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Thermal conductivity modeling of circular-wire nanocomposites

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A phonon Boltzmann equation solver using multiblock-structured grid system is developed and applied to study transverse thermal transport in silicon–germanium circular-wire nanocomposite (silicon nanowires embedded in germanium host matrix). Past studies usually assume geometric simplification for the circular-wire nanocomposite, so the heat transfer is actually modeled in a square-wire nanocomposite. To demonstrate geometry effect, phonon transport in both the circular-wire and square-wire nanocomposites are investigated with various wire spacings, volume fractions, and dimensions. In ballistic phonon transport, due to the smoothness of circular shape, the circular wire imposes less thermal resistance than the square wire. Nevertheless, in the geometric simplification, the wire spacing of the square-wire nanocomposite is larger than that of the circular-wire nanocomposite. The usual geometric simplification can overestimate the thermal conductivity of the circular-wire nanocomposite. The obtained results can provide essential information for the development of bulk-nanostructured thermoelectric devices. © 2010 American Institute of Physics. [doi:10.1063/1.3457230]

I. INTRODUCTION

Nanocomposites attract much attention for their potential application in thermoelectric (TE) devices.\textsuperscript{1–3} The performance of TE devices can be quantified by the TE figure of merit $ZT=\frac{S^2\sigma T}{k}$, here $S$ is the Seebeck coefficient, $\sigma$ the electrical conductivity, $T$ the temperature, and $k$ is the thermal conductivity. Nanocomposites have an extremely high interface density which dramatically reduces their lattice thermal conductivity as compared with their bulk sized equivalents. To design high-efficiency bulk-nanostructured TE devices, it is necessary to comprehensively understand the heat transfer in composite structures. Heat conduction in semiconductors and insulators is mainly through lattice vibrations. Theses vibrations travel within the medium as waves and can be regarded as pseudoparticles, called phonons.\textsuperscript{4} The prevailing approach for evaluating thermal conductivity of a composite is effective medium approximation (EMA).\textsuperscript{5} Although EMA can accurately predict the thermal conductivity for macrostructured composites, its predictions for nanocomposites cannot match with those based on phonon Boltzmann transport equation (BTE) model\textsuperscript{6,7} due to phonon size effect. To understand the mechanisms affecting carrier transport, molecular dynamics (MD) simulation\textsuperscript{8} provides the most accurate picture for phonon transport from atomic scale. Nanometer-scale composites are investigated based on MD for atomistic design.\textsuperscript{9,10} Nevertheless, atomistic simulations require tremendously huge computer power for realistic engineering problems. As an alternative, the phonon BTE is more efficient for the phonon transport from nanoscale to microscale.

Phonon transport can be well described with the phonon BTE as the length scale is much greater than phonon coherent length.\textsuperscript{11} In general, the phonon BTE is difficult to be analytically solved for realistic phonon dispersion and complex scattering events. Monte Carlo (MC) method, which can easily incorporate with the phonon dispersion and scattering processes, provides an alternative to solve the phonon BTE indirectly.\textsuperscript{12} However, the stochastic nature of MC leads to statistical error and long computation time is required to yield good statistical accuracy. For the phonon transport from nanoscale to microscale, the direct phonon BTE solver\textsuperscript{13} is an accurate and efficient way. A rigorous phonon transport solution should incorporate the phonon dispersion and the frequency- and temperature-dependence of the scattering process.\textsuperscript{14–16} Further, the phonon dispersion relation can be altered at nanoscale.\textsuperscript{17,18} For phonon transport in nanocomposites which is dominated by interface scattering, the major contribution to the thermal conductivity reduction comes from the interface scattering.\textsuperscript{19} Based on the dispersion model in which the average phonon mean free path (MFP) is estimated by taking bulk phonon dispersion relation into account,\textsuperscript{20} the thermal conductivities of superlattice predicted by phonon BTE model\textsuperscript{21,22} are in good agreement with the experimental results. Therefore, past studies on the phonon transport in nanocomposites\textsuperscript{7,22,23,25} applied the dispersion model. Phonon size effect can be obtained from these square- or cubic-geometric composites at nanoscale. Very recently, Hao et al.\textsuperscript{26} pointed out the importance of considering the frequency-dependent MFP at microscale to submicroscale. Their MC results for porous materials with square-cylinder pores can predict the strong size effect occurs in microporous material\textsuperscript{27} by taking account of the individual phonon behavior for different frequency bands and branches.

