

Scattering matrix formalism for interface heat conduction based on Monte Carlo evaluation of the phonon Boltzmann transport equation

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As electronic devices continue to advance, accurate thermal management at the nanoscale is becoming increasingly crucial in engineering design. While the phonon Boltzmann transport equation (BTE) is commonly used for this purpose, conventional boundary conditions, such as the acoustic mismatch model (AMM) and diffuse mismatch model (DMM), fail to accurately predict nanoscale heat transport. In this work, we evaluate an interfacial boundary condition based on the scattering matrix (S-matrix) formalism within a low-variance direct simulation Monte Carlo (DSMC) solution of the BTE. The S-matrix framework resolves frequency- and polarization-dependent phonon transmission and reflection, enabling us to examine how microscopic details, including anisotropic scattering neglected by traditional models, lead to large differences in interfacial thermal resistance at ideal and disordered silicon/germanium interfaces. We further demonstrate that while S-matrix data can be used to accurately tune DMM for larger systems of known materials, DMM remains unsuitable for simulating nanoscale devices. Our predictions show good agreement with experimental measurements, and can be used for more accurate nanoscale thermal design of real-world devices.

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I. INTRODUCTION

As electronic devices become more integrated and smaller, the issue of increased heat generation has emerged as a critical bottleneck, undermining operational performance and reliability [1,2]. The main sources of thermal resistance in solid systems are the interfacial structures, such as polycrystalline grain boundaries and heterostructures, making the accurate prediction of interfacial thermal resistance (ITR) essential for optimizing overall device performance.

Heat is primarily carried by phonons, the quantized modes of lattice vibration that possess wave-particle duality [3–5]. A phonon of frequency ω carries an energy of $\hbar\omega$, where $\hbar$ is the reduced Planck constant. Heat transport can be described using a phonon gas model and rigorously formulated through the phonon Boltzmann transport equation (BTE) [5], which tracks the phase-space distribution function of each phonon mode as it evolves, accounting for all relevant scattering processes. The phonon BTE has been solved by two different approaches: (i) deterministic schemes, which discretize and solve the governing integrodifferential transport equation, such as finite-element methods [6], discrete ordinates methods

[7,8], and finite-difference methods [9,10]; and (ii) stochastic schemes, such as Monte Carlo (MC) methods [11,12], which rely on statistical sampling. The latter are particularly well suited for simulating heat flow through complex and heterogeneous real-world structures, as they offer the flexibility of Lagrangian schemes to handle complex computational domains [13,14]. Consequently, MC-based BTE solvers are now widely recognized as an effective technique for quantitatively evaluating interfacial thermal resistance.

The phonon MC method was initially developed based on the standard direct simulation Monte Carlo (DSMC) algorithm for rarefied gas dynamics, and has since been used to simulate phonon evolution and thermal conductivity [15]. However, this original formulation, which simulates the full phonon distribution, is subject to significant statistical noise near equilibrium, resulting in a substantial computational burden. To address this issue, Péraud and Hadjiconstantinou developed the energy-based deviational DSMC method that only tracks small deviations from the equilibrium state [16,17]. While this framework is inherently applicable to multiple phonon branches [18], its implementation based on the relaxation time approximation (RTA) fails when non-resistive scattering processes dominate, as RTA does not conserve momentum [19]. In subsequent work, Péraud and Hadjiconstantinou addressed this limitation by implementing a scattering algorithm that strictly conserves both energy and momentum, enabling the DSMC scheme to achieve superior accuracy in the phonon hydrodynamic regime [20]. Since then, DSMC-based schemes have become the standard methodology for multiscale phonon transport calculations, and have been successfully applied to nanofilms [21,22],

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nanowires [23], superlattices [24], and other low-dimensional structures [25]. Although these schemes have been successfully applied to a wide range of single-phase materials, extending them to heterogeneous structures remains challenging, as the accuracy of boundary conditions at interfaces becomes paramount.

In BTE-based simulations, the interfacial boundary conditions are typically defined using two classical acoustic wave models, i.e., the acoustic mismatch model (AMM) [26] and the diffuse mismatch model (DMM) [27]. AMM assumes that the interface is atomically smooth and elastically continuous, which is most accurate at cryogenic temperatures, where the dominant phonon wavelengths are larger than the characteristic size of the interface. In this model, longitudinal and transverse phonons are partially transmitted across the interface or reflected according to their acoustic-impedance mismatch. By contrast, DMM assumes a fully rough, phase-randomizing interface, which is most accurate at elevated temperatures, where the typical phonon wavelengths are comparable to, or smaller than, the characteristic length of the interface. In this model, incident phonons lose coherence, and their energy is redistributed among available modes on either side of the interface according to the local phonon density of states (DOS). A key limitation of both models is that they neglect the intrinsic spectral dependence of phonon transmission and reflection, thereby preventing them from accurately capturing interfacial effects such as elastic mismatch, rough scattering, and chemical reconfiguration. As a result, their predictive accuracy is reduced, as evident from discrepancies with time-domain thermoreflectance (TDTR) measurements [28] and other simulation results [29,30].

The atomistic Green's function (AGF) approach has proven to be a powerful framework for investigating interfacial heat transport [31,32], as it gives frequency-dependent transmission spectra by solving the harmonic dynamical matrix based on both empirical and *ab initio* modeling. However, it is challenging to extract the transmission of individual phonon modes using the traditional AGF method, which is important for understanding the microscopic contributions of specific phonon modes to ITR at the quantum scale. Ong [33,34] extended the AGF method based on the concept of the Bloch matrix, enabling it to calculate the transmission dependence on the wavelength and polarization of phonons across different spectral modes. Using this extended scheme, the author quantitatively determined the respective contributions of the longitudinal acoustic (LA) and transverse acoustic (TA) phonon branches to the thermal transport in a nanotube junction and graphene edge structure. The author further developed a scattering matrix (S-matrix) method within the AGF framework, taking the bulk phonon eigenmodes as transport channels. The specific mode-to-mode scattering amplitudes can be obtained to construct a full scattering matrix describing the interfacial phonon transport behavior, including the transmission and reflection submatrices. Since the AGF framework contains the dynamical matrix of the interface region, the S-matrix method can also be employed to study the rough [35] and amorphous [36] interface structures. Yang *et al.* [36] integrated AGF-derived mode-resolved data into Monte Carlo simulations by summing the transmission coefficients into scalar values to calibrate their interface model for

amorphous silicon. However, their refinement primarily focuses on adjusting the transmission probability, while still assuming specular scattering when determining outgoing phonon states, which aligns with an AMM framework. In contrast, fully preserving the phase-space information and microscopic anisotropy of phonons at the interface is crucial to overcome the inherent limitations of the classical AMM and DMM models. This motivates us to develop an advanced interfacial boundary condition for the BTE based on the S-matrix method, and to embed the full S-matrix information within the DSMC framework, thus compensating for the shortcomings of the conventional DMM and its underlying physical assumptions, thereby enabling the precise prediction of interfacial thermal resistance.

In this paper, we establish a bridge between the particle-based description inherent to the DSMC scheme and the quantum-mechanical behavior of interfacial phonons, and further build a wavelength- and polarization-dependent boundary condition based on the S-matrix model. Using DSMC, we are now able to directly compare microscopic phonon dynamics, such as transmission and reflection processes, to explain the discrepancies in ITR predicted by the S-matrix and DMM approaches. Although tuning DMM with S-matrix data improves agreement at larger system scales by incorporating predominantly transmission effects, we show how its description of phonon scattering remains invalid at the nanoscale. We further show that the computational cost of using the S-matrix model is only twice as high as that of DMM, and that, when coupled with DSMC, the two can provide a practical and reliable framework for the engineering design of nanoscale heat transfer in solids. In Sec. II, we describe the S-matrix model and its integration into the DSMC framework. Section III presents results from the phonon-based DSMC simulations with the S-matrix method implemented, showing results for interfacial thermal resistance for both ideal and disordered Si/Ge interfaces. Section IV concludes the study.

II. METHODOLOGY

In Sec. II A, for completeness, we provide an overview of the S-matrix developed by Ong [33], along with an explanation of how the scattering matrix is extracted from our *ab initio* simulations. In Sec. II B, we describe its implementation as a boundary condition within the low-variance, phonon-based DSMC framework for solving the BTE developed by Péraud and Hadjiconstantinou [16,17].

