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Yunfeng Gu

College of Electronic and Mechanical Engineering, Nanjing Forestry University, Nanjing, P. R. China

ABSTRACT
The thermal conductance of isotopic-superlattice graphene nanoribbons randomly mixed with isotope defects is investigated by atomistic Green’s function method. The isotopic-superlattice structure reduces the thermal conductance, which changes non-monotonically as the superlattice period length decreases, and there exists a minimum thermal conductance at the critical period length. About 20% defects just further increase the reduction and shorten the critical period length. As the defect concentration in superlattice increases, the thermal conductance decreases monotonically in the zigzag nanoribbon, but in armchair nanoribbon the thermal conductance first decreases to its minimum value and then increases. The isotopic doping effect is particularly evident for large isotope mass, in armchair nanoribbons and for out-of-plane phonon modes. Isotope defects lead to additional phonon scattering in the superlattice structure, which is explained by analyzing the phonon transmittance.

1. Introduction
As an exciting new allotrope of carbon, graphene not only has remarkable electronic properties, but also has an extremely high thermal conductivity [1, 2]. In some situations, for example in the thermoelectric applications, the thermal transport must be suppressed without a large reduction of electronic conduction. One way to achieve this purpose is to use isotope engineered graphene structures [3–10]. There are 15 known isotopes of carbon, and 12C makes up almost 99% in nature. Various percentages of carbon isotopes can be introduced to modify the graphene by chemical vapor deposition [11]. The thermal conductivity of suspended graphene with 50% of 13C measured by the Raman optothermal method, is approximately one half of the value in the isotopically pure 12C graphene at 320 K [7].

Several theoretical studies exist regarding the isotope effects on the thermal properties of graphene. The key parameters to design isotope engineered graphene are the type and fraction of isotopes, and their distribution [5]. Various carbon isotopes are chemically almost identical, but have different mass. Larger mass discrepancy can induce smaller thermal conductivity [6, 8]. If various percentages of the 12C atoms are randomly substituted with the heavier 14C isotopes, the thermal conductivity of graphene nanoribbons is found to decrease rapidly before 10% doping, and decreases slowly after this doping percentage [4]. This interesting phenomenon is also found in the randomly isotope doped silicene nanosheets [12]. Jiang et al. [4] reveal that the relation of thermal conductivity versus isotope percentage is related to the localized phonon modes, whose number increases quickly (slowly) with increasing isotopic doping in low (high) isotopic doping region. Moreover, it should be noted that even for the same isotope percentage, the thermal conductivity varies in a significant range, which shows the importance of isotope distribution [5].
In addition to the random distribution, the superlattice distribution is often used in isotope engineered graphene structures. Using classical molecular dynamics simulation, Hu et al. [10] find that isotope mixing can reduce the thermal conductivities, and the reduction effect is more evident with the superlattice distribution than with the random distribution. It is found that the thermal conductivity of the isotopic-superlattice changes non-monotonically as the superlattice period length decreases, and there exists a minimum thermal conductivity as a result of two competing mechanisms, namely interfacial scattering and phonon tunneling effects [3, 6, 8]. By introducing defects, it is possible to further reduce the thermal conductivity of isotopic-superlattice. For example, the thermal conductivity of the 12C/13C superlattice can be further decreased if the 13C graphene portion is changed into a mixture of randomly distributed 12C and 13C isotope atoms with a number ratio of 1:1 [3]. Liu et al. [12] studied the isotopic silicene superlattice with interfaces roughened by randomly replacing half of the 28Si (30Si) atoms at the interfaces with 30Si (28Si) atoms. The rough interfaces reduce the thermal conductivity, and the non-monotonic dependence of thermal conductivity on period length can turn monotonic if heavy 42Si atoms are doped.

As discussed above, the isotope distribution can play an important role to design isotope engineered graphene structures having targeted properties. The isotopic graphene superlattices can be formed theoretically by alternatively feeding different isotope sources during the graphene growth process [3]. As a fact, it is an experimental challenge to precisely manipulate isotopic atoms. Therefore, in this work, the isotopic atoms are not assumed to be distributed strictly in superlattice pattern. Two layers of different isotopes in one period are considered. A few of different isotopic atoms randomly mixed into all the superlattice layers as defects will introduce additional phonon scattering effects, and change the thermal properties of isotopic-superlattices. This kind of semi-disordered isotopic-superlattice graphene nanoribbon studied here has both the characteristics of random distribution and superlattice distribution.