Phonon size effect can be demonstrated from the simple-geometric nanostructures, but many multidimensional problems of practical interest involve complex geometries. A Cartesian phonon BTE solver for the Cartesian grid system is insufficient for solving these practical problems. Past studies on heat transfer in complex-geometric nanocomposites

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adopted geometric simplifications to convert the complex geometry into a simpler one. Due to the ballistic nature of phonons, the geometry effect, which comes from shape, spacing, and orientation of nanostructures, will play an important role in ballistic phonon transport. Undoubtedly, one may anticipate the geometric simplification can lead to large errors in ballistic regime. Despite the importance of the geometry effect, there are only a few studies for phonon transport in complex-geometric nanostructures due to the complexity of tracing the three-dimensional (3D) phonon motions. Prasher studied transverse thermal conductivity of two-dimensional (2D) cylindrical-pore materials with ballistic-diffusive effective medium model. Moore et al. preformed MC to investigate the effect of sawtooth roughness in nanowires and pointed out the possibility of phonon backscattering. Liu et al. applied MC to investigate curvature effect of curved square nanowires. Sakurai et al. applied discrete ordinate radiation element method to study 2D and 3D cylindrical-pore materials.

Complex-geometric composite structures are hard to be modeled due to the presence of irregular material interfaces. Murthy and Mathur developed an unstructured finite volume method to study composites embedded with round rods. However, they imposed a completely absorbing boundary condition at the interface and Fourier law is assumed to hold within the rods. Thus, their analysis is suitable as the rod diameter is greater than the phonon MFP. On the other hand, although the unstructured grid system is very flexible for complex geometry, one must keep memory of the neighbors of each cell explicitly. Therefore, it is difficult to extend a Cartesian phonon BTE solver to an unstructured one without many changes in data structures of the phonon BTE solver. Contrarily, in a structured grid system [Fig. 1(a)], the logical structure underlying the connectivity between computational cells is identical to that of a Cartesian grid system, so it is relatively easy to extend a Cartesian phonon BTE solver to a structured phonon BTE solver. In computational fluid dynamics, the structured grid system is commonly used in multidimensional problems and has considerably less memory requirement for the same level of accuracy as compared to the unstructured grid system. Furthermore, a multiblock grid system, which contains two or more structured grid systems, is a very popular method due to its accuracy and flexibility to handle complicated geometries. We develop a structured finite volume method for the multiblock grid system which is suitable for investigating the phonon transport in nanostructures involve arbitrary geometries.

In this study, we focus on the geometry effect on phonon transport. To clarify, the block-structured phonon BTE solver with the dispersion model is performed for solving phonon transport in circular-wire and square-wire nanocomposites. By directly comparing the circular-wire and square-wire composite structures based on the same parameters, we can validate the rationality of the geometric simplification and assess more precisely the benefit of the geometry effect on TE efficiency enhancement.

II. THEORETICAL MODEL AND SIMULATION

In terms of phonon intensity \( I(\hat{r}, \hat{\Omega}, t) \) and equilibrium phonon intensity \( I_E(\hat{r}, t) \), the phonon BTE under relaxation time approximation can be expressed as

\[
\frac{\partial I}{\partial t} + \hat{v} \cdot \nabla I = \frac{I_E - I}{\tau},
\]

where \( \hat{r} = (x, y, z) \) is the position vector, \( \hat{\Omega} = (\mu, \eta, \zeta) \) = (cos \( \theta \), sin \( \theta \cos \phi \), sin \( \theta \sin \phi \)) is phonon radiative direction [Fig. 1(b)], \( t \) is time, \( \hat{v} \) is the phonon velocity, and \( \tau \) is the relaxation time. Here \( \tau = \Lambda / v \) and \( \Lambda \) is the phonon MFP which can be evaluated from the bulk thermal conductivity \( k_{\text{bulk}} = C v \Lambda / 3 \). In the dispersion model, the average phonon specific heat \( C \) and the phonon velocity \( v \) are estimated by approximating the bulk phonon dispersions of the acoustic branches with sine functions.