A. Extracting the interfacial phonon scattering matrix

The phonon scattering matrix is determined within the AGF framework. In the conventional AGF approach [37–39], the retarded Green's function of the interface region is computed from the dynamical matrices of the constituent materials, enabling the calculation of the total phonon transmission across the interface. However, this approach does not provide mode-resolved or polarization-dependent information, meaning it cannot distinguish how individual phonon modes or polarizations contribute to heat transport. To address this limitation, we adopt the extended AGF method developed by Ong [33]. A representative solid–solid interface is shown in

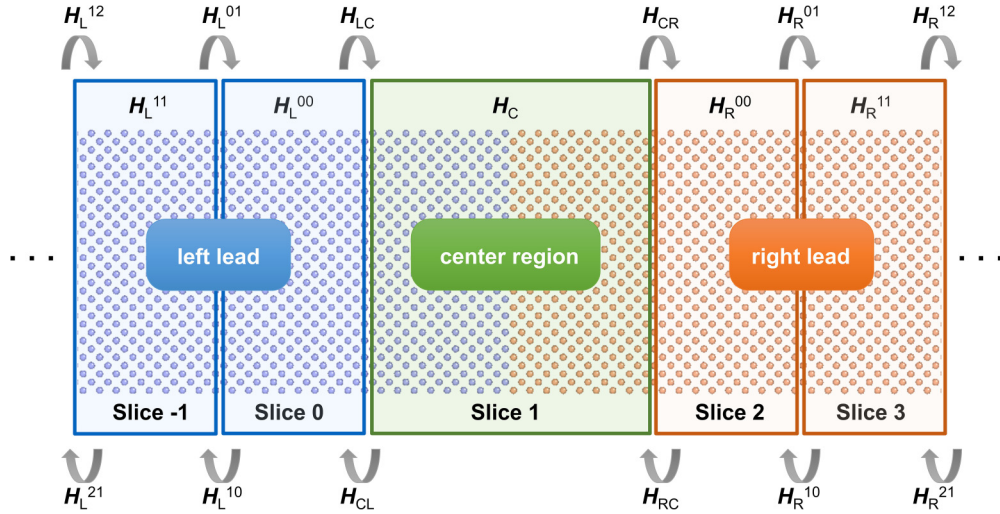


FIG. 1. Schematic diagram used in S-matrix model simulation, consisting of semiinfinite left/right leads and a center region representing the interface.

Fig. 1, and is divided into three regions: the semi-infinite left and right leads, and the central scattering region. Following the standard procedure, the system is then partitioned into slices, and the force-constant matrices (also called Hamiltonian matrices) within each slice and between adjacent slices are then calculated,

$$H = \begin{pmatrix} \cdots & \cdots & & & & & & & & \\ \cdots & H_L^{11} & H_L^{01} & & & & & & & \\ & H_L^{10} & H_L^{00} & H_{LC} & & & & & & \\ & H_L & H_{CL} & H_C & H_{CR} & & & & & \\ & & & H_{RC} & H_R^{00} & H_R^{01} & & & & \\ & & & & H_R^{10} & H_R^{11} & \cdots & & & \\ & & & & H_R & H_R & \cdots & \cdots & & \end{pmatrix}. \quad (1)$$

Each matrix is calculated using density functional theory (DFT), implemented via the Vienna *Ab initio* Simulation Package (VASP) [40–42]. The retarded surface Green's functions are obtained by

$$g_{\alpha,-}^{\text{ret}} = [(\omega^2 + i\eta)I_{\alpha} - H_{\alpha}^{00} - H_{\alpha}^{10} g_{\alpha,-}^{\text{ret}} H_{\alpha}^{01}]^{-1}, \quad (2)$$

$$g_{\alpha,+}^{\text{ret}} = [(\omega^2 + i\eta)I_{\alpha} - H_{\alpha}^{00} - H_{\alpha}^{01} g_{\alpha,+}^{\text{ret}} H_{\alpha}^{10}]^{-1}, \quad (3)$$

where $\alpha = L$ or R denotes the left and right leads, respectively. η is a positive infinitesimal introduced to ensure causality in the Green's function. The advanced surface Green's function can be obtained by taking the Hermitian conjugate of the retarded Green's function,

$$g_{\alpha,-}^{\text{adv}} = (g_{\alpha,-}^{\text{ret}})^{\dagger}, \quad (4)$$

$$g_{\alpha,+}^{\text{adv}} = (g_{\alpha,+}^{\text{ret}})^{\dagger}. \quad (5)$$

To obtain mode-resolved phonon transport properties at the interface, it is first necessary to identify all phonon modes that participate in transport, which can be derived from the advanced and retarded Bloch matrices of the left and right

leads, $F_{\alpha}^{\text{adv/ret}}(+)$ and $F_{\alpha}^{\text{adv/ret}}(-)$,

$$F_{\alpha}^{\text{adv/ret}}(+) U_{\alpha}^{\text{adv/ret}}(+) = U_{\alpha}^{\text{adv/ret}}(+) \Lambda_{\alpha}^{\text{adv/ret}}(+), \quad (6)$$

$$F_{\alpha}^{\text{adv/ret}}(-)^{-1} U_{\alpha}^{\text{adv/ret}}(-) = U_{\alpha}^{\text{adv/ret}}(-) \Lambda_{\alpha}^{\text{adv/ret}}(-)^{-1}, \quad (7)$$

$$F_{\alpha}^{\text{adv/ret}}(+) = g_{\alpha,+}^{\text{adv/ret}} H_{\alpha}^{10}, \quad (8)$$

$$F_{\alpha}^{\text{adv/ret}}(-)^{-1} = g_{\alpha,-}^{\text{adv/ret}} H_{\alpha}^{01}, \quad (9)$$

where U is a matrix whose columns are the eigenvectors of the Bloch matrix, corresponding to propagating or evanescent phonon modes. Specifically, $U_{\alpha}^{\text{ret}}(+)$ and $U_{\alpha}^{\text{ret}}(-)$ contain right-going and left-going modes, respectively, while $U_{\alpha}^{\text{adv}}(-)$ and $U_{\alpha}^{\text{adv}}(+)$ describe their time-reversed counterparts. Λ is a diagonal matrix whose elements take the form $e^{ik_n a}$, where k_n is the phonon wave vector associated with the n th eigenvector in $U_{\alpha}^{\text{adv/ret}}(+)$ or $U_{\alpha}^{\text{adv/ret}}(-)$. In addition, the calculation of individual phonon properties requires the eigenvelocity matrix $V_{\alpha}^{\text{adv/ret}}(\pm)$ with diagonal elements that correspond to the mode-resolved group velocities of the eigenvectors in $U_{\alpha}^{\text{adv/ret}}(\pm)$,

$$V_{\alpha}^{\text{adv/ret}}(+) = \frac{ia_{\alpha}}{2\omega} [U_{\alpha}^{\text{adv/ret}}(+)]^{\dagger} H_{\alpha}^{01} g_{\alpha,+}^{\text{adv/ret}} - (g_{\alpha,+}^{\text{ret/adv}})^{\dagger} H_{\alpha}^{10} U_{\alpha}^{\text{adv/ret}}(+), \quad (10)$$

$$V_{\alpha}^{\text{adv/ret}}(-) = -\frac{ia_{\alpha}}{2\omega} [U_{\alpha}^{\text{adv/ret}}(-)]^{\dagger} H_{\alpha}^{10} g_{\alpha,-}^{\text{adv/ret}} - (g_{\alpha,-}^{\text{ret/adv}})^{\dagger} H_{\alpha}^{01} U_{\alpha}^{\text{adv/ret}}(-). \quad (11)$$

Given Eqs. (10) and (11), the diagonal velocity-normalization matrices $F_{\alpha}^{\text{adv/ret}}(\pm)$ can be defined by

$$I_{\alpha}^{\text{adv/ret}}(+) = V_{\alpha}^{\text{adv/ret}}(+) \tilde{V}_{\alpha}^{\text{adv/ret}}(+), \quad (12)$$

$$I_{\alpha}^{\text{adv/ret}}(-) = V_{\alpha}^{\text{adv/ret}}(-) \tilde{V}_{\alpha}^{\text{adv/ret}}(-), \quad (13)$$

where $\tilde{V}_{\alpha}^{\text{adv/ret}}(+)$ and $\tilde{V}_{\alpha}^{\text{adv/ret}}(-)$ are diagonal matrices whose nonzero diagonal elements are the reciprocals of

the corresponding diagonal elements of $V_{\alpha}^{\text{adv/ret}}(+)$ and $V_{\alpha}^{\text{adv/ret}}(-)$. For phonon modes incident from the left (right)

side of the interface and transmitted to the right (left), the transmission matrix t_{RL} (t_{LR}) can be computed using the following expression:

$$t_{\text{RL}} = \frac{2i\omega}{\sqrt{a_{\text{R}}a_{\text{L}}}} [V_{\text{R}}^{\text{ret}}(+)]^{1/2} [U_{\text{R}}^{\text{ret}}(+)]^{-1} G_{\text{RL}}^{\text{ret}} [U_{\text{L}}^{\text{adv}}(-)^{\dagger}]^{-1} [V_{\text{L}}^{\text{adv}}(-)]^{1/2}, \quad (14)$$