This article is organized as follows. Section 2 presents the semi-disordered isotopic-superlattice graphene nanoribbons with zigzag (IS-ZGNR) edges and isotopic-superlattice graphene nanoribbons with armchair (IS-AGNR) edges, and introduces briefly the simulation method, i.e., the atomistic Green’s function (AGF) method [13]. In Section 3, the thermal conductance ratios of 12C/13C and 12C/22C superlattices are detailed, and the phonon transmittance as a function of frequency is discussed to reveal the phonon propagation mechanism. Finally, a concluding remark is given to summarize this work in Section 4.

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**Nomenclature**

- \( a \) bond length
- \( f \) Planck distribution
- \( G \) Green’s function matrix
- \( I \) identity matrix
- \( i \) unit of imaginary number
- \( K_S \) harmonic matrix of scattering region
- \( L \) superlattice period length
- \( L_C \) critical superlattice period length
- \( N_a \) number of dimer lines
- \( N_z \) number of zigzag lines
- \( n \) number of isotope defects in one superlattice layer
- \( n_0 \) number of atoms in one superlattice layer
- \( T \) temperature
- \( \theta^+ \) broadening constant, which is a positive infinitesimal number
- \( \Gamma \) broadening function, defined in Eq. (4)
- \( \gamma \) thermal conductance ratio defined in Eq. (6)
- \( \eta \) defect concentration defined in Eq. (1)
- \( \Sigma \) self-energy matrix

**Subscripts**

- \( I \) in-plane modes
- \( IS \) isotopic-superlattice
- \( LT \) left terminal
- \( O \) out-of-plane modes
- \( RT \) right terminal
- \( S \) scattering region

**Superscripts**

- \( A \) armchair edge type
- \( Z \) zigzag edge type
- \( \ast \) conjugate transpose of a matrix

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2. Model and method

2.1. Semi-disordered isotopic-superlattice

There are two kinds of semi-disordered isotopic-superlattice graphene nanoribbon: the first one has a zigzag edge shown in Figure 1a, and the other one has an armchair edge shown in Figure 1b. Herein, \( N_z \) and \( N_a \) denote respectively the number of zigzag lines and dimer lines [14]. The structures illustrated in Figure 1 are suitable to be studied by AGF method. There are three parts in the system: left terminal (LT), scattering region (S) and right terminal (RT). The terminals have a semi-infinite periodic structure, and serve as the heat reservoirs. The area enclosed by the dash line in Figure 1 stands for one period of the terminals. By using the AGF method, we can explore the phonon transport across the scattering region, which is an isotopic-superlattice structure composed of alternate layers of two different isotopes, highlighted by different background colors. The small and large balls respectively denote the \(^{12}\text{C} \) atoms and other carbon isotopes. It should be noted that the isotopic-superlattice studied in this article is not perfect. In the semi-disordered isotopic-superlattice graphene nanoribbons shown in Figure 1, a few of \(^{12}\text{C} \) atoms are not in the layer they belong to, but randomly exchange their positions with the carbon isotopes in the neighbor layer. In other words, all the superlattice layers are mixed with the same concentration of defects.

The period length of superlattice in Figure 1 is \( L \). In one period, there are two same size layers, and each layer is assumed to have \( n_0 \) atoms, \( n \) of which are different isotopes as defects. The defect concentration used to assess the disorder then is defined as

\[
\eta = 100\% \times \frac{n}{n_0}
\]  

(1)

For example, \( n_0 = 20 \) and \( n = 1 \) in the semi-disordered IS-ZGNR shown in Figure 1a, which means the defect concentration \( \eta = 5\% \).

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**Figure 1.** Schematic diagram of the (a) semi-disordered IS-ZGNR and (b) semi-disordered IS-AGNR. Small and large balls denote \(^{12}\text{C} \) and other carbon isotopes, respectively. The background color highlights the different layers of superlattice. Note: IS-ZGNR, isotopic-superlattice graphene nanoribbons with zigzag edges; IS-AGNR, isotopic-superlattice graphene nanoribbons with armchair edges.