The phonon intensity and equilibrium phonon intensity satisfy the conservation condition, so the equilibrium phonon intensity can be expressed as

\[
I_E = \frac{1}{4\pi} \int_{\Omega} I d\hat{\Omega} = \frac{C v T}{4\pi}.
\]

In ballistic phonon transport, the effective temperature merely represents local phonon energy because local thermal equilibrium cannot be established. The degree of nonequilibrium is characterized by Knudsen number (Kn) which is defined as the ratio of the phonon MFP to the characteristic size. The characteristic size chosen will depend on the problem under consideration. The wire dimension \( L_w \) denotes the diameter and width of the circular and square wires, respectively. The unit cell size \( L \) is the width of the unit cell. The wire volume fractions are \( \Phi_S = (\pi/4)L_w^2/L^2 \) and \( L_w^2/L^2 \) for the circular-wire and square-wire nanocomposites, respectively. The wire spacing \( d = L - L_w \) is the characteristic size.
or diffuse scattering. Recent study on interface roughness in transition regime as Kn is ranging from 0.1 to 10. When Kn is less than 0.1, the Fourier law is assumed to be valid. The transport is expressed as

\[ I(\bar{r}_B, \bar{\Omega}, t) - I_E(\bar{r}_B, t) = I(\bar{r}_P, \bar{\Omega}, t) - I_E(\bar{r}_P, t), \]

where \( \bar{r}_B \) and \( \bar{r}_P \) represent the boundary and corresponding periodic locations, respectively. The equilibrium intensity satisfies \( I_E(\bar{r}_B, t) - I_E(\bar{r}_P, t) = C_0 \Delta T / 4 \pi \). Here, \( \Delta T \) is the applied temperature difference. At y-directional boundaries, the implementation of periodic boundary condition is simply to set the phonon intensity at the boundary location to be identical as that at the corresponding periodic location. The heat flux is defined as \( q = \int_\Omega \mu d\bar{\Omega} \).

A block-structured phonon BTE solver for the multiblock-structured grid system is developed. The procedure contains two main steps. One is discrete ordinate method (DOM) for discretizing phonon radiative direction and the other is upwind finite volume scheme for solving linear advection equations in the multiblock-structured grid system. In the DOM, the phonon radiative direction \( \bar{\Omega} \) is divided into discrete directions \( \bar{\Omega}_k \) by discretizing \( \mu \) and \( \phi \) with Gauss–Legendre quadrature to achieve high-order integration accuracy and resolve the ray effect at nanoscale. The integration over the phonon radiative direction can then be approximated by a summation of the integrated value multiplying its weight \( w_i \) in each direction. As an example, the equilibrium phonon intensity can be represented as

\[ I_E = \frac{1}{4\pi} \sum_{k=1}^{N} w_i I_k, \]

where \( N \) is the total number of phonon radiative directions and subscript \( k \) represents the phonon radiative direction.

With the phonon intensity direction discretized, the original integral-differential phonon BTE is transferred into a set of advection equations with source terms. In each phonon radiative direction \( \bar{\Omega}_k \), the phonon BTE can be expressed as

\[ \frac{\partial I_k}{\partial t} + \bar{v} \cdot \nabla I_k = \frac{I_k - I_E}{\tau}. \]

