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Effect of spatial coherence on phonon transmission at interfaces

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Accurate phonon transmission coefficients are essential for controlling heat transport and designing phononic metamaterials. Conventional models for computing transmission coefficient are based on plane-wave solution and spectrum weighting, limiting their ability to capture actual phonon transport dynamics in multi-interface heterostructures. Here we develop an analytical framework that incorporates spatial coherence and validate it against time-domain wave-packet simulations. We show that spatial coherence strongly affects transmission in multi-interface systems, whereas it is negligible for a single interface. The developed framework is robust for various wave-packet profiles and can accurately resolve both transmission coefficient and the wave-packet dynamics in realistic multi-interface heterostructures. Our work provides a robust framework for exploring coherence effects in phonon transport, which may offer guidelines for thermal management and design of phononic metamaterials.

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I. INTRODUCTION

As the quanta of vibrational waves, phonons exhibit wave-like characteristics [1,2]. In recent years, the wave nature of phonons has garnered significant attention [3,4]. Both theoretical and experimental works have revealed that this wavelike behavior plays a crucial role in determining thermal properties of various solids [5–11]. For example, Ravichandran *et al.* [6] have highlighted the critical role of phonon coherence on heat conduction in superlattices. The destructive interference of phonons leads to the formation of phonon band gaps, which in turn suppresses the lattice thermal conductivity. Moreover, previous studies have demonstrated the feasibility to tailor the density of states and the group velocity of thermal phonons via interference phenomena [12–15]. Consequently, exploring phonon coherence and its manipulation strategy holds significant potential for controlling thermal transport properties in solids [16].

Building on these insights, accounting for the coherence-driven interference is crucial to study the phonon transport across multilayer heterostructures [17–24]. However, conventional theories are formulated at the single-interface level and do not explicitly track the phase evolution between successive interfaces, where interfacial spacing-dependent interference can strongly modulate the overall transmission. Moreover, existing methods such as the atomistic Green's function [25–27] are typically built on a plane-wave picture, thus lacking a characteristic length scale to quantify the phonon spatial coherence. Phonons in realistic materials have a finite coherent length, as described by the wave packet with the finite broadening as a characteristic length scale [28–31]. Consequently, the plane-wave solution fails to capture the complex interplay

between the wave-packet broadening and the finite interfacial spacing, which can critically shape the phonon transmission in multi-interface systems [32]. Therefore, an analytical framework beyond the plane-wave approximation is needed to efficiently quantify the coherence effects on phonon transmission in multi-interface systems.

More importantly, although existing methods such as weighted-averaging approach can provide the estimation of transmission coefficient, they do not provide direct access to the waveform dynamics [33–35]. For example, the spectrum-weighted approach [33] can estimate the transmission coefficient by combining plane-wave transmission with spectral weights. It retains only intensity information and discards the phase-resolved coherence among spectral components, which are essential for the reconstruction of the waveform dynamics. While the atomistic simulations can probe the real-time dynamics of wave-packet propagation [36], its application can be limited due to the computational cost for large-scale systems. Therefore, it is highly desirable to develop a theoretical framework that can efficiently model the wave-packet dynamics in order to greatly reduce the reliance on expensive time-domain simulations.

In this work, we theoretically investigate the effect of phonon spatial coherence on interfacial phonon transmission and validate our findings through phonon wave-packet simulations. Our results show that while spatial coherence has negligible impact on phonon transmission across a single interface, it plays a crucial role in the multi-interface system. The phonon transmission coefficient obtained from the plane-wave approximation fails to provide an accurate assessment of the actual phonon transmission in the multiple-interface system. To account for phonon spatial coherence, we propose an analytical method that explicitly incorporates finite spatial broadening. We demonstrate that the proposed method not only can accurately predict phonon transmission