$$t_{\text{LR}} = \frac{2i\omega}{\sqrt{a_{\text{L}}a_{\text{R}}}} [V_{\text{L}}^{\text{ret}}(-)]^{1/2} [U_{\text{L}}^{\text{ret}}(-)]^{-1} G_{\text{LR}}^{\text{ret}} [U_{\text{R}}^{\text{adv}}(+)^{\dagger}]^{-1} [V_{\text{R}}^{\text{adv}}(+)]^{1/2}, \quad (15)$$

where a_{L} and a_{R} are lattice constants for the left and right side materials. Each row and column of the transmission matrix corresponds to transmitted and incident phonon modes, respectively, with evanescent modes contributing zero owing to their vanishing group velocities. The squared magnitude $|\mathbf{t}|_{mn}|^2$ gives the transmission probability from an incident mode m to a transmitted mode n . Similarly, phonon reflection behavior at the interface can be represented by the reflection matrix r_{LL} (r_{RR}), which characterizes the amplitude of phonon modes reflected back into the left (right) lead,

$$r_{\text{LL}} = \frac{2i\omega}{a_{\text{L}}} [V_{\text{L}}^{\text{ret}}(-)]^{1/2} [U_{\text{L}}^{\text{ret}}(-)]^{-1} (G_{\text{L}}^{\text{ret}} - Q_{\text{L}}^{-1}) [U_{\text{L}}^{\text{adv}}(-)^{\dagger}]^{-1} [V_{\text{L}}^{\text{adv}}(-)]^{1/2}, \quad (16)$$

$$r_{\text{RR}} = \frac{2i\omega}{a_{\text{R}}} [V_{\text{R}}^{\text{ret}}(+)]^{1/2} [U_{\text{R}}^{\text{ret}}(+)]^{-1} (G_{\text{R}}^{\text{ret}} - Q_{\text{R}}^{-1}) [U_{\text{R}}^{\text{adv}}(+)^{\dagger}]^{-1} [V_{\text{R}}^{\text{adv}}(+)]^{1/2}, \quad (17)$$

where

$$Q_{\alpha} = (\omega^2 + i\eta)I_{\alpha} - H_{\alpha}^{00} - H_{\alpha}^{10} g_{\alpha,-}^{\text{ret}}(\omega) H_{\alpha}^{01} - H_{\alpha}^{01} g_{\alpha,+}^{\text{ret}}(\omega) H_{\alpha}^{10}. \quad (18)$$

Using the transmission and reflection matrices obtained from Eqs. (14) to (17), the rationalized smaller matrices $\bar{t}_{\text{RL}}$, $\bar{t}_{\text{LR}}$, $\bar{r}_{\text{LL}}$, and $\bar{r}_{\text{RR}}$ can be constructed by excluding the matrix components associated with evanescent modes, and retaining only propagating channels. Specifically, the matrix entries associated with any channel n for which the diagonal indicator satisfies $[I_{\alpha}^{\text{adv/ret}}(\pm)]_{nn} = 0$ are removed from t_{RL} , t_{LR} , r_{LL} , and r_{RR} . A scattering matrix can be constructed that relates the amplitudes of both transmitted and reflected phonons by combining $\bar{t}_{\text{RL}}$, $\bar{t}_{\text{LR}}$, $\bar{r}_{\text{LL}}$, and $\bar{r}_{\text{RR}}$,

$$S = \begin{pmatrix} \bar{r}_{\text{LL}} & \bar{t}_{\text{LR}} \\ \bar{t}_{\text{RL}} & \bar{r}_{\text{RR}} \end{pmatrix}. \quad (19)$$

Similarly, the rationalized smaller matrices $\bar{\Lambda}_{\alpha}^{\text{adv/ret}}(\pm)$ can be defined by removing the rows and columns associated with evanescent modes from $\Lambda_{\alpha}^{\text{adv/ret}}(\pm)$ in Eqs. (6) and (7). The mode-resolved transmission for the l th incoming phonon mode (moving towards the interface) in the left (right) lead, $\Xi_{\text{L},l}$ ($\Xi_{\text{R},l}$), and its corresponding wave vector $k_{\text{L},l}$ ($k_{\text{R},l}$) can be further determined by

$$\Xi_{\text{L},l} = [\bar{t}_{\text{RL}}^{\dagger} \bar{t}_{\text{RL}}]_{ll}, \quad \Xi_{\text{R},l} = [\bar{t}_{\text{LR}}^{\dagger} \bar{t}_{\text{LR}}]_{ll}, \quad (20)$$

$$k_{\text{L},l} = \frac{1}{a_{\text{L}}} \cos^{-1} \text{Re}[\bar{\Lambda}_{\text{L}}^{\text{adv}}(-)]_{ll},$$

$$k_{\text{R},l} = \frac{1}{a_{\text{R}}} \cos^{-1} \text{Re}[\bar{\Lambda}_{\text{R}}^{\text{adv}}(+)]_{ll}. \quad (21)$$

The mode-resolved reflection coefficient for the m th outgoing phonon mode (moving away from the interface) in the left (right) lead, $\xi'_{\text{L},m}$ ($\xi'_{\text{R},m}$), and its corresponding wave vector

can be obtained by

$$\xi'_{\text{L},m} = [\bar{r}_{\text{LL}} \bar{r}_{\text{LL}}^{\dagger}]_{mm}, \quad \xi'_{\text{R},m} = [\bar{r}_{\text{RR}} \bar{r}_{\text{RR}}^{\dagger}]_{mm}, \quad (22)$$

$$k_{\text{L},m} = \frac{1}{a_{\text{L}}} \cos^{-1} \text{Re}[\bar{\Lambda}_{\text{L}}^{\text{ret}}(-)]_{mm},$$

$$k_{\text{R},m} = \frac{1}{a_{\text{R}}} \cos^{-1} \text{Re}[\bar{\Lambda}_{\text{R}}^{\text{ret}}(+)]_{mm}. \quad (23)$$

The mode-resolved absorption coefficient for the n th outgoing phonon mode in the left (right) lead, $\xi_{\text{L},n}$ ($\xi_{\text{R},n}$), which quantifies the fraction of outgoing energy flux received from phonons incident from the opposite lead, can be obtained by

$$\xi_{\text{L},n} = [\bar{t}_{\text{LR}} \bar{t}_{\text{LR}}^{\dagger}]_{nn}, \quad \xi_{\text{R},n} = [\bar{t}_{\text{RL}} \bar{t}_{\text{RL}}^{\dagger}]_{nn}, \quad (24)$$

$$k_{\text{L},n} = \frac{1}{a_{\text{L}}} \cos^{-1} \text{Re}[\bar{\Lambda}_{\text{L}}^{\text{ret}}(-)]_{nn},$$

$$k_{\text{R},n} = \frac{1}{a_{\text{R}}} \cos^{-1} \text{Re}[\bar{\Lambda}_{\text{R}}^{\text{ret}}(+)]_{nn}. \quad (25)$$

Using $\bar{r}_{\text{LL}}$ and $\bar{r}_{\text{RR}}$ from Eq. (19), the phonon specularity parameter p can also be determined, which represents the ratio of the reflected intensity of a phonon with incident wave vector k_n to that of a phonon reflected with wave vector $-k_n$ at the interface,

$$p_{\text{L}}(k_n) = \frac{|\bar{r}_{\text{LL}}^{\dagger}]_{n\bar{n}}|^2}{\sum_m |\bar{r}_{\text{LL}}^{\dagger}]_{nm}|^2} = \frac{|\bar{r}_{\text{LL}}^{\dagger}]_{n\bar{n}}|^2}{|\bar{r}_{\text{LL}}^{\dagger} \bar{r}_{\text{LL}}]_{nn}}, \quad (26)$$

$$p_{\text{R}}(k_n) = \frac{|\bar{r}_{\text{RR}}^{\dagger}]_{n\bar{n}}|^2}{\sum_m |\bar{r}_{\text{RR}}^{\dagger}]_{nm}|^2} = \frac{|\bar{r}_{\text{RR}}^{\dagger}]_{n\bar{n}}|^2}{|\bar{r}_{\text{RR}}^{\dagger} \bar{r}_{\text{RR}}]_{nn}}. \quad (27)$$

B. Integration of the S-matrix model as a DSMC boundary condition

The complete description of phonon scattering at a solid-solid interface, as provided by the S-matrix, is incorporated as a boundary condition in the BTE. We illustrate this for the

