Phonon transport in single-layer boron nanoribbons

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Received 4 June 2016, revised 25 August 2016
Accepted for publication 30 August 2016
Published 26 September 2016

Abstract

Inspired by the successful synthesis of three two-dimensional (2D) allotropes, the boron sheet has recently been one of the hottest 2D materials around. However, to date, phonon transport properties of these new materials are still unknown. By using the non-equilibrium Green’s function (NEGF) combined with the first principles method, we study ballistic phonon transport in three types of boron sheets; two of them correspond to the structures reported in the experiments, while the third one is a stable structure that has not been synthesized yet. At room temperature, the highest thermal conductance of the boron nanoribbons is comparable with that of graphene, while the lowest thermal conductance is less than half of graphene’s. Compared with graphene, the three boron sheets exhibit diverse anisotropic transport characteristics. With an analysis of phonon dispersion, bonding charge density, and simplified models of atomic chains, the mechanisms of the diverse phonon properties are discussed. Moreover, we find that many hybrid patterns based on the boron allotropes can be constructed naturally without doping, adsorption, and defects. This provides abundant nanostructures for thermal management and thermoelectric applications.

Keywords: boron sheet, nanoribbons, thermal transport, pattern, anisotropic transport

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

1. Introduction

Thermal management is critical in electronics. Graphene is considered to be an outstanding thermal material because of its super-high thermal conductivity [1–4]. In thermal devices based on graphene, phonon transport needs to be modulated to obtain different functions and applications, such as phonon rectifiers [5, 6], phonon filters [7], phonon transistors [8, 9], and thermoelectric devices [10, 11]. Heterostructures and periodic patterns are frequently-used modulation structures, which can be obtained by adsorption [12, 13], doping [14], and defects [15, 16]. For example, periodic linear or rectangular patterns can be created by regular hydrogen adsorption [10, 12], while antidot periodic patterns can be formed by vacancy defects [16, 17]. It has been proven that periodic patterns indeed tune phonon transport effectively [11–13, 16]. However, to obtain the different patterns, the lattice of graphene must be destroyed and accurate experimental conditions are required [18, 19].

Boron is another element possessing rich chemical properties in addition to carbon [20–22]. Many two-dimensional (2D) single-layer boron allotropes have been predicted theoretically, such as α-, β-, and γ-boron [21–23]. In these boron sheets, boron exhibits more diverse bonds than carbon. It is known that, in the 2D carbon sheets, one carbon atom may have two, three, or four bonds with its nearest neighboring atoms, while one boron atom can have three to seven bonds connected with other boron atoms [21, 24, 25]. Because boron atoms appear to form triangular or hexagonal rings, almost all boron allotropes have close lattice geometries, which can be considered as inserting atoms to parts of hexagonal rings in a honeycomb lattice or removing parts of...
atoms from a triangular lattice [21, 26, 27]. A parameter, the so-called hexagonal vacancy density $\eta$ [21, 23], is used to describe the ratio of hexagon holes to the number of atomic sites in the original triangular lattice within one unit cell. Boron allotropes with different $\eta$ show different electronic properties, such as high anisotropy [21, 28] and superconductivity [29, 30], which have attracted much attention. More inspiringly, several boron allotropes have been synthesized successfully [28, 31]. Feng et al obtained $\beta_{12}$ and $\chi_3$ using molecular beam epitaxy on a Ag (111) surface [31]. A triangular boron sheet was reported by Mannix et al in their experiment [28]. This further suggests that boron materials are one of the hottest areas of research in a variety of fields. However, as far as we know, phonon transport in boron sheets has not been reported to date. An intriguing question is: what is the phonon transport ability of these 2D boron sheets? Moreover, boron allotropes consisting of triangular or hexagonal rings can form various patterns without destroying their pristine lattices, and thus provide rich hybrid structures to modulate thermal transport.

In this work, we study ballistic phonon transport in boron nanoribbons cut from three types of boron sheets, as shown in figure 1, by using the non-equilibrium Green’s function (NEGF) combined with first principles methods [32–35]. The three boron sheets show different phonon transports along zigzag and armchair directions, and the transport mechanisms are explained by phonon dispersion, bonding charge densities, and simplified models of atomic chains. Based on the three boron sheets, various hybrid boron structures with different patterns are proposed, and their potential applications are also suggested.