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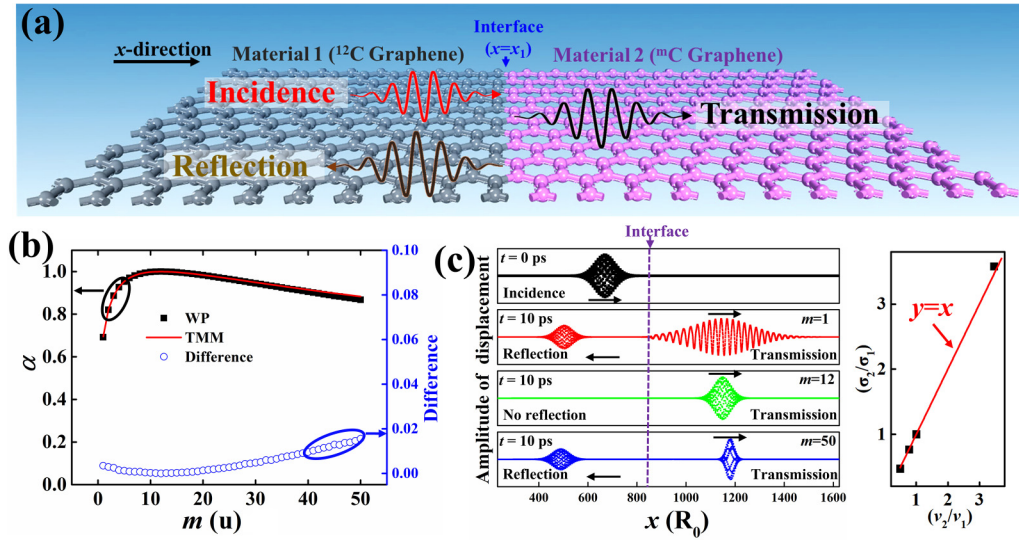


FIG. 1. (a) Schematic diagram of a single-interface system. The system consists of two graphene layers with different atomic masses. The graphene layer on the left, with carbon atoms of mass 12 u, represents the incidence (reflection) region. The graphene layer on the right, where the carbon atoms possess a varying mass of m in units of u, serves as the transmission region. (b) Transmission coefficients (left axis) obtained using wave-packet (WP) simulation with an incident wave packet width of 173 Å and wave vector $k_1 = 0.177$ (1/Å) and TMM, along with the differences (right axis) between these two methods. (c) Variation in the phonon broadening of the transmitted phonon wave packet with different m during WP simulations (left panel). The dashed line represents the position of the interface. The relationship between the group velocity (v_2) and the broadening of the wave packet (σ_2) in material 2, normalized by the corresponding values (v_1 and σ_1) in material 1 (right panel). Here R_0 denotes the graphene lattice constant and is used as the reference length scale for the system length.

coefficient across multiple interfaces, but also can faithfully resolve the dynamical behavior of finite-width wave-packet propagation in multi-interface heterostructures. This work provides a reliable framework for evaluating phonon transport in the multiple-interface system and offers valuable guidances for the design of phononic metamaterials.

The rest of the paper is organized as follows. The transmission of a phonon wave packet across a single interface is described in Sec. II. We then discuss in Sec. III the transmission of a phonon wave packet through multiple interfaces by comparing results from the transfer matrix method (TMM), wave-packet (WP) simulations, and the approach developed in this work. Finally, the conclusions are summarized in Sec. IV.

II. TRANSMISSION OF A PHONON WAVE PACKET ACROSS A SINGLE INTERFACE

A. Theory and simulation methods for the single-interface system

As depicted with Fig. 1(a), we first consider a single interface formed by two materials. A phonon mode is launched on the left side of the interface, and we calculate the energy transmission coefficient (α) across the interface. For a single-mode plane-wave phonon, the TMM is commonly used to calculate the transmission coefficient, which can simultaneously account for the wave vector and polarization [37]. To simplify the analysis, we focus on the case of normal incidence along the x direction (perpendicular to interface), for which no mode conversion occurs [37].

Let u_I be the atomic displacement of a given phonon mode in material I , and k_I denotes the wave vector. In the incident region (material 1), the atomic displacement amplitude can be

written as

$$u_1(x, t) = a_{1,i} e^{ik_1 x} e^{-i\omega t} + a_{1,r} e^{-ik_1 x} e^{-i\omega t}, \quad (1)$$

where $a_{1,i}$ and $a_{1,r}$ are the amplitudes of the incident and reflected waves, respectively. The atomic displacement in material 2 can be expressed as

$$u_2(x, t) = a_{2,t} e^{ik_2 x} e^{-i\omega t}, \quad (2)$$

where $a_{2,t}$ denotes the amplitude of the transmitted wave.