2.2. Atomistic Green’s function method

The study of phonon transport in the graphene nanoribbons is performed by the AGF method, which starts by building the harmonic matrix, obtained by the force constant method. In this method, the interactions between atoms are simply described by a few force springs connecting an atom with its neighbor atoms. The fourth nearest-neighbor approximation is used [15]. According to the AGF method, the Green’s function for the scattering region is defined as [16]

\[ G = \left((\omega + i0^+) I - K_S - \Sigma_{LT} - \Sigma_{RT}\right)^{-1} \]  

(2)

where \( \omega \) is the phonon frequency, and \( 0^+ \) is the broadening constant [17], which is a small positive number standing for the phonon energy dissipation in contacts [18]. \( i \) and \( I \) are the unit of imaginary number and the identity matrix, respectively. \( K_S \) is the scattering region harmonic matrix. \( \Sigma_{LT} \) and \( \Sigma_{RT} \) are the self-energy matrices of left and right terminals, respectively which play the role of energy-dependent boundary conditions [19]. Based on the Green’s function obtained by Eq. (2), the transmittance (or transmission coefficient) can be determined by [20, 21]

\[ \tau(\omega) = \text{Trace}(\Gamma_{LT}G\Gamma_{RT}G^*) \]  

(3)

where the broadening functions are in the form of

\[ \Gamma_\alpha = i(\Sigma_\alpha - \Sigma_\alpha^*) \]  

(4)

The superscript “*” represents the complex conjugate operation. Under the condition of ballistic phonon transport, the thermal conductance can be written in the form [22]

\[ \sigma = \frac{h}{2\pi} \int \tau(\omega) \frac{\partial f}{\partial T} \omega d\omega \]  

(5)

where \( f \) is the Planck distribution, and \( T \) is the temperature. \( h \) is the reduced Planck constant.

3. Results and discussion

In order to assess the effect of thermal conductance reduction by isotopic-superlattice structure, the thermal conductance ratio is defined as

\[ \gamma = \frac{\sigma_{IS}}{\sigma_{12}} \]  

(6)

where \( \sigma_{IS} \) and \( \sigma_{12} \) are the thermal conductance of isotopic-superlattice and pristine \(^{12}\text{C}\) graphene nanoribbon, respectively which can be calculated by Eq. (5).

The structure of the semi-disordered isotopic-superlattices is illustrated in Figure 1. The width of IS-ZGNR is set as \( N_z = 5 \) (i.e., \( 3N_z a/2 = 1.0875 \) nm), and the length of the scattering region is \( N_a = 144 \) (i.e., \( \sqrt{3}N_a a/2 = 18.0826 \) nm), where the bond length \( a = 0.145 \) nm. For the IS-AGNR, the width is \( N_a = 9 \) (i.e., \( 1.1302 \) nm), and the length of the scattering region is \( N_z = 80 \) (i.e., 17.4 nm). These parameters are kept the same in all the following simulations.

3.1. Thermal conductance in the ideal isotopic-superlattice

Figure 2 shows the thermal conductance ratio of the ideal \(^{12}\text{C}/^{13}\text{C}\) isotopic-superlattices, in which the defect concentration \( \eta = 0\% \), as a function of the superlattice period length \( L \) at room temperature (300 K). The dash line with dot symbols denotes the thermal conductance ratio of IS-ZGNR (\( \gamma_{Z}^{\text{IS}} \)). The in-plane phonon modes can be decoupled from the out-of-plane modes in graphene [23]. Therefore, the thermal conductance ratios of in-plane (\( \gamma_{IF}^{\text{IS}} \)) and out-of-plane (\( \gamma_{OF}^{\text{IS}} \)) phonon modes are also given, and denoted by the dash line with triangle symbols and dash line with square symbols, respectively. The total thermal conductance \( \sigma_{12} \) and its contribution from in-plane and out-of-plane phonon modes respectively are 1.7043, 1.0357 and 0.66857 nW/K for the pure \(^{12}\text{C}\) zigzag graphene
nanoribbon at room temperature, and 1.2034, 0.72563 and 0.47773 nW/K if the graphene nanoribbon has armchair edges. The thermal conductance ratios of IS-AGNR ($\gamma_A$, $\gamma_c^A$ and $\gamma_O^A$) are represented by solid lines with symbols in Figure 2.