To solve for the advection equation with source term, the multiblock grid system is utilized to discretize the spatial domain. In the multiblock grid system, the spatial domain is divided into several blocks and a structured grid system is constructed in each block domain. In a 2D structure grid system [Fig. 1(a)], each cell is an arbitrary quadrilateral bounded by four linear edges. Each cell has four cell vertices and the data value is presented at the cell center. Therefore, one can label the cells in a logical manner, indexing “rows” and “columns” by \( i \) and \( j \), then cell \( (i,j) \) has four neighbor cells \((i \pm 1,j)\) and \((i,j \pm 1)\). In each structure grid system, the donor-cell upwind method (DCU) for the advection equation is adopted. The stencil of DCU can be expressed as

\[ f_{k,i,j}^{n+1} = f_{k,i,j}^n - \frac{\Delta t}{A_{ij}} (h_{i+1/2,j} f_{k,i+1/2,j} - h_{i-1/2,j} f_{k,i-1/2,j} + h_{i,j+1/2} G_{k,i,j+1/2} - h_{i,j-1/2} G_{k,i,j-1/2}) + \frac{\Delta t}{\tau} (F_{k,i,j}^n - F_{k,i,j}^n), \]
where superscript $s$ is the time step index, $\Delta t$ is the time step size, $A_{ij}$ is area of cell $(i,j)$, $h_{i,j+1/2}$ and $F_{k,i+1/2,j}$ are length and phonon intensity flux of edge $(i+1/2,j)$, and $h_{i,j+1/2}$ and $G_{k,i+1/2,j}$ are length and normal phonon intensity flux of edge $(i,j+1/2)$. The phonon radiative fluxes $F_{k,i+1/2,j}$ and $G_{k,i+1/2,j}$ present the fluxes of phonon intensity $I_k$ across cell edges $(i+1/2,j)$ and $(i,j+1/2)$, respectively. The phonon radiative fluxes are calculated based on upward propagation directions across the cell edges as

\[
F_{k,i+1/2,j} = v \left( J_{k,i+1/2,j} + \frac{1}{2} J_{k,i+1/2,j} \right) + \frac{1}{2} J_{k,i+1/2,j} - J_{k,i+1/2,j},
\]

\[
G_{k,i+1/2,j} = v \left( J_{k,i,j+1/2} + \frac{1}{2} J_{k,i,j+1/2} \right) + \frac{1}{2} J_{k,i,j+1/2} - J_{k,i,j+1/2},
\]

where $J_{k,i+1/2,j}$ and $J_{k,i,j+1/2}$ are the dot products of phonon radiative direction $\hat{\Omega}_k$ with the normal vectors $\hat{n}_{i+1/2,j}$ and $\hat{n}_{i,j+1/2}$ [Fig. 1(a)].

The multiblock system of the circular-wire composite [Fig. 2(c)] is used in our simulation. In the multiblock grid system, two structured grid systems, including host and wire grid systems, are connected to each other at the interface. In the host material domain, a grid system is generated by producing the cell vertexes in the manner of polar coordinate $(R, \Theta)$. The radius $R$ is interpolated between the wire shape and square unit cell. To increase the spatial resolution, the cell sizes are reduced near wire boundary ($R = L_w/2$) and diagonals ($\Theta = \pi/4, 3\pi/4, 5\pi/4$, and $7\pi/4$). In the wire domain, from the cell vertexes on the interface, a grid system is produced by transfinite interpolation. To better illustrate the multiblock grid system, a course $20 \times 160$ host grid system and a $40 \times 40$ wire grid system are drawn in Fig. 2(c). A similar mesh system is used for the square-wire composite. For the boundary conditions of the host grid system, the periodic boundary condition is applied at locations $x = \pm 0.5$, $y = \pm 0.5$, and $\Theta = 7\pi/4$. For the interface boundary conditions of the host and wire grid systems, the diffusive interface condition is imposed. The interaction between the host and wire grid system is involved through the interface condition.

To reduce the computing time for steady state solution, an efficient implicit lower-upper symmetric Gauss–Seidel solution algorithm is adopted and the block-structure phonon BTE solver is parallelized by decomposing the phonon radiative directions. The steady solution is obtained as the maximum deviation of the equilibrium phonon intensity between two successive iterations is less than $10^{-6}$. Then, the effective thermal conductivity can be calculated by $k = \bar{q}L/\Delta T$, here $\bar{q} = \int q dy/L$ is the average heat flux. The following dimensionless units are used to present the numerical results

\[
\hat{x} = \frac{x}{L}, \quad \hat{y} = \frac{y}{L},
\]