2. Model and simulation methods

Three types of boron sheets are considered, as shown in figures 1(b)–(d); these are named boron 1, 2, and 3, respectively. Boron 1 and 2 have been synthesized successfully [31], while boron 3 is a boron allotrope that is highly stable even if it has not been reported to have been experimentally synthesized [23, 36]. All of them can be viewed as boron structures by periodically inserting atoms into honeycomb or periodically removing atoms from triangular lattices. Different insertion or removal methods lead to distinct patterns and atomic densities of boron allotropes. To study the phonon transport properties along different edges and directions, 2D sheets are always cut into quasi-one-dimensional (Q1D) nanoribbons. For example, graphene has two typical

![Figure 1. Atomic structures of graphene and three types of boron sheets: graphene (a), boron 1 (b), boron 2 (c), and boron 3 (d). The solid atoms between the red and blue lines represent zigzag-edged nanoribbons (ZNRs) and armchair-edged nanoribbons (ANRs), respectively, whose widths are labeled as $W_Z$ and $W_A$. The dark green atoms in (b), (c), and (d) represent the inserted atoms in the honeycomb structure.](image-url)
nanoribbons: ZNRs (G-ZNRs) and ANRs (G-ANRs). Similarly, boron 1/2/3 can also be cut into zigzag and armchair-edged nanoribbons, named as B1/2/3-ZNRs and B1/2/3-ANRs, respectively. The two types of boron nanoribbons are denoted by solid atoms in figures 1(b)–(d), whose widths are labeled as \( W_2 \) and \( W_3 \), respectively.

Ballistic phonon transport properties of the boron nanoribbons can be calculated by using the NEGF method combined with first principle calculations. Each nanoribbon can be divided into three parts: left lead, right lead, and the center scattering region. In order to investigate the intrinsic transport properties of boron nanoribbons, the three parts are set to be homogeneous to avoid scattering between them. According to the NEGF scheme, the retarded Green’s function of the nanoribbon is expressed as \( [33, 34, 37–39] \):

\[
G' = \left[ (\omega + i0^+)\gamma I - K^c - \sum_{L,R}\frac{r}{L} - \sum_{R}\frac{r}{R} \right]^{-1}, \tag{1}
\]

where \( \omega \) is the frequency of phonons; \( K^c \) is the mass-weighted harmonic force constants matrix of the center region, and \( \sum_{\beta} = V^{C}\beta'V^{C} \) (\( \beta = L, R \), corresponding to the left and right) denotes the self-energy of the (left or right) lead \( \beta \), in which \( V^{C}\beta = (V^{C})^T \) is the coupling matrix of the lead \( \beta \) to the center region and \( g_{\beta}^C \) is the surface Green’s function of the lead. Once the retarded Green’s function \( G' \) is obtained, we can calculate the transmission coefficient \( T[\omega] \) and then the thermal conductance \( \kappa \) of the nanoribbon:

\[
T [\omega] = Tr \{ G^T[I] G[I] \}, \tag{2}
\]

\[
\kappa (T) = \frac{k}{2\pi} \int_{0}^{\infty} T [\omega] \omega \frac{\partial f(\omega)}{\partial T} d\omega, \tag{3}
\]

where \( \Gamma_{\beta} \) is \( i(\sum_{\beta} - \sum_{a}^a) = -2imV^{C}\beta'V^{C} \) is the coupling function of the lead \( \beta \) and \( f(\omega) = \{ \exp\left[\frac{\omega - \mu}{kT}\right] - 1 \}^{-1} \) is the Bose–Einstein distribution function for heat carriers at the leads. In addition, the phonon spectrum of the nanoribbons can be obtained from the generalized eigenvalue method:

\[
\left( \omega^2 I - K_{ii} \right) \begin{pmatrix} I \\ 0 \end{pmatrix} = \lambda \begin{pmatrix} K_{ii} & 0 \\ 0 & I \end{pmatrix} \begin{pmatrix} I \\ 0 \end{pmatrix}. \tag{4}
\]

After diagonalizing this generalized eigenvalue matrix, one can get the eigenvalues \( \lambda \). By setting the traveling waves eigenvalue to be \( (\lambda = \epsilon^{i\omega}) \), the wave number \( q \) for a special \( \omega \) is found. And then, the phonon spectrum of the nanoribbons is obtained.