Next, the stress in material 1 and material 2 can be expressed by $S_I(x, t) = C_I \frac{\partial u_I(x, t)}{\partial x}$, where C_I is an appropriate elastic constant. The displacement and stress must satisfy the continuity conditions at the interface:

$$u_1(x_1, t) = u_2(x_1, t), \quad (3a)$$

$$S_1(x_1, t) = S_2(x_1, t), \quad (3b)$$

where x_1 is the interface position [see Fig. 1(a)]. Note that without loss of generality we can set $a_{1,i} = 1$. Based on the above equations, the transmitted amplitude $a_{2,t}$ can be obtained as

$$a_{2,t} = \frac{2C_1 k_1}{C_1 k_1 + C_2 k_2} = \frac{2\rho_1 v_1}{\rho_1 v_1 + \rho_2 v_2}. \quad (4)$$

The energy fluxes for the incident wave and the transmitted wave are given by [37]

$$P_i = \frac{1}{2} \rho_1 \omega^2 v_1 a_{1,i}^2, \quad (5)$$

$$P_t = \frac{1}{2} \rho_2 \omega^2 v_2 a_{2,t}^2, \quad (6)$$

where v_1 and v_2 denote the phonon velocity in material 1 and material 2, respectively. Therefore, we can define the energy

transmission coefficient α as

$$\alpha = \frac{P_t}{P_i}. \quad (7)$$

To validate the α calculated from the TMM, we employ the phonon WP simulation approach [36,38] that can account for the finite broadening of phonons in space to compute α . The WP approach provides a phase-resolved real-space description of phonon propagation and thus naturally captures spatial coherence, phase evolution, and interference effects. Owing to these features, it has been widely used and benchmarked in the literature for validating the coherent phonon transport theories [38,39]. Since realistic effects such as interfacial roughness, anharmonicity, and mode coupling can substantially degrade phonon coherence [5,40], we exclude these effects in our simulations and only consider sharp interfaces at low temperature where the coherent phonon transport is largely preserved.

It is worth noting that the phonon coherence underlying the WP approach refers to the preservation of relative phases among the constituent k components within a selected phonon branch, which is termed as *intrinsic coherence* [10] and is particularly strong at low temperatures. At elevated temperature, the phonon coherence can also originate from the overlapping of phonon branches due to the anharmonicity induced phonon mode broadening, which is termed as *mutual coherence* [10] and becomes increasingly important at high temperatures. When anharmonic broadening makes phonon linewidths comparable to the frequency separation between adjacent branches, these branches overlap in the frequency domain and no longer behave as fully independent transport channels [8]. In this work, we limit our investigation at low temperature and focus on the intrinsic coherence of phonon wave packet in real space.

The schematic diagram is depicted with Fig. 1(a), and the whole simulation domain is a single-layer graphene. To create the interface, material 1 is composed of carbon atoms with mass of 12 u (atomic mass unit), while material 2 is composed of artificial carbon atoms with varying mass m in the unit of u. In this toy model, two materials share the same interaction potential for simplicity but with different masses, and the variation of mass is used to tune the mismatch degree between two materials in order to obtain a smoothly varying trend. The variation of m in our model provides a straightforward way to tune the acoustic impedance contrast across the interface without altering the bonding network. In order to examine the validity of the developed theory, the range of m explored in this work spans from the weak to strong impedance mismatch.

All structures have been optimized at 0 K. The WP simulation in this work was performed by using the LAMMPS package [41] with the optimized Tersoff potential [42]. The Tersoff type potential has been widely used in the literature for various systems like graphene, *h*-BN, Si, and their interfaces [43–48]. It should be pointed out that the momentum-space transmission method (MSTM) does not depend on the specific potential, and different potentials mainly influence the elastic constants, which can be incorporated into the analytical framework accordingly. Here, the C–C bond length is set as 1.44 Å, and the time step is set at 0.5 fs. The atomistic system used has a length of 8632 Å, a width of 60 Å, and a vacuum layer in the z direction of 20 Å. In material 1, the initial profile

of a Gaussian phonon wave packet with wave vector k_1 and branch index λ is set as [49]

$$u_{j\lambda\beta}(x, 0) = A \varepsilon_{j\lambda\beta} e^{ik_1(x-x_c)} e^{-\frac{(x-x_c)^2}{2\sigma_1^2}}, \quad (8)$$

where $u_{j\lambda\beta}(x, 0)$ represents the β component of displacement at $t = 0$ for atom j in primitive cell, and $\varepsilon_{j\lambda\beta}$ is the phonon eigenvector component. The wave packet has the amplitude A and spatial broadening σ_1 centered at x_c in real space. Once k_1 is specified, $\varepsilon_{j\lambda\beta}$ and ω are determined from the phonon dispersion relation by diagonalizing the dynamical matrix. In this work, we limit our simulation to the case of normally incident wave packet with one-dimensional spatial broadening, as the modeling of oblique phonon incidence would require a two-dimensional wave packet with substantially larger simulation domain. In our simulations, we use the transverse acoustic (TA) phonon mode with $k_1 = 0.177$ (1/Å) as a representative example. The amplitude A is set as $A = 0.01R_0$, where $R_0 = 2.46$ Å corresponds to the graphene lattice constant and is used as the length unit in our study. The spatial broadening σ_1 is set as $\sigma_1 = 173$ Å. This value is consistent with typical coherence lengths observed in experiments involving coherent acoustic phonons in semiconductor systems, where similar wave-packet broadening has been reported, particularly for wavelengths on the order of tens of nanometers [50–54]. This consistency ensures that our model parameters are physically relevant in realistic system and can be experimentally accessible.