It is seen from Figure 2 that when the superlattice total length is fixed, there exists a non-monotonic dependence of thermal conductance on the period length, which has been reported in many literatures [3, 6, 8]. The decreasing of period length leads to the increasing of the number of interface, and therefore enhances the interfacial scattering. This is the reason why the thermal conductance of isotopic-superlattice is lower than the value of the pristine 12C graphene nanoribbon, and initially decreases as the period length decreases. Moreover, the thermal conductance will have a transition from decreasing to increasing as the period length decreases further. This is the result of two competing mechanisms, namely interfacial scattering and phonon tunneling effects [3, 6, 8]. To explain this phenomenon, Ouyang et al. [8] calculated the phonon transmittance with different superlattice period lengths. However, only the out-of-plane modes in IS-ZGNR were studied in their work. It appears in Figure 2 that for both in-plane and out-of-plane modes in IS-ZGNR or IS-AGNR, the thermal conductance ratio versus the period length shows the similar behaviors. Moreover, thermal conductance of out-of-plane modes is more likely to be reduced than that of in-plane modes. Having almost the same width and length, the thermal conductance ratio in IS-AGNR is smaller than that in IS-ZGNR, which is also discovered by Xie et al. [6].

3.2. Thermal conductance in the semi-disordered isotopic-superlattice

Figure 3 illustrates the thermal conductance ratio in the semi-disordered 12C/13C isotopic-superlattice graphene nanoribbons with different defect concentration defined in Eq. (1). To avoid the possible fluctuations due to random distribution [5], the results are obtained by averaging over ten independent distributions with the same defect concentration.

There is an interesting phenomenon in the randomly isotope doped graphene nanoribbon found by Jiang et al. [4]: the thermal conductivity decreases rapidly with increasing doping in low doping region, and the reduction slows down in high doping region. The underlying mechanism is the localization of phonon modes. The same phenomenon also can be discovered in Figure 3a. It appears that a small defect concentration, say $\eta = 10\%$ or $20\%$, does not change the behaviors between $\gamma$ and $L$ dramatically, but can further reduce the capability of phonon thermal transport in IS-ZGNR. When $L$ equals the critical superlattice period length $L_C$ which is about 1.5 nm, thermal conductance ratio has.

Figure 2. Thermal conductance ratio $\gamma$ in the ideal 12C/13C IS-ZGNR and IS-AGNR as a function of the superlattice period length $L$ at room temperature (300 K). The superscripts “A” and “Z” stand for the armchair and zigzag respectively. The subscripts “I” and “O” indicate the in-plane and out-of-plane modes, respectively. Note: IS-ZGNR, isotopic-superlattice graphene nanoribbons with zigzag edges; IS-AGNR, isotopic-superlattice graphene nanoribbons with armchair edges.
a minimum value, which is 0.8657, 0.8439 and 0.8374 for η = 0, 10 and 20%, respectively. With the further increase of η, γ is reduced slowly, especially if L is approximately equal to L_C. If η approaches 50%, γ will not vary with L apparently, because the two layers in the superlattice period as shown in Figure 1 become the same material with randomly distributed isotopes, and there are no interface scattering by the mass discontinuities. The isotope random distribution can help to get the minimum thermal conductance in the zigzag graphene nanoribbons.

Figure 3 displays the thermal conductance ratio in the semi-disordered 12C/13C IS-AGNR with different defect concentration defined in Eq. (1). Strictly speaking, the superlattice structure has a certain degree of damage in the semi-disordered 12C/13C IS-AGNR because of a small fraction of defects (η = 17%). However, these random defects just reduce the value of thermal conductance ratio which still has the shape of a basin. The same phenomenon is found in the semi-disordered 12C/13C IS-ZGNR in Figure 3a. Different from in Figure 3a, as η further increases, the thermal conductance ratio exhibits a transition from the decrease to the increase, especially when the superlattice period length is comparable to the critical length L_C. In the end, the superlattice distribution (η = 0%) of isotopes can lead to a more reduction of γ than the random distribution (η = 50%). This kind of phenomenon is also reported in Hu et al. [10]. In the armchair graphene nanoribbon, the minimum thermal conductance can be achieved not in the ideal isotopic-superlattice or in the disordered nanoribbon, but in the semi-disordered isotopic-superlattice.