The force constant \( K^c \) in equation (1) can be calculated from the first principles method based on the following form \( [40, 41] \):

\[
K_{ij}^{xy} = \frac{\partial^2u_{ij}}{\partial x\partial y}, \tag{5}
\]

where \( K_{ij}^{xy} \) is the force constant between the \( i \)th and \( j \)th neighboring atoms in the \( x \) and \( y \) directions, and \( u_{ij} \) is the total energy between the \( i \)th and \( j \)th atoms, respectively. That is, the force constant \( K_{ij}^{xy} \) is calculated from the second derivative of potential energy with small displacements in \( \partial x \) and \( \partial y \). In the first principles calculations, the generalized gradient approximation with Perdew–Burke–Ernzerhof exchange-correlation potential is adopted, with plane wave cut-off energy 450 eV. The total energy convergence is chosen as \( 1.0 \times 10^{-8} \) eV, and structure optimization is performed until the force acting on each atom is less than \( 1.0 \times 10^{-7} \) eV Å\(^{-1}\). In addition, the calculations are performed on \( 5 \times 5 \times 1 \) supercell structures. Then the force constant matrix of any nanoribbons can be obtained based on the interatomic force constant. In order to accurately describe the interactions between atoms, the considered force constants are up to the third neighboring atom in each direction. Take the B1-ZNR as an example, as shown in figure S1 in the supplementary material (SM)—the third neighboring interaction well describes the phonon transport properties. In addition, the edge effect of the nanoribbons has been considered here. After structural optimizing, the bond lengths on the edges change, which leads to the corresponding variation of force constant. Detailed information regarding this issue can be found in figure S2 in the SM.

### 3. Results and discussion

In figures 2(a) and (b), the thermal conductance \( \kappa \) for ZNRs and ANRs of the three types of boron sheets as a function of temperature \( T \) are shown \( (W_{2/3} \approx 5.0 \) nm\), respectively. The \( \kappa \) for G-ZNRs and G-ANRs are also shown for comparison. All the \( \kappa \) curves increase with \( T \) because the phonon modes are gradually excited by high temperatures, which is different from the temperature dependence of diffusive transport due to the omission of phonon-phonon scattering. Both the G-ANRs and G-ZNRs have higher \( \kappa \) values than those of the boron nanoribbons. The three types of boron sheets exhibit diverse phonon transport abilities. For the ZNRs, the \( \kappa \) of the B1-ZNR is the highest, while that of the B3-ZNR is the lowest, as shown in figure 2(a). Moreover, the former is nearly two times that of the latter. For the ANRs, the \( \kappa \) values of the three boron sheets have little difference (see figure 2(b)). This implies that the three boron sheets possess a completely different transport anisotropy.

Previous studies reported that 2D materials have different dependence relationships between \( \kappa \) and \( T \) \([37, 42–44]\). For example, many 2D materials exhibit \( T^2 \) and \( T^3 \) dependences of \( \kappa \) \([42, 43]\), while a \( T^{1.5} \) dependence has been found in graphene and boron nitride \([37, 42, 44]\). We fit the \( \kappa \) curves of boron nanoribbons in figures 2(a) and (b) by the following formula:

\[
\kappa(W, T) = (a_1 + b_1 W) T + (a_2 + b_2 W) T^{1.5}
+ (a_3 + b_3 W) T^2, \tag{6}
\]

where \( a_i \) and \( b_i \) are parameters. The optimal fitting parameters for the boron nanoribbons are given in table 1. It is found that, similar to graphene, the \( T^{1.5} \) term in equation (6) has an important contribution to \( \kappa \). The detailed analysis of the contributions of \( T \), \( T^{1.5} \), and \( T^2 \) is given in the SM.

Figures 2(c) and (d) present the dependences of \( \kappa \) on the width \( W_{2/3} \) of boron ZNRs and ANRs \((T = 300 \) K),
respectively. Because the number of phonon channels depends linearly on the widths of the nanoribbons, nearly all the $\kappa$ values vary linearly as the $W_{Z/A}$ increases. The edge effect induces the $\kappa$ values of small width nanoribbons to slightly deviate from the lines. Meanwhile, at the small widths, the $\kappa$ differences of the nanoribbons are small. The main reason for this is that there are relatively few phonon modes in the narrower nanoribbons, and only relatively low-frequency phonons are activated at room temperature (see figure S5 in the SM). One can find that the slopes of the lines are different. The B1-ZNR has the largest slope that is close to graphene’s at room temperature. The slope of the B3-ZNR is the smallest, and thus the difference in $\kappa$ between the B3-ZNR and the B1-ZNR increases with the width. However, the difference in $\kappa$ between boron ANRs is very small with an increase in width. Therefore, the anisotropies of $\kappa$ in the boron sheets will increase with the widths.