B. Results and discussion for the single-interface system

In this work, we focus on the acoustic phonon branches, which exhibit linear dispersion and relatively high group velocities, enabling clear tracking of wave-packet propagation. Moreover, given the fact that acoustic phonons dominate thermal transport in most crystalline materials, investigating their dynamics is essential for elucidating the fundamental mechanisms of phonon-mediated heat conduction. As shown in Fig. 1(b), the phonon transmission coefficient α obtained from TMM (solid line) matches well with wave-packet simulation results (squares) when varying the mass in material 2. In fact, the group velocity v of the acoustic branches in the linear region is approximately independent of the wave vector. For two graphene sheets with different atomic masses, the velocities of their acoustic branches are related by a multiplicative factor as $v_1/v_2 = \sqrt{m_2/m_1}$. Therefore, all modes within the same linear acoustic branch exhibit the same α according to Eqs. (5)–(7). Consequently, in the case of a single interface, α obtained from the phonon wave packet aligns with the value predicted by the TMM. Moreover, the reflected and transmitted waves retain the same waveform as the incident wave [see Fig. 1(c)]. When m varies up to 50 u, the difference between WP and TMM predictions remains negligible [below 2%, see circle in Fig. 1(b)]. This minor discrepancy is due to the presence of interfacial phonon modes [55,56], which is excluded in the analytical framework. Unlike the hard-boundary assumption used in the continuity equation during derivation, molecular dynamics simulations inherently capture interfacial phonon modes that deviate significantly from those in the bulk material [57,58]. These interfacial modes are spatially

localized and their amplitudes decay exponentially with the distance away from the interface, leading to a gradual rather than abrupt transition across the interface [59–61]. Although the interaction between phonons and these localized interfacial modes may also sustain phase-correlated dynamics in the near-interface region at low temperature [62], such dynamics is conceptually different from the phonon spatial coherence considered in this work, which refers to the propagation of phase-preserving phonon wave packets with finite-width across heterostructures. The presence of interfacial modes alters the local phonon field, causing deviations from the idealized hard-boundary model and thereby compromising the accuracy of coherent-phonon transport predictions. Nevertheless, their overall impact on the transmission coefficient is minor and can be safely neglected in the present analysis.

It is worth noting that the spatial coherence length of a phonon wave packet varies across different materials and is generally proportional to the phonon group velocity in each material [63]. In material 2, its wave-packet broadening is thus given by

$$\sigma_2 = \frac{v_2}{v_1} \sigma_1. \quad (9)$$

The left panel of Fig. 1(c) illustrates the evolution of the phonon wave packet as it propagates towards the right side of the interface with varying mass. The top panel represents the shape of the wave packet in material 1 at initial time ($t = 0$ ps). The remaining three plots show the shape of the wave packet at the same instantaneous time ($t = 10$ ps) after transmission into material 2 with varying mass. It is clearly observed that as the mass in material 2 decreases, the broadening of the wave packet becomes more substantial. As shown in the right panel of the Fig. 1(c), we compare the group velocity and broadening of the wave packet propagating into material 2 with those of the initial wave packet in material 1. The observed linear proportionality further confirms the validity of Eq. (9). Although the variation in the spatial broadening of phonon wave packet does not impact the transmission coefficient in single-interface systems, it significantly influences wave-packet transmission in multi-interface systems, which will be discussed in the next section.

III. TRANSMISSION OF PHONON WAVE PACKET THROUGH MULTIPLE INTERFACES

A. TMM theory for the multiple-interface system

Next, we consider a system with multiple interfaces, which is more common in practical applications, such as superlattices or thin film systems. We also consider the incidence of plane-wave phonons or Gaussian wave-packet phonons to a multi-interface system. Under the plane-wave assumption, the TMM can also be used to obtain the final α for the multiple-interface system because it accounts for multiple transmissions and reflections between interfaces. The atomic displacement amplitude in layer I can be expressed as

$$u_I(x, t) = a_{I,t} e^{ik_I x} e^{-i\omega t} + a_{I,r} e^{-ik_I x} e^{-i\omega t}, \quad (10)$$