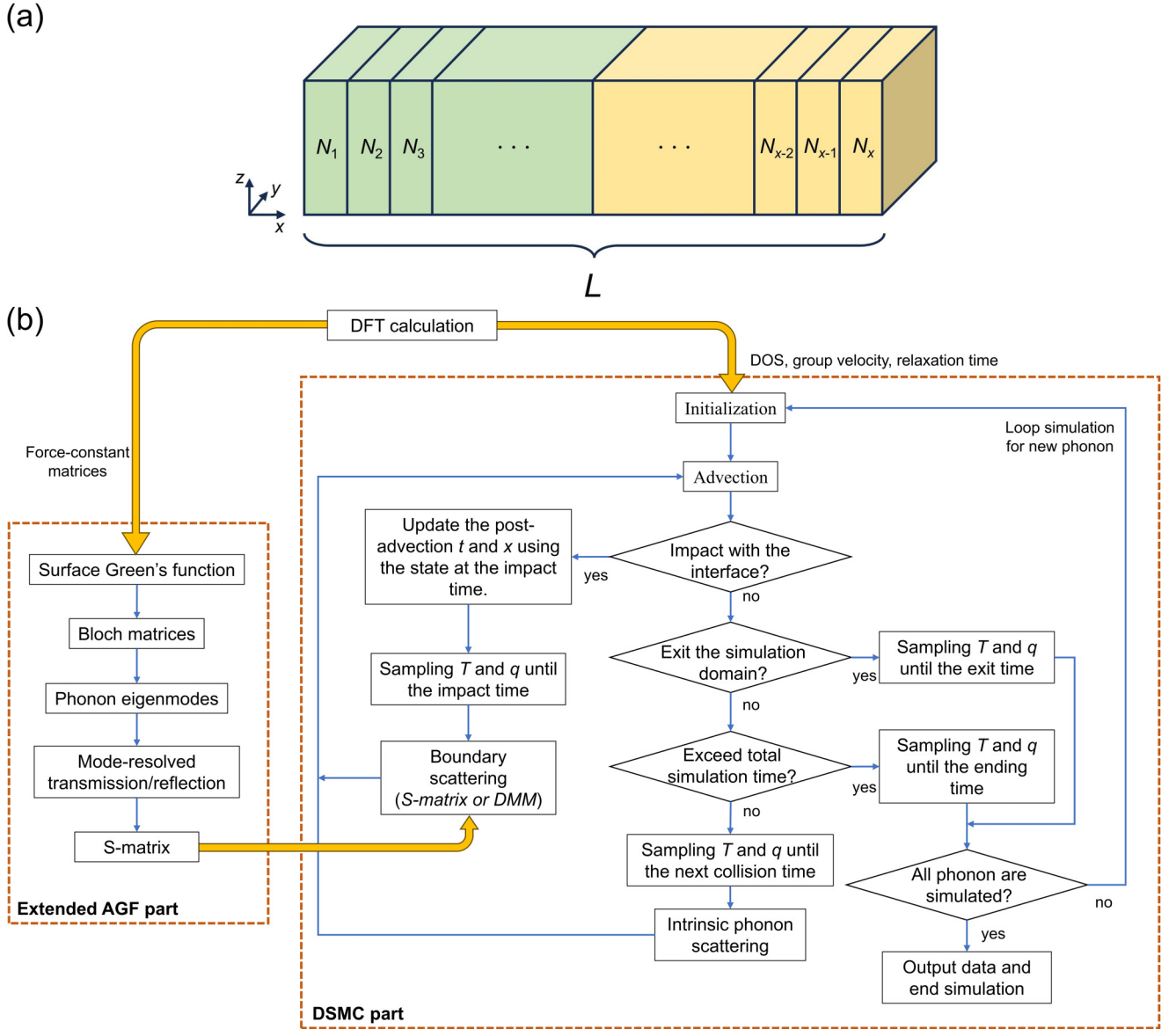


FIG. 2. (a) The one-dimensional configuration of the DSMC simulation applied to the solid-solid interface. (b) Phonon-based DSMC algorithm flow chart, including the implementation of the S-matrix model. Data required by the S-matrix model and the initialization information are obtained using prior and separate DFT/AGF simulations, as indicated.

one-dimensional steady heat flux across a system composed of two materials in contact, with an interface mediating phonon transport, as shown in Fig. 2(a). In this model, the total length L of the system is discretized along the transport direction (x axis) into N_x individual grid cells, each with a spatial width of Δx , where the green and yellow regions represent two distinct materials meeting at a central interface. The steady-state BTE is solved using the energy-based deviational DSMC scheme developed by Péraud and Hadjiconstantinou [16,17], which we will hereafter refer to simply as “DSMC” for brevity. This scheme is constructed upon a reformulation of the governing equation in terms of the deviational phonon energy, which significantly reduces the variance in Monte Carlo simulations and thereby enhances computational efficiency, i.e.,

$$v_g(\omega, \mathbf{p}) \cdot \nabla e^d = -\frac{e^d - (e_{\text{loc}}^{eq} - e_{T_{eq}}^{eq})}{\tau(\omega, \mathbf{p}, T)}, \quad (28)$$

where $e^d = e - e_{T_{eq}}^{eq}$ denotes the deviational phonon energy, with the energy distribution $e = \hbar\omega f$ and equilibrium energy distribution $e_{T_{eq}}^{eq} = \hbar\omega f_0(T_{eq})$ at equilibrium temperature T_{eq} , v_g is the group velocity vector, τ is the phonon relaxation time, and $e_{\text{loc}}^{eq} = \hbar\omega f_0(T_{\text{loc}})$ represents the pseudoequilibrium energy distribution at the local pseudoequilibrium temperature T_{loc} .

The corresponding steady-state variance-reduced DSMC/S-matrix algorithm for solving the BTE is summarized in the flowchart shown in Fig. 2(b). In this algorithm, energy packets are represented as N computational particles, and the simulation advances through three main steps: initialization, advection, and sampling.

In the initialization step, each particle is then either created inside the domain, representing the initial temperature distribution, or injected from one of the isothermal boundaries.

Particles generated inside the domain are placed uniformly and assigned properties such as frequency, density of states, group velocity, and relaxation time sampled from DFT calculations performed in VASP [40–42]. Those entering from the boundaries are drawn from boundary-weighted distributions that ensure the correct energy flux without recalculating the full phonon spectrum at every emission.

In the advection step, each particle's position is updated over a prescribed time step Δt according to its group velocity. If a particle encounters the solid-solid interface, its post-collision state is determined using a Monte Carlo sampling process in two possible ways: (a) the mode-resolved scattering probabilities from the S-matrix, as expressed in Eqs. (20) and (22), whereby a random number is generated and compared against the cumulative distribution of all possible transmission and reflection probabilities to select the corresponding outgoing phonon mode; or (b) the DMM boundary condition that accounts for the full phonon dispersion relations of both materials [27,43,44], i.e.,

$$\Xi_L(\omega) = \frac{\sum_j D_R^j(\omega) v_R^j(\omega)}{\sum_i D_L^i(\omega) v_L^i(\omega) + \sum_j D_R^j(\omega) v_R^j(\omega)}, \quad (29)$$

where D and v denote the density of states and phonon velocity at frequency ω , respectively. If the particle does not encounter the interface during the time step, it undergoes intrinsic scattering according to the scattering probability function $P = 1 - \exp(-\Delta t/\tau)$. When a particle encounters the interface a scattering event occurs, and the particle is absorbed and reemitted from its current location according to the local pseudoequilibrium temperature. In the sampling step, each particle contributes to the macroscopic quantities (e.g., temperature T_{loc} and heat flux q_{loc}) within its respective cell. Sampling for a particle terminates when it exits the simulation domain or when the time exceeds the simulation time.

By repeating advection, scattering, and sampling for all particles throughout the simulation, the macroscopic temperature distribution and heat flux profile of the system are obtained by

$$T = \sum_{i=1}^N \frac{\sigma_i \varepsilon_{\text{eff}}}{C_V \Delta x} + T_{eq}, \quad (30)$$

$$q = \sum_{i=1}^N \sigma_i \varepsilon_{\text{eff}} v_{x,i}, \quad (31)$$

where C_V is the volume heat capacity, σ_i is the sign of the i th energy packet, ε_{eff} is the effective energy of each packet, and $v_{x,i}$ is the x component of the phonon group velocity vector, where its sign explicitly accounts for the direction of energy transport (forward or backward).