Figure 2. Thermal conductance $\kappa$ of (a) the G-ZNR, the B1-ZNR, the B2-ZNR, and the B3-ZNR, and (b) the G-ANR, the B1-ANR, the B2-ANR, and the B3-ANR as a function of temperature at $W_{Z/A} \approx 5.0$ nm, respectively. Thermal conductance $\kappa$ of (c) the G-ZNR, the B1-ZNR, the B2-ZNR, and the B3-ZNR, and (d) the G-ANR, the B1-ANR, the B2-ANR, and the B3-ANR as a function of widths $W_{Z/A}$ at $T = 300$ K, respectively.

Table 1. The values of fitting parameters $a_i$ and $b_i$ ($i = 1, 2, 3$) in equation (6).

<table>
<thead>
<tr>
<th></th>
<th>$a_1 \times 10^{-3}$</th>
<th>$b_1 \times 10^{-4}$</th>
<th>$a_2 \times 10^{-4}$</th>
<th>$b_2 \times 10^{-4}$</th>
<th>$a_3 \times 10^{-6}$</th>
<th>$b_3 \times 10^{-5}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>B1-ZNR</td>
<td>2.70</td>
<td>-2.61</td>
<td>-1.61</td>
<td>8.63</td>
<td>1.68</td>
<td>-2.83</td>
</tr>
<tr>
<td>B2-ZNR</td>
<td>2.25</td>
<td>-3.14</td>
<td>-0.85</td>
<td>8.70</td>
<td>-0.63</td>
<td>-2.86</td>
</tr>
<tr>
<td>B3-ZNR</td>
<td>3.83</td>
<td>-1.11</td>
<td>-5.00</td>
<td>5.12</td>
<td>13.2</td>
<td>-1.85</td>
</tr>
<tr>
<td>B1-ANR</td>
<td>3.25</td>
<td>-1.50</td>
<td>-2.47</td>
<td>5.31</td>
<td>5.00</td>
<td>-1.81</td>
</tr>
<tr>
<td>B2-ANR</td>
<td>4.25</td>
<td>-1.38</td>
<td>-4.94</td>
<td>5.24</td>
<td>13.9</td>
<td>-1.93</td>
</tr>
<tr>
<td>B3-ANR</td>
<td>2.70</td>
<td>-1.10</td>
<td>-1.21</td>
<td>4.86</td>
<td>-0.96</td>
<td>-1.71</td>
</tr>
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</table>
To directly compare the anisotropies of the intrinsic transport properties of boron nanoribbons, the scaled thermal conductivities $\sigma/L$ for both ZNRs and ANRs at 300 K are shown in figure 3. Thermal conductivity $\sigma$ is calculated by

$$\sigma = \kappa/S \times L,$$

where $S = W_z/L \times h$ is the cross-sectional area ($h = 0.32$ nm is the thickness of the boron sheets) [45] and $L$ is the mean free path of phonons. Because $L$ has not been reported, here we calculate the $L$ scaled thermal conductivities $\sigma/L$ for both ZNRs and ANRs at 300 K. The inserted blank dots represent the corresponding values of graphene nanoribbons.

Figure 3. (a) Scaled thermal conductivities $\sigma/L$ of boron ZNRs as a function of $W_z$ at $T = 300$ K. (b) Scaled thermal conductivities $\sigma/L$ of boron ANRs as a function of $W_A$ at $T = 300$ K. The inserted blank dots represent the corresponding values of graphene nanoribbons.

Figure 4. Phonon spectrums of a unit of (a) the G-ZNR and the G-ANR, (b) the B1-ZNR and the B1-ANR, (c) the B2-ZNR and the B2-ANR, and (d) the B3-ZNR and the B3-ANR. The units of different nanoribbons are shown in figure 1 with the black dashed box.