where $a_{I,t}$ and $a_{I,r}$ represent the amplitudes of transmitted and reflected waves in layer I , respectively. Here, it is convenient to introduce a 2×2 matrix $\mathbf{h}_I$ defined as

$$\mathbf{h}_I(x) = \begin{bmatrix} e^{ik_I x} & e^{-ik_I x} \\ C_I k_I e^{ik_I x} & -C_I k_I e^{-ik_I x} \end{bmatrix}, \quad (11)$$

where C_I is the elastic constant in layer I . Besides, we define two-component column vectors $\mathbf{w}_1 = [a_{1,i}, a_{1,r}]^T$ for the first layer and $\mathbf{w}_I = [a_{I,t}, a_{I,r}]^T$ for the remaining layers. It is convenient to express the continuity condition of the displacement and stress fields at the interfaces as

$$\begin{aligned} \mathbf{h}_1(x_1)\mathbf{w}_1 &= \mathbf{h}_2(x_1)\mathbf{w}_2, \\ \mathbf{h}_2(x_2)\mathbf{w}_2 &= \mathbf{h}_3(x_2)\mathbf{w}_3, \\ &\dots \\ \mathbf{h}_{n-1}(x_{n-1})\mathbf{w}_{n-1} &= \mathbf{h}_n(x_{n-1})\mathbf{w}_n. \end{aligned} \quad (12)$$

Eliminating the intermediate vectors $\mathbf{w}_2 \sim \mathbf{w}_{n-1}$ in Eq. (12) yields a relation between the incident phonon wave amplitudes $\mathbf{w}_1$ and the transmitted phonon wave amplitudes $\mathbf{w}_n$ as

$$\mathbf{w}_n = \mathbf{M}\mathbf{w}_1, \quad (13)$$

where $\mathbf{M}$ is the “transfer matrix” given by

$$\begin{aligned} \mathbf{M} &= [\mathbf{h}_n(x_{n-1})]^{-1} [\mathbf{h}_{n-1}(x_{n-1})] [\mathbf{h}_{n-1}(x_{n-2})]^{-1} [\mathbf{h}_{n-2}(x_{n-2})] \\ &\dots [\mathbf{h}_2(x_1)]^{-1} [\mathbf{h}_1(x_1)]. \end{aligned} \quad (14)$$

The solution of Eq. (13) yields the amplitudes $a_{n,t}$ of the transmitted wave in the transmitted region and $a_{1,r}$ of the reflected wave in the incident region. The transmission coefficient α can then be obtained via Eq. (7).

However, due to the spatially varying amplitude of the phonon wave packet, the situation in the multiple-interface system differs fundamentally from that of a single interface. In such system, the amplitude of the wave packet interacting with each interface is nonuniform, as it is modulated by a Gaussian envelope. As a result, each interface experiences a different incident amplitude, making it difficult to directly evaluate the overall transmission as in the case of single interface. Moreover, since the wave packet does not exhibit a stationary amplitude like a plane wave, the multiple reflections and transmissions are wave-vector dependent. These complications make the cumulative propagation in the multiple-interface system highly nontrivial.

B. TMM and simulation results for the two-interface system

To demonstrate the effect of phonon spatial coherence on the transmission coefficient α in the multiple-interface system, we consider a two-interface heterostructure shown in Fig. 2(a) as the simplest example. This heterostructure is composed of a ^{13}C isotopic graphene sheet with the length L sandwiched by two ^{12}C graphene sheets, which correspond to the incident region and transmission region, respectively. The same approach can be further extended to the multiple-interface system without loss of generality.

We first investigate the influence of wave-packet broadening on phonon transmission by simulating wave packets with different spatial widths and analyzing their behaviors across varying interfacial length L . Significant differences