\[
\hat{T} = \frac{T - T_0}{\Delta T}, \quad \hat{q} = \frac{4\pi q}{C_0 v_0 \Delta T},
\]

where $C_0$ and $v_0$ are the specific heat and phonon velocity of the host material, respectively. The reference temperature $T_0$ is 300 K and the constant temperature difference $\Delta T$ is 1 K. The bulk thermal conductivities of silicon (Si) and germanium (Ge) are 150 and 60 W/mK at room temperature $T = 300$ K. The parameters of Si and Ge are taken from Yang and Chen. The MFP of Si and Ge are 268 nm and 198 nm, respectively. In our simulation, a $40 \times 480$ host grid system and a $120 \times 120$ wire grid system are used. The phonon radiative direction is divided by discretizing $\mu(-1+1)$ into 80 directions and $\phi(0-\pi)$ into 30 directions. Therefore, the total number of phonon radiative directions used is $N=2400$.

To ensure the grid independence of the solution, several finer grid systems are extensively tested and the relative deviation in effective thermal conductivity between current and finer grid systems is less than 0.5%.

In this work, the block-structured phonon BTE solver with the dispersion model and diffusive interface condition is presented for 2D composite structures. We note that this procedure can be readily extended to 3D geometries and take account of the interface roughness and realistic phonon dispersion without much effort.

### III. RESULT AND DISCUSSION

To ensure the correctness of our block-structured phonon BTE solver, we simulate transverse thermal transport of the square-wire Si–Ge nanocomposites for several wire volume fractions and dimensions. Based on the same parameters, the predicted thermal conductivities of the Si–Ge square-wire nanocomposites are compared with those obtained using the Cartesian phonon BTE solver. As shown in Fig. 3, our predictions are in good agreement with phonon BTE solutions using the Cartesian grid system for a wide range of wire volume fractions ($\Phi_{Si}=0.2-0.8$).

### A. NONEQUILIBRIUM PHONON TRANSPORT

The steady state results (effective temperature and heat flux) for transverse heat transport of the circular-wire Si–Ge nanocomposites ($\Phi_{Si}=0.2$) with $L_w=10$ and 500 nm are presented in Figs. 5 and 6, respectively. Simple calculation gives the ratio $L/L_w=1.982$ for $\Phi_{Si}=0.2$. As the wire dimension is 10 nm, the phonon transport is in ballistic regime ($Kn=20.2$). The temperature contour within the unit cell [Fig. 4(a)] is highly nonuniform. The maximum temperature occurs in front of the circular wire (located at $R=0.5L_w/L$ and $\Theta=\pi$) and the minimum temperature occurs behind the wire (located at $R=0.5L_w/L$ and $\Theta=0$). The temperature distribution is asymmetric along the $y$-axis and symmetric with respect to the $x$-axis. We note that, in ballistic regime, local thermal equilibrium cannot be established and thus the effective temperature merely represents local phonon energy. Since almost no intrinsic scattering occurs, ballistic phonon transport occurs dominantly.
transport is dominated by interface scattering. In the host medium, phonons can drift freely until they collide with the interface. The region in front of the wire can receive higher energy phonons come from upstream flow region outside the unit cell. Consequently, the relative higher temperature occurs in front of the wire. Although only a unit cell domain is used, this nonlocal transport, which may take place over a range of several characteristic sizes, can be captured by imposing the periodic boundary condition. On the other hand, since very few phonons can arrive in the rear of the wire without been scattered, a low-temperature area appears behind the wire (as a shadow). Because phonons drift ballistically in the medium, interface scattering contributes the major part of phonon energy loss. Due to thermal resistance of the interface, temperature drop across the interface is formed. To better illustrate the temperature drop, the temperature profiles along the $x$-direction at three different $y$-locations are plotted in Fig. 4(b). Besides, according to Fourier heat conduction based theories, the temperature gradient along $y=0$ line should produce negative heat fluxes in the host medium. Nevertheless, from the heat flux distribution [Fig. 4(c)], the heat fluxes are always positive. Contrary to macrocomposite, the heat flux distribution is entirely opposite in ballistic regime. That is, although the bulk thermal conductivity of the wire material Si is greater than that of host Ge, the heat flow is found to avoid the Si wire. Relatively large heat flux appears around the top and bottom of the unit cell. This indicates ballistic phonons automatically choose the pathway in which no interfaces exist. When the wire dimension is increased to 500 nm, the phonon transport is in transition regime ($Kn=0.4$). The temperature contour [Fig. 5(a)] is close to the temperature distribution that one can expect in macrocomposites. The maximum and minimum temperatures occur at the $x$-directional boundaries $x=-0.5$ and 0.5, respectively. In transition regime, phonons suffer more intrinsic scattering in the medium as compared with ballistic transport, so interface scattering contributes the minor portion of the phonon energy loss. Therefore, the temperature distribution is uniformly varying from high temperature to low temperature. From the temperature profiles [Fig. 5(b)], the temperature
drop is much smaller as compared with ballistic transport. Because interface scattering is less dominant, the heat flux distribution is more uniform [Fig. 5(c)]. More phonons pass through the Si wire because Si contains less intrinsic scattering than host Ge.