To directly compare the anisotropies of the intrinsic transport properties of boron nanoribbons, the scaled thermal conductivities $\sigma/L$ for both ZNRs and ANRs at 300 K are shown in figure 3. Thermal conductivity $\sigma$ is calculated by

$$\sigma = \kappa/S \times L,$$
conductivity. One can find from figure 3 that, with an increase in width, the thermal conductivities drop at first and then approach converged values. The different transport abilities of the ZNRs are shown again (see figure 3(a)), while the difference between the ANRs is small (see figure 3(b)). We define \( \varepsilon = 1 - (\sigma/L)_{\text{ANR}}/(\sigma/L)_{\text{ZNR}} \) to identify the anisotropic degree of phonon transport in the different boron sheets. Then, \( \varepsilon = 39.1\%, 50.2\%, \) and \(-17.4\%\) for boron 1, 2, and 3, respectively. This indicates that boron 1 and 2 possess very strong transport anisotropies (\( \varepsilon \approx 20\% \) for graphene) [46]. The thermal conductivities of the ZNRs are much higher than those of the ANRs. Interestingly, the anisotropy of boron 3 is a negative value, i.e. thermal conductivities of ANRs are higher than those of ZNRs. The different transport characteristics on one hand demonstrate wide ranges of thermal conductivities of boron sheets, and on the other hand show diverse transport phenomena.

Phonon transport properties are related to the phonon dispersions. To explain the difference of phonon transport in the boron sheets, as shown in figure 4, the phonon spectra of the boron nanoribbons and also graphene nanoribbons are given. The comparison of the phonon spectra reveals that the frequency ranges and the acoustic phonon velocities determine transport abilities. For example, the phonon dispersions of the B1-ZNR are much closer to those of the G-ZNR, and thus it has the highest thermal conductivity in all boron nanoribbons. In contrast, the lower thermal conductivity of the B3-ZNR is because of its small group velocities of both optical and acoustic phonons. The different anisotropies of boron sheets are also reflected by the spectra. The group velocities of acoustic phonons in the B1 and B2 ZNRs are obviously faster than those in the ANRs, while the case of boron 3 is opposite. Therefore, the anisotropies of the former

**Figure 5.** BCD contours for (a) graphene, (b) boron 1, (c) boron 2, and (d) boron 3, respectively. Black circles represent the positions of atoms and black lines represent strong bonds.

**Figure 6.** Normalized \( \kappa \) of simplified models of atomic chains corresponding to graphene and boron nanoribbons. The inset figures are simplified models of atomic chains where the parameters of mass \( m \) and force constant \( K \) are shown.
two are opposite to that of the third one. In addition, it is
noted that there exist quadratic acoustic branches in the
spectra, which are responsible for the $T^{1.5}$ dependence in
equation (6) [42].

The different phonon transport properties in the boron
sheets can be understood from their bonding charge densities
(BCDs) [47], which are the charge density difference between
the valence charge density of the system and the superposition
of the valence charge density of the neutral constituent atoms.
Figures 5(a)–(d) show BCD contours of ground-state gra-
phene and boron 1, 2, and 3, respectively. They directly
reflect the strength of interactions between atoms. In
figure 5(a), electrons are evenly distributed between the car-
bon atoms and thus form a honeycomb geometry, which has
been explained as an intrinsic reason for the high conductivity
of graphene [42, 44]. The BCD contour of boron 1 is
somewhat similar to that of graphene except the interactions
are weaker, as shown in figure 5(b). Therefore, its phonon
transport properties are mostly close to those of graphene. Seen from figures 5(c) and (d), boron 2 and 3 have completely
different contours. In boron 2, the BCD contour exhibits strong directionality: along the zigzag direction the contour
forms channels while the channels are truncated along the
armchair direction. This is the cause of the high transport
anisotropy. In boron 3, the contour forms channels along both
zigzag and armchair directions. However, the channels along
the armchair direction are linear, while those along the zigzag
direction are zigzag. The former are more advantageous to
transport, and thus the thermal conductivity along the arm-
chair direction is higher than that along the zigzag direction.
Consequently, boron 3 has inverse anisotropy compared to
boron 1 and 2. Meanwhile, the contour of boron 3 implies that
the interactions between atoms are weaker, which results in
low acoustic phonon velocities and thermal conductivity.