Figure 4 illustrates the thermal conductance ratio γ in the 12C/22C superlattice to reveal the effect of larger mass discrepancy on γ by replacing 13C atoms in the 12C/13C superlattice with the heavier 22C atoms. The error bars in Figure 4 indicate the maximum and minimum results of the ten independent calculations. It is found that the thermal conductance ratio in 12C/22C IS-ZGNR shown in Figure 4 is far smaller than that in 12C/13C IS-ZGNR shown in Figure 3a, both in the case of ideal superlattice (η = 0%) and in the case of semi-disordered superlattice (η = 20%). Just like the phenomena shown in Figure 3a, the randomly distributed heavier 22C atoms with η = 20% do not change the behavior of γ versus L dramatically, and moreover tend to reduce γ more evidently compared to the η = 0% case than 13C atoms do. Figure 4 also demonstrates that the effect of reducing γ due to the larger mass discrepancy is stronger in IS-AGNR than in IS-ZGNR. Adding the contribution from the randomly distributed heavier 22C atoms with η = 17%, γ in semi-disordered 12C/22C IS-AGNR can be reduced to about 0.25.

The large mass discrepancy between 12C and 22C amplifies the isotope doping effect. Figure 4, therefore, can more clearly reveal another phenomenon: the random defects decrease the value of the critical superlattice period length L_C. For the γ^Z, L_C is about 1.5 and 1 nm when η equals 0 and 20%, respectively. For the γ^A, L_C is about 2.5 and 1.7 nm when η equals 0 and 17%, respectively. As discussed above, the interfacial scattering and phonon tunneling effect are the two competing forces that govern the thermal conductance.
mechanisms in ideal superlattice. When \( L < L_C \), the phonon tunneling effect will outweighs the interface scattering [8]. The decrease of \( L_C \) shown in Figure 4 means that, together with the interface scattering, the additional scattering introduced by the random defects competes against with the phonon tunneling effect.

### 3.3. Phonon transmittance

According to Eq. (5), the thermal conductance is calculated on the basis of the phonon transmittance. Therefore the phonon transmittance of IS-ZGNR and IS-AGNR shown in Figure 5 can provide a more in-depth perspective. As a comparison, the transmittance in the pristine \( ^{12}\text{C} \) nanoribbon is denoted by the dash line in Figure 5a, b for the zigzag edge, and in Figure 5c, d for the armchair edge. Without scattering in the pristine case, the dash line has a set of quantization plateaus as a function of frequency \( \omega \) taking only integer values, which equal the number of phonon subbands crossing frequency \( \omega \). The thermal conductance \( \sigma_{12} \) in Eq. (6) is calculated based on the transmittance in the pristine case.

The solid lines in Figure 5 indicate the transmittance in the ideal superlattice, which means that \( \eta = 0\% \). The periodic length is set as 1.5069 nm for IS-ZGNR, and 1.74 nm for IS-AGBR. Because of the interfacial scattering introduced by the superlattice structure, the transmittance denoted by the solid line will be significantly reduced compared to the dash line, especially at the higher frequency range [6]. The comparison between Figure 5a, b, or between Figure 5c, d, shows that the reduction of transmittance in the \( ^{12}\text{C}/^{22}\text{C} \) superlattice is more evident than in the \( ^{12}\text{C}/^{13}\text{C} \) superlattice. The reason is that the interface scattering is stronger in \( ^{12}\text{C}/^{22}\text{C} \) superlattice which has larger phonon spectra mismatch arises between the \( ^{12}\text{C} \) and \( ^{22}\text{C} \) layers. Moreover, the allowed maximum frequency will decrease as atomic mass rises according to the phonon dispersion relations [6, 10]. Therefore, the heavy atom layer plays the role of low pass filter, which will prevent the transport of high frequency phonons. As a result, the phonon transmittance is degraded to zero when the frequency is above a cutoff frequency, which is about 1,550 cm\(^{-1}\) in the \( ^{12}\text{C}/^{13}\text{C} \) superlattice shown in Figure 5a–c, and has a smaller value about 1200 cm\(^{-1}\) in the \( ^{12}\text{C}/^{22}\text{C} \) superlattice shown in Figure 5b, d.

