using coarse grids of 20 × 20 × 1 k-points with 10 × 10 × 1 q-points, and then interpolated to dense meshes of 200 × 200 × 1 k-points with 100 × 100 × 1 q-points. The vacuum distance of 30 Å is adopted to simulate the monolayer structure, and all the calculated transport coefficients are renormalized with respect to the interlayer distance of graphite (3.35 Å).

3. Results and discussion

Single-layer BX is sp2 bonded with the B and X atoms arranged in a hexagonal honeycomb lattice (see figure S1 of the supplementary material (available online at stacks.iop.org/JPhysCM/31/385701/mmedia)). Similar to that of graphene, the primitive cell of BX monolayer contains two atoms, and each B atom is three-fold coordinated to the neighboring X atoms. The calculated B–X bond lengths of BP, BAs, and BSb monolayers are 1.86 Å, 1.96 Å, and 2.16 Å, respectively, which are in good agreement with previous theoretical results [43]. Figures 1(a)–(c) show the phonon dispersion relations of the BX monolayers calculated by DFPT (the computation details is given in section 2 of the supplementary material), where there is no imaginary frequency guaranteeing the dynamic stability of these systems. Besides, the in-plane Young’s modulus (141.9 N m⁻¹, 121.5 N m⁻¹, and 90.8 N m⁻¹ for the BP, BAs, and BSb, respectively) are comparable with that of the MoS2 monolayer [44] and obviously larger than that of the phosphorene [45], indicating the mechanical stability of these systems. Moreover, we see from figure 1(d) that the B–X distance varies slightly around the equilibrium bond length during the *ab initio* molecular dynamics (AIMD) simulation at 1400 K, suggesting the high temperature stability of the BX series. Similar to those found in graphene [46] and hexagonal BN [47], we see that all the optical branches of BX monolayers exhibit very weak dispersions, which suggests that their lattice thermal conductivities should be mainly contributed by the acoustic phonons. With increasing atomic mass of the X elements, we find that the maximum phonon frequency becomes smaller, indicating the gradually lower lattice thermal conductivity [48].

Figures 2(a)–(c) plot the lattice thermal conductivities of BP, BAs, and BSb monolayers as a function of temperature, respectively. For each system, we see that the lattice thermal conductivity along the armchair direction is slightly lower than that along the zigzag direction. At room temperature, the κl of BP, BAs, and BSb monolayers are 240 (312) W m⁻¹ K⁻¹, 27.6 (36.3) W m⁻¹ K⁻¹, and 18.7 (26.3) W m⁻¹ K⁻¹ along the armchair (zigzag) direction, respectively. To further confirm the reliability of the results, we have done additional calculations of the lattice thermal conductivity of graphene using
Figure 1. The phonon dispersion relations of (a) BP, (b) BAs, and (c) BSb monolayers. (d) gives the AIMD calculated B–P, B–As, and B–Sb distances at 1400K, where the yellow dashed lines indicate the corresponding equilibrium bond length.

Figure 2. The temperature dependent lattice thermal conductivities of (a) BP, (b) BAs, and (c) BSb monolayers. (d) shows the room temperature phonon relaxation times of them.
Table 1. Comparison of acoustic phonon group velocities (at 300 K) of BX monolayers.

|     | ZA (km s$^{-1}$) | TA (km s$^{-1}$) | LA (km s$^{-1}$) |
|-----|-----------------|-----------------|-----------------|
| BP  | 3.2             | 7.9             | 13.9            |
| BAs | 1.6             | 6.2             | 10.1            |
| BSb | 1.4             | 4.1             | 7.5             |