FIG. 5. (Color online) (a) Temperature distribution, (b) temperature profiles along x-direction, and (c) heat flux distribution of the circular-wire Si–Ge nanocomposite ($\Phi_{Si}=0.2$) for $L_w=500$ nm.

B. Effect of wire shape

To demonstrate the effect of wire shape on ballistic transport, the transverse heat transport in the circular-wire and square-wire Si–Ge nanocomposites are compared based on the same values of wire spacing. For $d=10$ nm, the temperature contours (Fig. 6) and heat flux contours (Fig. 7) show dissimilar features between the circular and square wires ($L_w=20$ nm). Due to ballistic phonon transport ($Kn =19.8$), the temperature contours are nonuniform for both cases. The temperature distributions are asymmetric with respect to the y-axis and symmetric along the x-axis. As mentioned earlier, a temperature peak can be clearly obtained in front of the circular wire [Fig. 6(a)]. The square shape has discontinuous surface tangent at corners while the circular shape has continuous variation in surface slope. Since the interface has an abrupt change at the square corners, two
temperature peaks occur at the corners in front of the square wire [Fig. 6(b)]. Moreover, the maximum temperature in the square-wire Si–Ge nanocomposite is greater than that in the circular-wire Si–Ge nanocomposite. On the other hand, the minimum temperature in the square-wire Si–Ge nanocomposite is less than that in the circular-wire Si–Ge nanocomposite. The shadow behind the square wire is darker compared with the circular wire. Consequently, the heat fluxes in the circular-wire Si–Ge nanocomposite are larger than those in the square-wire Si–Ge nanocomposite. To better demonstrate the effect of wire shape, the thermal conductivity of the Si–Ge nanocomposites as a function of wire dimension for $d=10$, 20, and 30 nm is drawn in Fig. 8. With a fixed wire spacing, the thermal conductivity of the circular-wire nanocomposite is obviously larger than that of the square-wire nanocomposite. Specifically, the circular-wire nanocomposite can yield about 24% higher thermal conductivity than the square-wire nanocomposite ($L_w=20$ nm) for the wire spacing $d=10$ nm. Accordingly, the circular wire imposes less thermal resistance to the heat flow when compared with the square wire. Besides, from Fig. 8, one can also obtain that thermal conductivity is very sensitive to the wire spacing. As the wire spacing is decreased, the thermal conductivity of the composite decreases. We note that altering the wire spacing is equivalent to changing the wire volume fraction of a composite structure. The discussions about the effect of wire volume fraction on phonon transport can also be found in past studies.6,7,23