The dot lines in Figure 5 indicate the transmittance in the semi-disordered superlattice. The defect concentration \( \eta = 20\% \) for IS-ZGNR, and \( \eta = 17\% \) for IS-AGBR. A small fraction of randomly
distributed isotopes can introduce additional defect scatterings in superlattice structure, denoted by the difference between solid line and dot line in Figure 5. It is obvious that the defect scattering is stronger in high frequency range, and in semi-disordered $^{12}\text{C}/^{22}\text{C}$ superlattice with large mass discrepancy between $^{22}\text{C}$ and $^{12}\text{C}$. The transmittance tuned by the ideal $^{12}\text{C}/^{22}\text{C}$ superlattice is

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure5.png}
\caption{Phonon transmittance as a function of the frequency. In each figure, the solid and dot lines correspond to the ideal and semi-disordered superlattice, respectively. In (a) and (b), the period length of IS-ZGNR is 1.5069 nm, and $\eta = 20\%$ for the semi-disordered superlattice. In (c) and (d), the period length of IS-AGNR is 1.74 nm, and $\eta = 17\%$ for the semi-disordered superlattice. The dash line denotes the pristine $^{12}\text{C}$ ZGNR in (a) and (b), and the pristine $^{12}\text{C}$ AGNR in (c) and (d). Note: IS-ZGNR, isotopic-superlattice graphene nanoribbons with zigzag edges; IS-AGNR, isotopic-superlattice graphene nanoribbons with armchair edges.}
\end{figure}

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure6.png}
\caption{Phonon transmittance as a function of the frequency for the semi-disordered $^{12}\text{C}/^{13}\text{C}$ IS-AGNR with the period length $L = 1.74$ nm. The defect concentration $\eta = 0$, 17 and 50$\%$ in (a), (b) and (c), respectively. Note: IS-AGNR, isotopic-superlattice graphene nanoribbons with armchair edges.}
\end{figure}
represented by the solid line, which shows intensive oscillations in the frequency range from 0 to 1,200 cm\(^{-1}\) in Figure 5b–d. As a comparison, the transmittance tuned by the semi-disordered \(^{12}\text{C}/^{22}\text{C}\) superlattice is represented by the relatively flat dot lines, significantly reduced and approaches to zero when the frequency is above about 800 cm\(^{-1}\) in the semi-disordered IS-ZGNR shown in Figure 5b, and about 500 cm\(^{-1}\) in the semi-disordered IS-AGNR shown in Figure 5d. The defect scattering discussed above is the cause of the thermal conductance reduction associated with defect concentration discovered in Figures 3 and 4.

Figure 3b demonstrates that as the defect concentration increases, the thermal conductance undergoes a transition from decreasing to increasing for the IS-AGNR. The reason can be disclosed by Figure 6. The comparison between Figure 6a, b illustrates that as the rising of the defect concentration from 0 to 17%, the phonon transmittance is reduced, more apparently at higher frequencies. Then the thermal conductance decreases correspondingly as shown in Figure 3b. When the defect concentration increases further and the superlattice interfaces begin to be destroyed, the oscillations of phonon transmittance due to the interface scattering are partly smoothed out and the quantization plateaus are gradually recovered as shown Figure 6c. As a result depicted in Figure 3b, the thermal conductance rises again.

4. Conclusion

The thermal conductance in the IS-ZGNR and IS-AGNR is investigated by using the AGF method. Simulation results indicate that the isotopic-superlattice modulation can reduce the thermal conductance more effectively in IS-AGNR than in IS-ZGNR. Moreover, the thermal conductance of out-of-plane modes is more likely to be reduced than that of in-plane modes. Such reduction effect can be promoted by enlarging the isotope mass discrepancy. The thermal conductance changes non-monotonically as the superlattice period length decreases, and there exists a minimum thermal conductance at the critical period length.

In the semi-disordered isotopic-superlattice, all the layers are randomly mixed with a fraction of different isotopes as defects. These defects lead to additional phonon scattering in the superlattice structure. When the defect concentration is about 20%, the thermal conductance still changes non-monotonically with the superlattice period length, but the value is further reduced, and the critical period length \(L_C\) decreases. As the defect concentration increases, the thermal conductance decreases monotonically in IS-ZGNR, but in IS-AGNR the thermal conductance first decreases to its minimum value and then increases. This phonon transport mechanism in the semi-disordered isotopic-superlattice is explained by analyzing the phonon transmittance.

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ORCID

Yunfeng Gu http://orcid.org/0000-0001-8089-9869

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