III. RESULTS AND DISCUSSION

A. Phonon scattering dynamics at Si/Ge interfaces

We employ the scattering matrix approach to investigate phonon scattering dynamics at silicon/germanium interfaces, including both ideal and disordered configurations, as illustrated in Fig. 3. The ideal interface is constructed by aligning a heterostructure along the [111] crystallographic direction

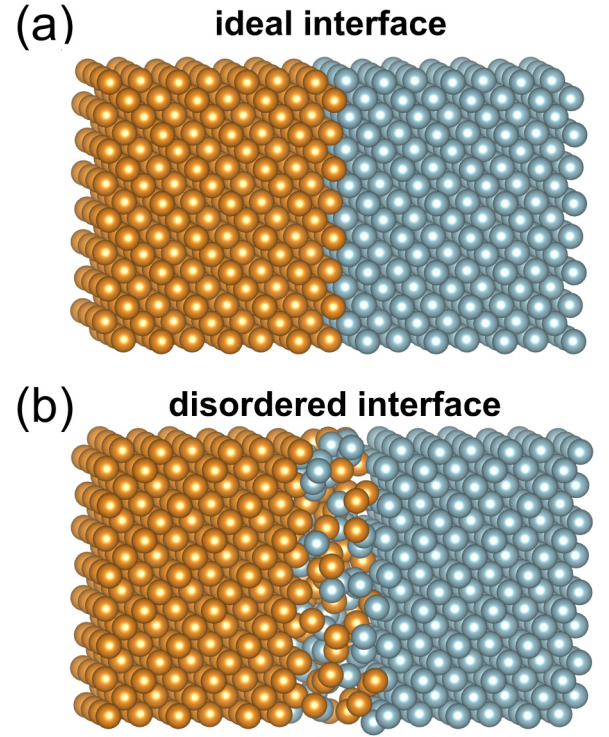


FIG. 3. Atomic configurations of (a) ideal and (b) disordered Si/Ge interfaces.

of Si and Ge. To generate the disordered interface, the four atomic layers near the interface are locally annealed while keeping the positions of all other atoms fixed, in order to introduce structural disorder without affecting the bulk regions. This process is carried out using molecular dynamics (MD) simulations performed in the Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) [45].

To elucidate the different interfacial phonon dynamics predicted by the S-matrix and DMM models, we first compare schematic diagrams of interfacial phonon transmission and reflection processes derived from the S-matrix with those from the DMM, as shown in Fig. 4. Here, an ideal interface is used for illustration. The same qualitative behavior is also observed at the disordered interface. In these diagrams, the length and direction of arrows represent the magnitude and direction of phonon velocities, where black arrows are the incoming phonon modes, blue arrows are transmission, and red arrows indicate reflection, with color intensity encoding the transmission/reflection probability. For the DMM model, as given in Eq. (29), all incoming phonon modes at a fixed frequency possess a transmission probability that depends solely on ω . Upon reaching the interface, these phonons lose memory of their initial momentum information and undergo diffuse scattering. The outgoing transmitted and reflected phonons follow a three-dimensional Lambertian distribution [46], consistent with the diffuse scattering assumption, with the distribution sampled using the inverse transform method. The S-matrix model reveals a strong directional dependence and pronounced anisotropy in phonon transmission and reflection, which stands in contrast to the diffuse scattering nature of the DMM model. At the same frequency, different

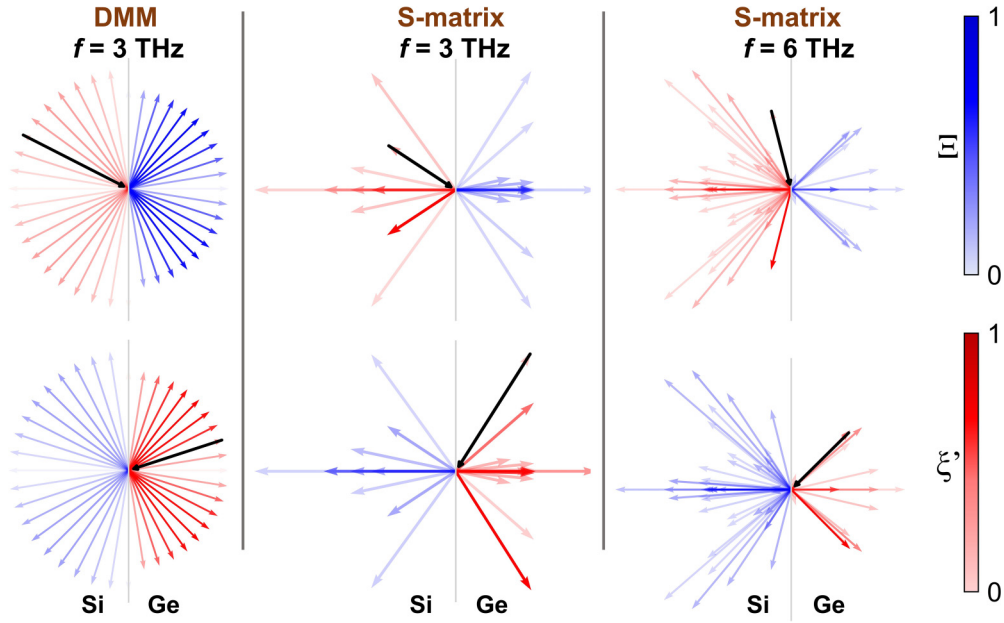


FIG. 4. Scattering patterns of phonon transmission and reflection for the S-matrix and DMM models taken from the ideal interface case at specific incoming phonon frequencies.

incoming phonon modes exhibit distinct scattering patterns, as evidenced by the varying color depths of the arrows in Fig. 4.

The mode-resolved transmission and reflection results from the S-matrix model are projected onto their respective bulk phonon dispersion curves, as demonstrated in Fig. 5, using data for the ideal Si/Ge interface as a representative example. Specifically, Figs. 5(a) and 5(b) illustrate the mode-resolved transmission and reflection for phonons incident from the left side (Si), whereas Figs. 5(c) and 5(d) depict these parameters for phonons incident from the right side (Ge). Taking the two panels on the left as an example, along all the dispersion curves, half of the phonon modes possess positive velocities, corresponding to rightward propagation (Si to

Ge) and participation in transmission processes, whereas the other half have negative velocities, propagating leftward and contributing to reflection processes. The transmission at the wave vector k_i and the reflection at the wave vector $-k_i$ sum to unity. On the Si side, only phonons with frequencies below 11.5 THz contribute to transmission, corresponding to the cutoff frequency on the Ge side. Phonons in silicon exceeding this frequency exhibit zero transmission. Heat transport across the interface is predominantly governed by acoustic branches in the frequency range from 0 to 6 THz, including both longitudinal acoustic (LA) and transverse acoustic (TA) branches, as evident from the transmission distribution plotted in Figs. 5(a) and 5(c).

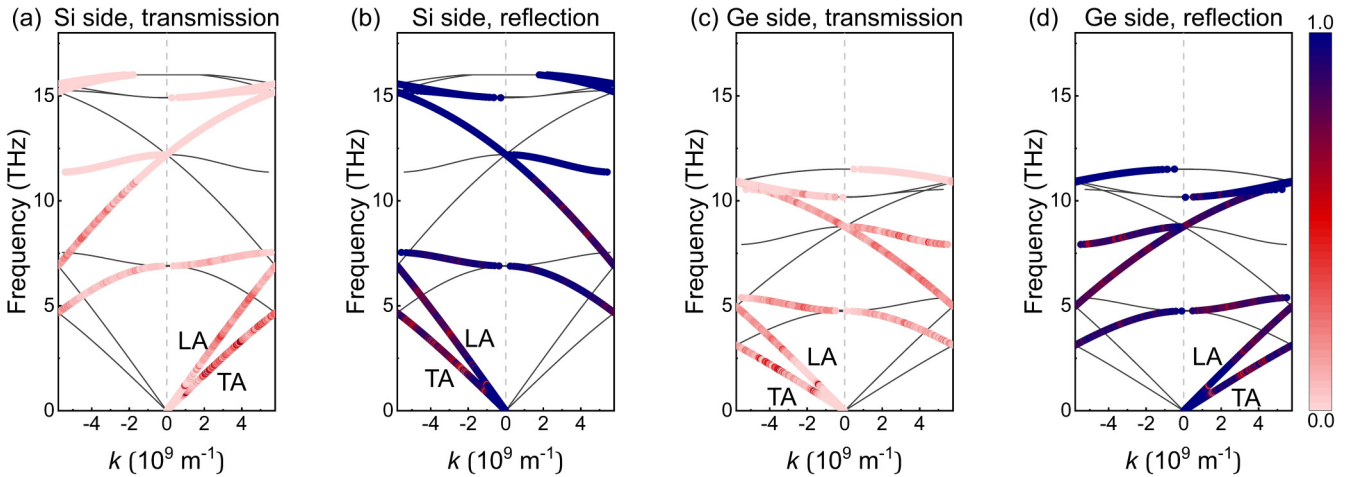


FIG. 5. Mode-resolved phonon transport properties at the Si/Ge interface, illustrated here for the ideal interface, (a), (b) Transmission and reflection for phonons incident from the Si side. (c), (d) Transmission and reflection for phonons incident from the Ge side. The black lines indicate the phonon dispersion curves for bulk Si and Ge obtained from the AGF part simulation in Sec. II A, while the colored dots represent individual phonon modes, with color intensity corresponding to the transmission/reflection probability, as shown in the legend on the right panel.