To further understand the relations between pattern geo-
metries and phonon transport properties, we use simpler atomic
chain models to simulate different nanoribbons. Q1D graphene
and boron nanoribbons consist of periodic units along the
transport direction. When each unit is simplified to one or sev-
eral atoms, the nanoribbons are equivalent to one-dimensional
atomic chains [48]. For comparison, the simplified models of
different nanoribbons are given in the inset of figure 6: the
G-ZNR, G-ANR, B1-ZNR and B2-ZNR have perfect stripe
geometries, and thus can be simplified to monatomic chains; the
B1-ANR and B2-ANR are constructed by alternative sub-units,
and thus are simplified to diatomic chains consisting of two
kinds of lattices, and the B3-ZNR and B3-ANR are more
complicated, and coupled diatomic chains are used to represent
them. Based on classical theory, the transport properties related to the vibration frequency of the lattice $\omega (=\sqrt{K/m})$ are determined by the lattice mass $m$ and force constant $K$ between lattices. Graphene nanoribbons consist of hexagonal rings, while boron nanoribbons consist of empty and filled hexagonal rings. Therefore, we can normalize the $m$ and $K$ of different nanoribbons based on the hexagonal rings. For example, if the mass of a unit including empty rings is $m$, that including filled rings can be set as $1.2m$, which is calculated from a reduced mass ratio of different rings and its own vibration properties. Meanwhile, the force constant $K$ can be normalized by the strength of the interaction between the units, which is calculated by the number of bonds times $K$ of each bond. The detailed values of $m$ and $K$ are shown in the insets of figure 6. As a result, the thermal properties of different nanoribbons can be described by different atomic chains. Figure 6 shows $\kappa$ values of the corresponding simplified models. One can find that the simplified models reproduce the phonon transport characteristics of the boron nanoribbons. This not only explains the origination of diverse transport properties in the three types of boron sheets, but also provides an effective method to predict the phonon properties of boron allotropes with other patterns. One can simplify other boron allotropes to atomic chains according to structure patterns and interaction strength, and then the normalized $\kappa$ value can be predicted from simplified atomic chains with the NEGF method.

As mentioned above, with the character that boron allotropes consisting of triangular or hexagonal rings can form various patterns without destroying their pristine lattices. In figure 7, some patterns based on boron 1, 2 and 3 are proposed and several potential applications are suggested. For the analogous geometry to graphene thermal devices, similar potential thermal functions and applications are expected to be found in those boron patterns. Figures 7(a)–(c) present perpendicular, parallel and array patterns constructed by boron 1 and 3, and figure 7(d) presents a hybrid pattern constructed by three types of boron nanoribbons. Because the transport properties of boron 1, 2 and 3 are different, these patterns will modulate thermal transport in different ways, and thus various functions and related devices are expected to be obtained, such as thermoelectric devices with reduced thermal conductances or phonon filters. In figure 7(e), a triangular heterostructure is constructed by boron 1 and 3. It can serve as a phonon rectifier because of the big asymmetry of geometry and the difference of phonon properties between two sides. Figure 7(f) shows a three-terminal T-shaped junction consisting of boron 1, 2 and 3. It may be a potential phonon transistor where boron 1 and 2 are two leads while boron 3 serves as a gate. Besides boron 1, 2 and 3, there are many other boron allotropes consisting of triangular or hexagonal rings [21, 23, 24]. Therefore, many hybrid patterns can be constructed naturally without doping, adsorption and defects, to fulfill the demands of thermal management.

4. Conclusion

In summary, we have studied ballistic phonon transport in three types of boron sheets with different edges, using a combined method of NEGF and first principles calculations. The boron sheets exhibit diverse phonon transport abilities and different anisotropies. The highest thermal conductivity is comparable to that of graphene, while the lowest thermal conductivity is less than half of graphene’s. Moreover, boron 1 and 2 exhibit stronger transport abilities along the zigzag edges than the armchair edges, while the case of boron 3 reveals the opposite. The phonon dispersions and BCD contours reveal the origins of the transport properties. The boron nanoribbons are simplified to atomic chains to further explore the difference between the transport properties, which provides an effective method to predict phonon transport of other boron allotropes. Hybrid patterns based on the boron sheets are constructed. All the hybrid structures have natural interfaces without doping, adsorption and defects. Some potential applications of hybrid boron sheets in thermal devices, such as rectifier and transistors, are proposed. With the analytic formula of thermal conductivity with respect to the width and temperature of these three base units, the thermal conductance of the hybrid structures is ready to be predicted. Our study is useful in material and devices design for thermal management and thermoelectric applications. It should be noted that here we only studied ballistic transport properties in boron nanoribbons, while phonon scattering plays an important role in the thermal transport, especially in the diffusive region and high temperature. We expect to study these complicated effects in future research.

Acknowledgments

This work was supported by the National Natural Science Foundation of China (Nos. 51376005 and 11474243).

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