the same method and calculation parameters, and the result of 5660 W m$^{-1}$ K$^{-1}$ agrees well with that reported previously [49]. By comparison, it is clear that $\kappa_l$ decreases by one order of magnitude from BP to BAs and BSb monolayers. To have a deep understanding, we compare the acoustic phonon group velocities ($v_{ph}$) of these BX monolayers at 300 K. As listed in table 1, the $v_{ph}$ of each acoustic phonon mode in the BAs and BSb monolayers are obviously smaller than that in the BP system rooted from the larger lengths of the B–As and B–Sb bonds [5]. Such an observation suggests much lower lattice thermal conductivities in the BAs and BSb monolayers owing to the relation of $\kappa_l \propto v_{ph}^4$. The decreasing phonon group velocities from the BP, BAs to BSb are consistent with their reducing highest acoustic phonon frequencies (see figures 1(a)–(c)) [48]. Note that several previous works suggested that the ZA modes contribute most to the lattice thermal conductivity of graphene-like structures due to the selection rules [50–52]. Here we find that the group velocities of ZA modes for BAs and BSb monolayers are close to those of the good thermoelectric materials with intrinsic low $\kappa_l$, such as Bi$_2$Te$_3$ [53] and PbTe [54]. Moreover, we see from figure 2(d) that the phonon relaxation time ($\tau_{ph}$) of the acoustic modes in the BP monolayer are dramatically larger than those of the BAs and BSb systems, which can be attributed to the weaker anharmonicity of the B–P bond [55]. Indeed, compared with that of the BP monolayer (1.36), the absolute values of the Grüneisen parameters ($\gamma$) for the BAs (2.94) and BSb (2.75) systems are much higher caused by bigger mass difference of the B and X atoms [56]. Such an observation can be also found in the group-VA monolayer where the phosphorene exhibits a much larger lattice thermal conductivity than those of the PAs and PSb monolayers [57]. Note that such higher $\gamma$ values are comparable to those of bulk SnSe [58] and Bi$_2$Te$_3$ [56]. It should be mentioned that although the $\gamma$ of the BAs monolayer is relatively higher than that of the BSb, the larger $v_{ph}$ of the former compensates its stronger anharmonicity and consequently leads to a relatively higher lattice thermal conductivity of the BAs systems.

Figures 3(a)–(c) plot the HSE band structures of the BP, BAs, and BSb monolayers, respectively. Similar to those of the graphene [21] and hexagonal BN [24], both the conduction band minimum (CBM) and valance band maximum (VBM) of these BX series are located at the K point in the Brillouin zone. The band gaps of BP, BAs, and BSb monolayers are calculated to be 1.37 eV, 1.18 eV, and 0.61 eV, respectively, which decrease with increasing atomic mass of the X elements. As can be found in the inset of figure 3(c), the CBM and VBM of the BSb monolayer are mainly contributed by the p$_z$ orbitals of the B and Sb atoms, respectively. Similar pictures can be also

found in the BP and BAs monolayers, indicating that the band gaps of the BX series are determined by the energy difference between the p$_z$ orbitals of the B and X atoms ($\Delta E_{p_z}$). From the BP to the BAs and BSb monolayers, the $\Delta E_{p_z}$ decreases and is responsible for the reduced band gap. Our calculated results are consistent with previous study using a tight-binding analysis [43]. On the other hand, it can be found that the energy dispersions around the VBM and CBM become stronger when going from the BP to BAs and BSb monolayers, which means gradually lower band effective masses ($m^*_b$) of the BX series (the computation details are given in section 2 of the supplementary material). Indeed, the $m^*_b$ of hole (electron) for the BP, BAs, and BSb monolayers are calculated to be 0.183 (0.195) $m_e$, 0.165 (0.173) $m_e$, and 0.105 (0.106) $m_e$, respectively. Such an observation suggests that higher carrier mobility ($\mu$) and thus larger electrical conductivity could be found in the BSb monolayer. Besides, the almost identical $m^*_b$ of hole and electron in the BSb monolayer indicates that the electronic transport properties of p- and n-type systems may be comparable, which is very desirable in thermoelectric modules. Note that the $m^*_b$ of BX series are obviously lower than those of the typical thermoelectric material such as SnSe [59]. However, the total density of states effective mass ($m^*_b$os = $N_v m^*_b$ for 2D system) can still be large because of moderate band degeneracy ($N_v = 4$), which will lead to a higher Seebeck coefficient [60]. Figure 3(d) displays the energy-dependent carrier relaxation time of the BP, BAs, and BSb monolayers at 300 K. For both the p- and n-type systems, it is obvious that the relaxation time of the BSb around the band edge is relatively higher than those of the BP and BAs monolayers. This is reasonable since the BX series exhibit similar deformation potential constants (~2.3 eV and ~3.8 eV for the p- and n-type systems, respectively) but distinct $m^*_b$ mentioned above. Such finding also suggests that although the strong anharmonicity in the BAs and BSb monolayers can greatly suppress the $\tau_{ph}$ and $\kappa_l$, it hardly affects the $\tau_c$ and the electronic transport.