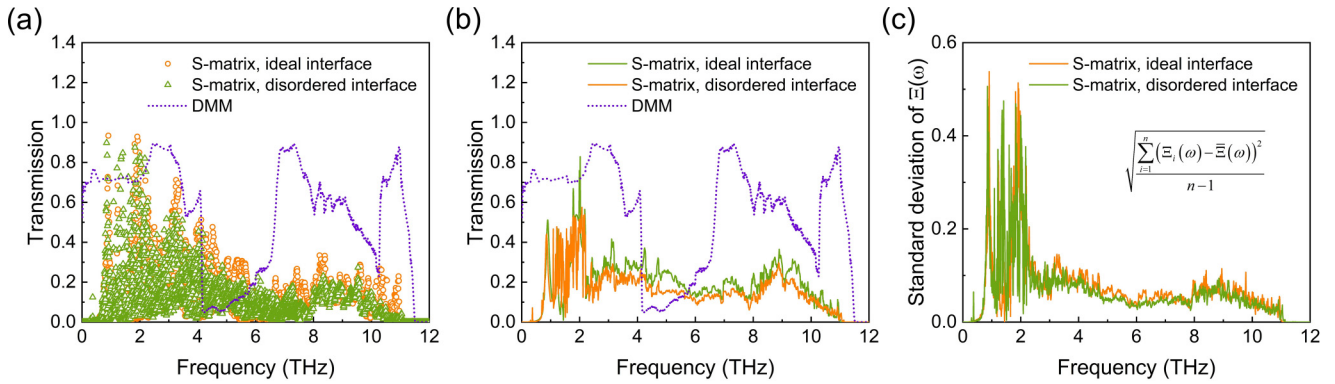


FIG. 6. (a) Mode-resolved and (b) average transmission at each frequency calculated by the S-matrix vs the DMM curve. (c) Standard deviation of transmission for ideal and disordered interfaces from S-matrix calculation.

It is not intuitive to compare the ideal and disordered interfaces by projecting the mode-resolved transmission onto the phonon dispersion curves. Accordingly, Figs. 6(a) and 6(b) present the mode-resolved transmission and mean transmission at each frequency obtained from the S-matrix model for the ideal and disordered interfaces, alongside the corresponding DMM curve for comparison. The enhanced interfacial scattering in the S-matrix model results in lower transmission compared to the DMM. The disordered interface does not significantly alter the mode-resolved transmission trend, but the disruption of interfacial bonding caused by disordered atoms reduces the overall transmission magnitude. A comparison of the integrated areas under the mean transmission curves for the ideal and disordered interfaces in Fig. 6(b) shows an approximately 20% reduction caused by the disordered structure. In addition, the apparent cutoff frequency of the S-matrix model is approximately 0.4 THz lower than that of the DMM. This deviation reflects the fundamental differences in the physical assumptions and numerical behavior of the two models. The DMM, based on the “memory-loss” assumption, is essentially a DOS-driven statistical model. As long as a nonzero DOS exists near the physical cutoff frequency, it assigns a finite and often significant transmission to those modes, regardless of the actual coupling strengths between phonon modes. In contrast, the S-matrix model, as a wave-based scattering approach, explicitly captures the weak intermodal coupling near the cutoff regime of the Ge side. As phonon wavelengths approach the scale of interatomic spacings, severe mode mismatch suppresses the coupling between modes, causing the transmission magnitude to drop sharply and producing the observed offset in the apparent cutoff frequency between the two models [35].

To better characterize the directional dependence of interfacial scattering, we quantify the degree of anisotropy captured by the S-matrix model using the standard deviation of transmission at each frequency, as shown in Fig. 6(c). This metric reflects the spread in transmission probabilities across different incident phonon modes, with higher values indicating stronger mode-dependent variations and, therefore, more pronounced anisotropic scattering. Notably, the transmission and reflection exhibit identical standard deviations, as they are complementary quantities constrained by energy conservation and their sum equals unity for each phonon mode. The anisotropic transmission and reflection behaviors

are primarily observed in acoustic phonons below 2 THz. Above this frequency, the standard deviation of the transmission and reflection decreases to below 0.1. Additionally, introducing the interfacial disorder does not substantially affect the anisotropy, as the standard deviation profile for the disordered interface closely resembles that of the ideal interface. These results underscore the importance of mode- and direction-resolved scattering information in accurately describing phonon transport across interfaces, especially in the low-frequency acoustic regime.

The specularity parameter is another key quantity that characterizes the complexity of phonon transport at the interface, and can be determined using Eqs. (26) and (27). As shown in Fig. 7, the specularity is not uniformly distributed but exhibits a clear frequency dependence, with higher values observed at low frequencies. It is important to note that a low specularity value does not imply fully diffuse reflection. Instead, phonons are reflected back into specific modes based on a mode-resolved probability. Analogous to the treatment of transmission, the standard deviation of the specularity parameter is demonstrated in Fig. 7(c). At low frequencies, the standard deviation of p reaches 0.6, indicating strong anisotropy. As frequency increases, the anisotropy weakens progressively, and the standard deviation of p decreases to around 0.2. In contrast to conventional DMM approaches, which prescribe a constant specularity (set to 0 in the implementation used below, corresponding to fully diffuse reflection), the present S-matrix treatment retains its frequency and mode dependence, thereby capturing the selective nature of interfacial scattering.

In summary, our analysis reveals that the microscopic phonon dynamics at the interface differ significantly between the DMM and S-matrix models. The S-matrix approach captures strong mode-dependent transmission characteristics, offering greater physical fidelity.

B. Interfacial thermal resistance

In this section, the DSMC framework is employed to investigate the macroscopic characteristics of phonon transport across the interface. As a preliminary step, we validate the DSMC algorithm by simulating bulk Si and Ge systems independently, using phonon parameters from *ab initio* calculations. In the bulk simulation domain, a total of 10^8 phonon

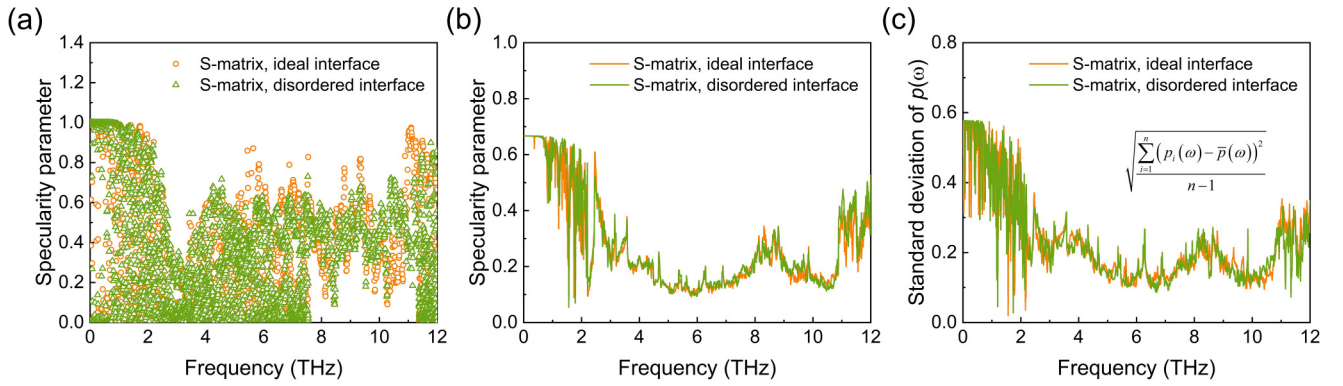


FIG. 7. (a) Mode-resolved and (b) average specular parameter at each frequency calculated by the S-matrix model. (c) Standard deviation of specular parameter for ideal and disordered interfaces from S-matrix calculation.

particles are randomly initialized and propagated according to the advection and scattering procedures described in Sec. II B. Isothermal boundary conditions are applied at both ends of the simulation domain ($T_L = 301$ K and $T_R = 299$ K), with an initial temperature of 299 K and a reference temperature of $T_{eq} = 300$ K. Any incident phonons at these boundaries are fully absorbed and reemitted in accordance with the equilibrium Bose-Einstein distribution corresponding to the prescribed temperatures, ensuring that the boundaries maintain the intended thermal conditions [16]. The system evolves until the simulation time exceeds a predefined limit of 600 ns, at which point a steady state is reached. The macroscopic temperature and heat flux distributions are then obtained using Eqs. (30) and (31).