C. Rationality of geometric simplification

Geometric simplification is commonly adopted for phonon transport in nanocomposites.6,7,26 To study the phonon transport for the circular-wire composite structure, in the geometric simplification, one replaces the circular wire by the square wire with the same wire dimension and volume fraction. Because the circular shape is smoother than the square shape, one may naturally anticipate that the geometric simplification can underestimate the thermal conductivity of the circular-wire composite structure, especially in ballistic regime. Figure 9 shows the thermal conductivity of the Si–Ge nanocomposites as a function of wire volume fraction.
for \( \Phi_{\text{Si}} \) from 0.2 to 0.7. It should be noted that, because the restriction \( L_w < L \), the wire volume fraction of the circular-wire composite structure cannot exceed \( \pi/4 \). For both the circular-wire and square-wire Si–Ge nanocomposites, we can observe that the larger the wire volume fraction is the lower the thermal conductivity will be. Therefore, the effect of wire volume fraction on ballistic phonon transport can be obtained for both circular and square wire shapes. Nevertheless, contrary to one’s expectation, the circular-wire Si–Ge nanocomposite is found to yield lower thermal conductivity than the square-wire Si–Ge nanocomposite. Furthermore, the discrepancy in thermal conductivity increases as the wire volume fraction is increased. For \( L_w = 10 \) nm, the thermal conductivities of the circular-wire Si–Ge nanocomposites are about 1% and 12% smaller than those of the square-wire Si–Ge nanocomposites with \( \Phi_{\text{Si}} = 0.2 \) and 0.7, respectively. In the geometric simplification, due to a fixed wire volume fraction \( \Phi_{\text{Si}} \) is maintained, the wire spacings of the circular-wire and square-wire nanocomposites are \( d = \left( \sqrt{\pi/4}/\Phi_{\text{Si}} - 1 \right)L_w \) and \( (\sqrt{1/\Phi_{\text{Si}}}-1)L_w \), respectively. Thus, the wire spacings of the square-wire composite structures are about 26% and 230% larger than those of the circular-wire composite structures for \( \Phi_{\text{Si}} = 0.2 \) and 0.7, respectively. Although the thermal resistance is increased with the square wire, the benefits thereof can be overcompensated by much wider wire spacing as compared to the circular-wire nanocomposite. As a result, the geometric simplification overestimate the thermal conductivity of the circular-wire nanocomposite. Figure 10 shows the thermal conductivities of the Si–Ge nanocomposites as a function of wire dimension for \( \Phi_{\text{Si}} = 0.2, 0.5, \) and 0.7. The deviation in thermal conductivity is increased as the wire dimension is decreased. Apparently, the geometric simplification will lead to large error in ballistic regime. On the other hand, the geometric effect is decreased as the wire dimension is increased and the approximation can be considered as adequate. Specifically, for \( \Phi_{\text{Si}} = 0.5 \), the thermal conductivities of the circular-wire Si–Ge nanocomposites are about 11% and 3% lower than those of the square-wire Si–Ge nanocomposites with \( L_w = 10 \) nm and 500 nm, respectively.

IV. CONCLUSION

We have developed a block-structured phonon BTE solver to study phonon transport in arbitrary geometries. The phonon transport in both the circular-wire and square-wire Si–Ge nanocomposites for various wire spacings, volume fractions, and dimensions is extensively investigated to demonstrate the effect of wire shape and validate the rationality of the geometric simplification. Results show that the geometry effect can no longer be ignored as phonon transport is in ballistic regime. The geometric simplification can overestimate the thermal conductivity of the circular-wire composite structure. Specifically, for \( L_w = 10 \) nm, the thermal conductivity of the square-wire Si–Ge nanocomposite is about 13% greater than that of the circular-wire Si–Ge nanocomposite (\( \Phi_{\text{Si}} = 0.7 \)). The geometry effect is decreased as the wire dimension is increased. For \( L_w = 500 \) nm, the thermal conductivity of the circular-wire Si–Ge nanocomposite (\( \Phi_{\text{Si}} = 0.2 \)) is nearly 99% of its square counterpart. The predicted thermal conductivity based on the geometric simplification is very close to the actual thermal conductivity of the circular-wire composite structure as the wire dimension is approaching micrometer scale. The obtained results can be useful for the design of high-efficiency TE devices. Our block-structured phonon BTE solver can serve as a very useful analysis tool for investigating heat transfer in realistic engineering problems from nanoscale to macroscale.

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