Using the Boltzmann transport theory and inserting the above-mentioned k-dependent carrier relaxation time, we can evaluate the electronic transport properties of the BX monolayers. As an example, we list in table 2 the room temperature $S$, $\sigma$, $\kappa_e$, power factor ($S^2\sigma$), and carrier mobility ($\mu$) of p-type BX series along the armchair direction. It is obvious that $S^2\sigma$ of the BSb and BAs monolayers are much higher than that of the BP system, which is attributed to the simultaneously larger Seebeck coefficient and electrical conductivity originated from the lower carrier concentration and smaller $m^*_b$, respectively. Compared with that of good thermoelectric material SnSe [59], the BX monolayers show much larger power factors due to their ultrahigh carrier mobilities (even comparable with that of graphene for the BAs and BSb monolayers [61]) and moderate band degeneracy. As a consequence, excellent thermoelectric figure-of-merit $ZT = S^2\sigma T/((\kappa_e + \kappa_l))$ can be expected in the BX monolayers. Note that the $\kappa_l$ of BP system is quite high, which could be significantly decreased by using a bilayer structure to enhance the $ZT$ value, as discussed in our previous work [62]. Here we focus on the thermoelectric performance of BAs and BSb monolayers. Figures 4(a) and (b) plot the temperature dependent $ZT$ values of the BAs and...
BSb monolayers, respectively. Due to relatively larger band gaps, the best thermoelectric performance of the BAs monolayer is achieved at a higher temperature of 1300 K compared with that at 700 K for the BSb system. The corresponding \( ZT \) values as a function of carrier concentration are plotted in figures 4(c) and (d), where we find that both systems exhibit better \( p \)-type thermoelectric performance along the armchair direction. To have a fully understanding of the anisotropic characteristics, using the BSb monolayer as an example, we summarize in table 3 the optimized \( ZT \) values and the corresponding transport coefficients at 700 K along both the zigzag and armchair directions. We see that the Seebeck coefficients (absolute value) of BSb monolayer along the armchair direction are larger than those along the zigzag direction for both \( p \)- and \( n \)-type systems due to the lower optimized carrier concentrations. Note that the anisotropy of transport coefficients is determined by the so-called transport tensor [39] where the carrier relaxation time is treated as a scalar. On the other hand, due to smaller hole mobility caused by larger effective mass, we see smaller hole electrical conductivity along the zigzag direction even at a higher carrier concentration, leading to a lower power factor compared with that along the armchair direction. As a consequence, the \( p \)-type \( ZT \) values along the armchair direction are higher than those along the zigzag direction. In the case of \( n \)-type system, however, the obviously larger electrical conductivity along the zigzag direction compensates the slightly smaller Seebeck coefficient and consequently leads to a higher power factor. Even so, we still find a higher \( n \)-type \( ZT \) values along the armchair direction since the larger lattice thermal conductivity dramatically suppress the thermoelectric performance along the zigzag direction. Similar pictures can be found in the BP and BAs monolayers. The electronic transport coefficients of all the BX systems at the optimized temperature are plotted as a functional of carrier concentration in sections 3–5 of the supplementary material. At the optimized hole concentration of \( 5.7 \times 10^{19} \text{cm}^{-3} \) (\( 2.7 \times 10^{19} \text{cm}^{-3} \)), the highest \( ZT \) value of 3.7 (3.3) can be obtained for the BAs (BSb) monolayer, which exceeds the target value of 3.0 for the practical applications of thermoelectric materials and are also obviously higher than that of the BP bilayer system discussed in previous work [62]. Although there is currently no experimentally reported \( ZT \) values