The resulting thermal conductivity is compared with experimental data [47–51], as shown in Fig. 8. Each data point was obtained by averaging five independent simulations. The resulting statistical uncertainty is found to be less than 0.5%. As the system length L increases, the thermal conductivity calculated from DSMC simulations monotonically approaches the

bulk values. This trend is typical of systems with finite-size effects (see, e.g., Ref. [52]), where the equilibrium isothermal boundary conditions that are used to impose a temperature gradient differ fundamentally from the nonequilibrium nature of the phonon distributions present near such boundaries in nanoscale systems. These results confirm the validity of the input phonon parameters used in our simulations. The results also highlight that meaningful predictions of bulk behavior can only be obtained when the simulation domain is sufficiently large to mitigate boundary-induced nonequilibrium effects.

We then simulate phonon transport through a combined Si and Ge heterostructure, with similar isothermal boundary conditions applied at both ends to induce a small temperature gradient across the system (ΔT) of 2 K, and incorporating either S-matrix or DMM-type boundary conditions at the interface. After the DSMC simulation reaches steady state, the temperature profile in the x direction is measured by averaging the cell temperatures over the steady-state time domain. The system-averaged heat flux per unit interface area q is also computed. The interfacial thermal resistance is then calculated as $ITR = \Delta T_{\text{interface}}/q$, where $\Delta T_{\text{interface}}$ is determined using a standard interpolation method. Bulk regions in the Si and Ge domains are identified, and a least-squares linear fit is applied to the temperature profiles. The temperature discontinuity at the interface, obtained from the extrapolated fits, provides the value of $\Delta T_{\text{interface}}$. We select the temperature profile of the 2000-nm system for illustration in Fig. 9(a), as this length effectively eliminates boundary effects associated with smaller scales, while clearly capturing the interfacial temperature jump and nonequilibrium effects. The temperature profile calculated using the S-matrix model exhibits a more pronounced $\Delta T_{\text{interface}}$ compared to that from the DMM model. The reduced transmission of the S-matrix model [recall Figs. 6(a) and 6(b)] increases the resistance encountered by phonons attempting to cross the interface, resulting in an accumulation of energy near the interface and a sharper temperature discontinuity.

The ITRs calculated using the S-matrix and DMM boundary conditions differ significantly because of the distinct phonon scattering mechanisms, as shown in Fig. 9(c). The error bars in the figure represent the standard deviation derived from five independent simulations. Note that, at small system lengths, the assumed isothermal boundary conditions may

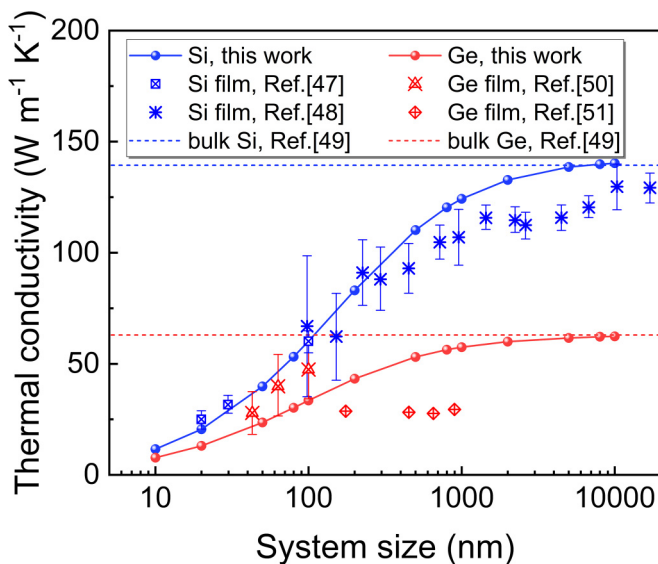


FIG. 8. Validation of the DSMC code, showing the thermal conductivity as a function of system size L compared with experimental data [47–51].

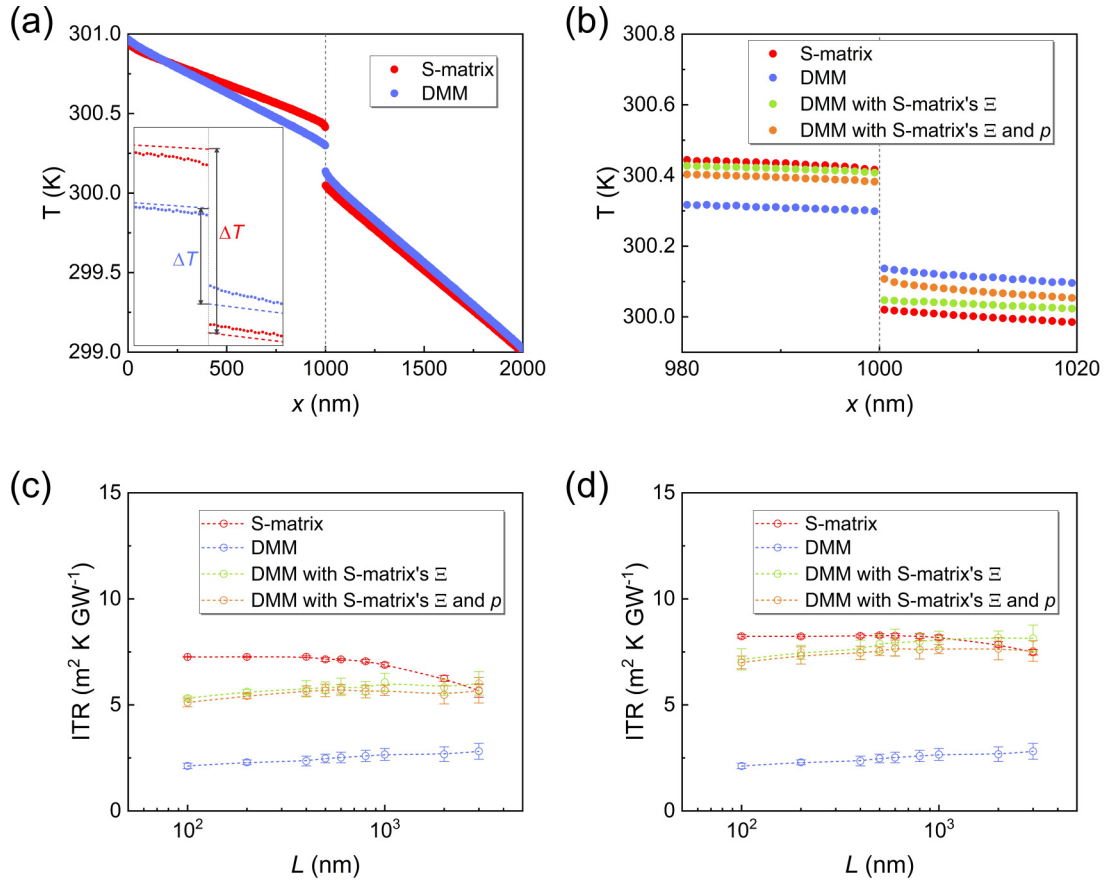


FIG. 9. (a) Temperature profiles across the Si/Ge interface obtained from DSMC simulations with S-matrix and DMM boundary conditions. (b) Zoomed-in view of the temperature profiles near the ideal Si/Ge interface. ITR predictions of the (c) ideal and (d) disordered Si/Ge interfaces obtained from the S-matrix model, the conventional DMM model, and the modified DMM model incorporating transmission and specularly parameters extracted from the S-matrix model.

introduce non-negligible artifacts because of the absence of phonon thermalization. However, since both models have the same boundary conditions at the edges of the simulation domain, the discrepancy in ITR highlights intrinsic differences in interfacial scattering, especially the anisotropy captured by the S-matrix. The DMM model assumes fully diffusive scattering, which randomizes the phonon direction regardless of the incident phonon mode. In contrast, the S-matrix model features lower transmission and retains strong correlations between incident and transmitted/reflected phonon modes. As a result, the transmitted/reflected phonons exhibit more pronounced anisotropy in both velocity and direction, yielding a higher ITR of around $5.7 \text{ m}^2 \text{ K GW}^{-1}$. We further confirm that, in the limit of large L , the discrepancy in ITR predicted by both the DMM and S-matrix models remains effectively constant across the temperature range 200–500 K.

To investigate the origin of this discrepancy, we modify the DMM boundary condition by replacing the transmission probability [originally prescribed by Eq. (29)] with the average transmission probability values obtained directly from the S-matrix method [see orange data points in Fig. 6(b)]. This treatment aligns with the scheme proposed by Yang *et al.* [36], although we maintain a fully diffusive scattering assumption here, unlike their specular treatment. In a second set of simulations, we also incorporate the specularly parameter

$p_{L/R}(\mathbf{k}_n)$ calculated by Eqs. (26) and (27) to further refine the treatment of phonon reflection. These two modifications to the DMM boundary condition allow us to isolate the impact of the transmission magnitude and angular redistribution, enabling a more detailed understanding of how interfacial coherence influences thermal resistance.