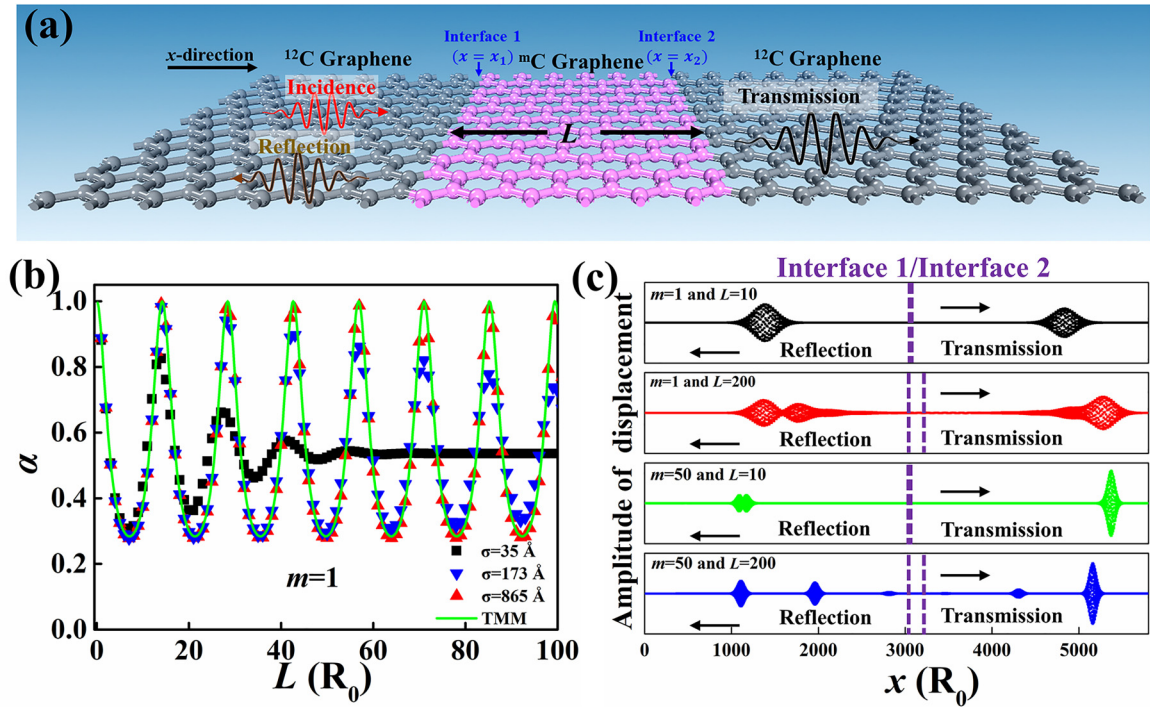


FIG. 2. (a) Structural schematic of a two-interface system. For simplicity, we employ a two-interface system consisting of two graphene layers with different atomic masses. The carbon atoms on the left and right sides have a mass of 12 u, serving as the incidence and transmission regions, respectively. The carbon atoms in the middle graphene layer have a mass of m . (b) The transmission coefficients of phonon wave packets with wave vector $k_1 = 0.177 \text{ (1/\AA)}$ and different broadening through a middle layer with $m = 1$ u varying with the length L of the interfacial layer. Phonon wave packets with larger broadening show better agreement with TMM, while those with smaller broadening exhibit significant discrepancies from the TMM results. (c) The snapshots at $t = 10 \text{ ps}$ for the reflected and transmitted wave packets after passing through the two-interface structure exhibit notable deviations from the initial Gaussian profile, particularly for larger m and L values. The σ_1 of the incident phonon wave packet is set as $\sigma_1 = 173 \text{ \AA}$. The vertical dashed lines denote the position of the interface.

are observed in Fig. 2(b) between the transmission coefficients obtained from wave-packet (WP) simulations with small spatial broadening $\sigma = 35 \text{ \AA}$ and $\sigma = 173 \text{ \AA}$ (symbols) and those from the TMM (solid line). As the interfacial length L increases, the WP transmission exhibits characteristic oscillations superimposed on an overall decay. In particular, broader wave packets ($\sigma = 865 \text{ \AA}$) result in a slower decay of the transmission, as they more closely resemble the plane-wave behavior. This trend demonstrates that spatial broadening, closely related to the phonon coherence length, plays a crucial role in determining transmission characteristics in multi-interface systems. In contrast, the transmission predicted by the TMM shows purely periodic oscillations without decay, corresponding to the idealized limit of infinitely broad wave packets or perfectly coherent plane waves. This discrepancy underscores the limitations of TMM in accounting for finite coherence length effects on phonon transport in realistic materials.

Another important finding is that the Gaussian wave packet gradually deviates from its initial shape after passing through multiple interfaces. Figure 2(c) presents snapshots at the same time instance for the reflected and transmitted wave packets under four representative configurations, highlighting how the atomic mass and interfacial spacing influence wave-packet evolution through cumulative transmission and reflection. In the first panel ($m = 1$ and $L = 10$), the wave packet retains its initial Gaussian profile, indicating minimal distortion under

weak modulation and short propagation distance. The second panel ($m = 1$ and $L = 200$) shows that even with the same mass, a longer interfacial spacing introduces notable distortion and spreading, as the wave packet undergoes strong internal reflections and interference within the interfacial layer in the middle.