![Figure 3. The band structures of (a) BP, (b) BAs, and (c) BSb monolayers calculated by using the HSE functional. The inset in (c) shows the orbital-decomposed band structures of BSb system around the Fermi level. (d) is the energy-dependent carrier relaxation time of BX monolayers at 300 K. The Fermi level is at 0 eV.](image)

![Table 2. The room temperature electronic transport coefficients of \( p \)-type BX monolayers at the optimized carrier concentration along the armchair direction.](table)
for our investigated BX monolayers, using the same theoretical approach, our previous work [63] well reproduced the experimentally measured $ZT$ values [64] of the well-studied thermoelectric material Bi$_2$Te$_3$. In a recent work [65], by considering the scattering from all the phonon modes, we have accurately predicted the $ZT$ values of typical thermoelectric material SiGe, which are also consistent with those reported previously [66]. It is thus reasonable to expect that our calculated $ZT$ values for the BX monolayers are reliable. On the other hand, it is interesting to find that along the zigzag direction, the $p$- and $n$-type $ZT$ values of BSb monolayer are almost identical to each other, which is quite beneficial for fabrication of thermoelectric modules with comparable efficiencies.

4. Summary

In summary, our theoretical work suggests that the graphene-like BAs and BSb monolayers could achieve considerably larger $ZT$ which even exceed the target value of thermoelectric applications. As opposite to that of graphene, such a record high performance originates from the moderate band gap and obviously lower thermal conductivity, which is believed to be rooted in the presence of two different hexagonal sublattices. Experimentally, the graphene-like BX monolayers could be prepared by mechanical cleavage or chemical vapor deposition similar to the synthesis of single-layer hexagonal BN [67, 68]. In general, the underlying design principle of our theoretical study could be used to find high performance thermoelectric materials in other 2D systems such as layered InP$_3$ [69], PBi [57], and transition metal dichalcogenides [70–72].

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Table 3. The electronic, phonon, and thermoelectric transport coefficients of BSb monolayer at 700 K along the armchair and zigzag directions.

| Type | Direction | $n$ ($10^{19} \text{cm}^{-3}$) | $S$ ($\mu\text{V K}^{-1}$) | $\sigma$ ($10^3 \text{S cm}^{-1}$) | $S^2\sigma$ ($\text{W m}^{-1} \text{K}^{-2}$) | $\kappa_e$ ($\text{W m}^{-1} \text{K}^{-1}$) | $\mu$ ($\text{m}^2 \text{V}^{-1} \text{K}^{-1}$) | $m^*$ ($m_e$) | $\kappa_l$ ($\text{W m}^{-1} \text{K}^{-1}$) | $ZT$ |
|------|-----------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|-------|
| $p$  | Armchair  | 2.72            | 263             | 9.12            | 0.063           | 5.42            | 0.209           | 0.098           | 7.79            | 3.3   |
|      | Zigzag    | 2.99            | 256             | 9.06            | 0.059           | 5.73            | 0.189           | 0.111           | 10.9            | 2.5   |
| $n$  | Armchair  | 2.79            | -254            | 8.22            | 0.053           | 5.18            | 0.184           | 0.112           | 7.79            | 2.9   |
|      | Zigzag    | 2.88            | -247            | 9.83            | 0.060           | 5.48            | 0.213           | 0.100           | 10.9            | 2.6   |

Figure 4. The temperature dependent $ZT$ values of (a) BAs and (b) BSb monolayers. (c) and (d) are respectively the $ZT$ values of BAs at 1300 K and BSb at 700 K, plotted as a function of carrier concentration.
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