As shown in Figs. 9(b) and 9(c), incorporating the lower transmission derived from the S-matrix model leads to a significant increase in $\Delta T_{\text{interface}}$ and the DMM-predicted ITR. However, incorporating the mode-resolved specularly parameter extracted from the S-matrix model has only a relatively minor impact on ITR. This adjustment leads to a reduction of only about $0.3 \text{ m}^2 \text{ K GW}^{-1}$ at L of 2000 nm, suggesting that the transmission modification is the dominant factor influencing the ITR prediction if the specularly parameter is small (as seen in Fig. 7, where p remains below 0.2 across a wide frequency range). It is worth noting that the modified DMM performs differently depending on the size of the system. For large L , it accurately predicts interfacial transport behavior, comparable to DSMC simulations using the full S-matrix boundary condition. By contrast, significant discrepancies arise at small L , highlighting the dominant role of microscopic phonon dynamics at the interface and demonstrating that even the modified DMM is inadequate for nanoscale systems.

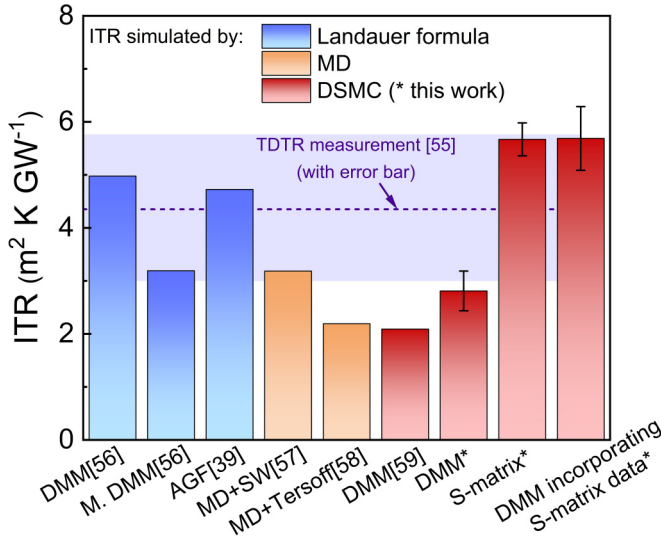


FIG. 10. Comparison of ITR with reported experimental [55] and simulation data [39,56–59] in the literature for the same Si/Ge case.

We further apply both the S-matrix and the modified DMM models to compute the ITR across the disordered interface, as shown in Fig. 9(d). The conventional DMM model accounts only for bulk phonon properties and therefore fails to capture the influence of localized interfacial structural complexity. As a result, its prediction remains unchanged compared to the ideal interface case [see Fig. 9(b)]. In contrast, the disordered structure suppresses phonon transmission in the S-matrix model, leading to an increase in ITR by more than $2 \text{ m}^2 \text{ K GW}^{-1}$ compared to the ideal interface. Meanwhile, the ITR predicted by the modified DMM model incorporating the transmission and specular parameters derived from the S-matrix model matches that of the S-matrix at large system sizes. These results highlight the capability of the modified DMM model to further capture interfacial disorder effects. We note that while our simulation framework incorporates intrinsic three-phonon scattering within the bulk leads, the S-matrix model based on the harmonic AGF framework is inherently elastic, and therefore neglects inelastic scattering events occurring strictly at the interface. The absence of these inelastic channels prevents high-frequency phonons in silicon from contributing to interfacial transport, potentially leading to an overestimation of the interfacial thermal resistance [53,54].

In Fig. 10, we compare the values of interfacial thermal resistance obtained in this work with previous simulation and experimental studies that use TDTR data as a benchmark. We find that the DSMC result based on the standard DMM model significantly underestimates the interfacial thermal resistance, while the result incorporating the S-matrix boundary condition shows much closer agreement. It is worth noting that integrating the DMM-based transmission function using the Landauer formula can lead to increased interfacial thermal resistance, bringing the prediction to appear closer to experimental results. Specifically, the modified Landauer formula combined with DMM (M. DMM) employs the bulk distribution (f_{bulk}) instead of the traditional equilibrium distribution (f_{eq}), thereby incorporating the non-equilibrium effects of the

TABLE I. Comparison of computing time in our DSMC simulations using the different boundary conditions.

Boundary condition	Computing time (s)
DMM	1281
S-matrix	2901
DMM incorporating S-matrix data	1769

populations on both sides of the interface. However, despite this improvement, the model still assumes isotropic diffuse scattering at the interface. As demonstrated in this work, the standard DMM model fails to accurately describe the microscopic phonon dynamics at the interface and does not take into account the directionality and mode resolution of phonon interactions.

Having established the accuracy benefits of the S-matrix boundary condition, we then evaluate its computational cost. Table I compares the computing times for DSMC simulations using the different boundary conditions. The incorporation of the S-matrix model leads to a moderate increase in computational cost for the DSMC simulations. In the case of the S-matrix boundary condition, the simulation requires evaluating the specific transmission probabilities associated with each individual matrix element in the S-matrix during each interface collision, and subsequently determining the postcollision phonon state based on these probabilities. This process results in a computing time that is approximately 2.5 times slower than that required for simulations using the standard or modified DMM boundary conditions.

IV. CONCLUSIONS

In this work, we have developed and implemented a mode-resolved interfacial boundary condition for the phonon Boltzmann transport equation by embedding the scattering matrix (S-matrix) formalism within a low-variance DSMC framework. Unlike conventional acoustic or diffuse mismatch models, the S-matrix approach provides direct access to wavelength- and polarization-dependent phonon transmission and reflection, thereby capturing microscopic details of anisotropic and mode-specific scattering that strongly influence interfacial thermal resistance. Through simulations of ideal and disordered Si/Ge interfaces, we demonstrated that the S-matrix model consistently predicts lower transmission and higher interfacial thermal resistance than DMM, in closer agreement with experimental measurements. Our results further show that while DMM can be empirically tuned with S-matrix data to recover large-scale averages, its intrinsic isotropic and frequency-averaged assumptions render it unsuitable for nanoscale device modeling.

The integration of the S-matrix into DSMC establishes a practical framework that balances computational efficiency with physical fidelity, requiring only a modestly higher cost compared to DMM. This approach bridges the gap between atomistic quantum transport descriptions and mesoscopic stochastic simulations, thereby enabling predictive and scalable modeling of nanoscale heat transfer across interfaces. The S-matrix model in our current framework is inherently

elastic and therefore neglects inelastic scattering at the interface. Future developments could extend this approach to incorporate interfacial anharmonicity by including higher-order force constants in the self-energy terms, enabling the study of more complex interface morphologies, alloyed or chemically modified junctions, and multiphase device architectures such as solid–liquid interfaces. Such developments will provide critical tools for the rational design of next-generation nanoscale electronic and energy-conversion technologies, where accurate prediction of interfacial thermal resistance is essential for performance and reliability.

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DATA AVAILABILITY

The data that support the findings of this article are openly available [60].

APPENDIX: COMPUTATIONAL DETAILS

The *ab initio* calculations were performed using VASP with the projector augmented wave (PAW) method [40–42]. The exchange–correlation interaction was described by the local density approximation (LDA), and a plane-wave energy cutoff

of 500 eV was applied with an energy convergence criterion of 10^{-8} eV.

To obtain the phonon properties for the DSMC simulations, the harmonic lattice dynamic calculations were first performed using the finite-displacement method implemented in the PHONOPY package, employing a $4 \times 4 \times 4$ supercell expanded from the primitive cell with a $5 \times 5 \times 5$ Monkhorst-Pack k -point mesh. The calculated phonon group velocities and DOS were used as inputs for DSMC simulations. Subsequently, for the anharmonic properties required to determine the phonon scattering times in the DSMC collision operator, third-order interatomic force constants (IFCs) were calculated using the PHONO3PY package [61]. $4 \times 4 \times 4$ supercells based on the primitive cells were constructed for both Si and Ge with a finite atomic displacement of 0.03 Å. The phonon scattering times were computed on a $25 \times 25 \times 25$ reciprocal-space mesh and were integrated into the DSMC simulations.

For the construction of the Hamiltonian matrices required for the AGF calculations, a separate set of harmonic calculations was performed consistent with the device geometry. The bulk leads, represented by H_L and H_R , were modeled using $3 \times 3 \times 3$ supercells (containing 216 atoms) expanded from the conventional unit cell. For the central scattering region, a 432-atom supercell was constructed by assembling $3 \times 3 \times 3$ expansions of the Si and Ge conventional unit cells along the x direction. Based on the harmonic calculations for this supercell, H_C was extracted from the scattering region, which spans the central four conventional unit cells. H_{LC} and H_{RC} were derived from the interactions between this scattering region and the buffer layers, defined as the single conventional unit-cell blocks at both terminals of the x direction. The disordered interface maintains the identical atomic count (432 atoms) as the ideal structure, with structural disorder introduced specifically within the four atomic layers at the Si/Ge junction.

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