Increasing the atomic mass in the interfacial layer leads to stronger reflection and transmission amplitude mismatches even for a small interfacial spacing ($m = 50$ and $L = 10$), which in turn produce a more pronounced deviation from the original wave-packet shape. The fourth panel ($m = 50$ and $L = 200$) combines both effects, large atomic mass and long interfacial spacing, resulting in significant broadening, asymmetry, and waveform reshaping in both transmitted and reflected components. These comparisons clearly demonstrate that the increase of both atomic mass and interfacial spacing can amplify the cumulative effect of multiple reflections and transmissions, leading to more substantial deviations from the initial wave-packet shape. This result emphasizes the critical role of internal interference dynamics on phonon transport across layered media.

These results indicate that the transmission of the wave packet differs significantly from that obtained using the TMM in the presence of finite spatial broadening. For the multiple interfaces, using the plane-wave assumption to estimate the phonon transmission coefficient can lead to significant deviations from the actual situation. Therefore, it is essential

to develop effective approaches for precisely assessing the transmission coefficient of phonon wave packets, accounting for the spatial broadening effect.

C. MSTM theory for the multiple-interface system

The observed discrepancy between wave-packet simulations and the TMM results underscores the limitations of conventional analytical approaches that assume perfectly coherent and infinitely extended plane waves. Therefore, it becomes essential to develop new computational frameworks that go beyond idealized assumptions and explicitly incorporate the spatial coherence effect. Here, we propose the momentum-space transmission method (MSTM) for the analytical determination of the transmission coefficient α in multi-interface systems, which can consider the spatial coherence in phonon transport processes, a missing feature in purely plane-wave-based models like the TMM. For simplicity, we also illustrate this method using the simple two-interface model shown in Fig. 2(a). The same principle can be straightforwardly extended to the multiple-interface system with increased calculation complexity. In these analytical calculations, we set the same parameters as those used in wave-packet simulations, including the incident wave vector and waveform, as well as the mass and elastic constants for each material in the system.

In the momentum space, the initial wave packet in the incident region can be written as

$$\langle k' | \psi(t=0) \rangle = B\sqrt{2\pi}\sigma_1 e^{-\left[\frac{\sigma_1^2(k'-k_1)^2}{2}\right]} e^{ik'x_c}, \quad (15)$$

which describes the Fourier transform of a real-space Gaussian wave packet of Eq. (8). Here, B is the amplitude of the wave packet in momentum space, k' represents the wave-vector variable and k_1 represents wave vector of the incident wave packet, and x_c is the center position of the wave packet in real space. Its time evolution is then given by

$$\langle k' | \psi(t) \rangle = \int_{-\infty}^{+\infty} \langle k | \varphi_k \rangle e^{-i\omega t} \langle k' | \psi(t=0) \rangle dk', \quad (16)$$

where φ_k denotes the eigenmodes that contribute to the formation of the wave packet. These states are expressed explicitly in coordinate representation as

$$\langle x | \varphi_{k'} \rangle = \begin{cases} a_{1,i} e^{ik'x} + a_{1,r} e^{-ik'x}, & x < x_1 \\ a_{2,t} e^{ik''x} + a_{2,r} e^{-ik''x}, & x_1 < x < x_2 \\ a_{3,t} e^{ik'x}, & x > x_2 \end{cases} \quad (17)$$

where $k'' = \sqrt{\frac{m}{12}}k'$ represents the wave vector in material 2, while x_1 and x_2 are the positions of interface 1 and interface 2, respectively. The incident amplitude is set as $a_{1,i} = 1$ and the rest coefficients $a_{1,r}$, $a_{2,t}$, $a_{2,r}$, and $a_{3,t}$ are determined by the continuity condition of the wave function, similar to Eq. (3) in the TMM, and can be expressed as

$$a_{1,r} = \frac{i}{2\Omega} \left(\frac{C_2 k''}{C_1 k'} - \frac{C_1 k'}{C_2 k''} \right) \sin[k''(x_2 - x_1)] e^{-ik'(x_2 - x_1)}, \quad (18)$$

$$a_{2,t} = \frac{1}{2\Omega} \left(1 + \frac{C_1 k'}{C_2 k''} \right) e^{-i(k' + k'')(x_2 - x_1)}, \quad (19)$$

$$a_{2,r} = \frac{1}{2\Omega} \left(1 - \frac{C_1 k'}{C_2 k''} \right) e^{-i(k' - k'')(x_2 - x_1)}, \quad (20)$$

$$a_{3,t} = \frac{1}{\Omega} e^{-ik'(x_2 - x_1)}, \quad (21)$$

where $\Omega = \cos[k''(x_2 - x_1)] - \frac{i}{2} \left(\frac{C_2 k''}{C_1 k'} + \frac{C_1 k'}{C_2 k''} \right) \sin[k''(x_2 - x_1)]$.

Fourier transformation of $\langle x | \varphi_{k'} \rangle$ in Eq. (17) gives five terms proportional to the coefficients $a_{1,t}$, $a_{1,r}$, $a_{2,t}$, $a_{2,r}$, and $a_{3,t}$, respectively. Substituting these terms into Eq. (16) with the initial state in Eq. (15), we obtain

$$\begin{aligned} \langle k | \psi(t) \rangle = & i \frac{B}{\sqrt{2\pi}} \sigma_1 \int_{-\infty}^{+\infty} [g_{1,i}(k') + g_{1,r}(k') + g_{2,t}(k') \\ & + g_{2,r}(k') + g_{3,t}(k')] e^{i\alpha(k',t)} dk', \end{aligned} \quad (22)$$

where different terms are given by

$$o(k', t) = -ik'v_1 t - \frac{ik'(x_2 - x_1)}{2} + ik'x_c - \frac{\sigma_1^2(k' - k_1)^2}{2}, \quad (23)$$

$$g_{1,i}(k') = \frac{1}{k - k' + i0^+} e^{ik'(x_2 - x_1)/2}, \quad (24)$$

$$g_{1,r}(k') = \frac{a_{1,r}}{k + k' + i0^+} e^{ik'(x_2 - x_1)} e^{ik(x_2 - x_1)/2}, \quad (25)$$

$$g_{2,t}(k') = \frac{-2ia_2^t}{k - k''} \sin\left[\frac{1}{2}(k - k'')(x_2 - x_1)\right] e^{ik'(x_2 - x_1)/2}, \quad (26)$$

$$g_{2,r}(k') = \frac{-2ia_2^r}{k + k''} \sin\left[\frac{1}{2}(k + k'')(x_2 - x_1)\right] e^{ik'(x_2 - x_1)/2}, \quad (27)$$

$$g_{3,t}(k') = \frac{-a_3^t}{k - k' - i0^-} e^{ik'(x_2 - x_1)} e^{-ik(x_2 - x_1)/2}. \quad (28)$$

In this framework, the wave-packet line shape can be described by the term $e^{i\alpha(k',t)}$. By specifying this term, one can prescribe an arbitrary spectral profile, while the remaining MSTM formulation provides a line-shape-independent transfer kernel for modeling phonon transport across different materials and interfaces.

The above derivation can be readily generalized to the oblique phonon incidence. In that case, the complexity is significantly enhanced in order to account for the multiple polarizations and mode conversion, which requires a polarization-resolved determination of the reflected and transmitted amplitudes at each interface [52]. In order to reduce the computational complexity and focus on the finite broadening effect, we restrict our discussion to the normal-incidence case in this work.

Previous work [64] has shown that if only the asymptotic behavior and the transmission after the collision is of interest, the structural terms $g_{1,i}(k')$, $g_{1,r}(k')$, and $g_{3,t}(k')$ are sufficient.

Therefore, we can calculate the transmission coefficient as

$$\alpha = \frac{\int_{-\infty}^{+\infty} |2\pi i \text{Res}(g_{3,t}(k'))|^2 e^{-\sigma_1^2(k'-k_1)^2} dk'}{\int_{-\infty}^{+\infty} (|2\pi i \text{Res}(g_{1,r}(k'))|^2 + |2\pi i \text{Res}(g_{3,t}(k'))|^2) e^{-\sigma_1^2(k'-k_1)^2} dk'}, \quad (29)$$

where Res is the notation for the residue. The MSTM framework explicitly resolves the k -dependent transmission and reflection, thereby capturing coherent interference effects, which are generally absent in disorder-averaged or frequency-only descriptions without the phase information [65,66].

D. MSTM and simulation results for the two-interface system

To verify the accuracy of our proposed method and better understand the role of phonon broadening, we study the phonon transport across a two-interface heterostructure, as illustrated in Fig. 2(a), by systematically varying two key parameters of material 2: the atomic mass m and the length L . In the following simulations and analytical calculations, we use Gaussian wave packet with a fixed spatial width of $\sigma = 173 \text{ \AA}$.

We first compare the transmission coefficient as a function of the interfacial layer mass for different lengths. When the interfacial length is relatively short ($L = 10R_0$), the results obtained from the TMM, wave-packet simulations, and MSTM are in good agreement [Fig. 3(a)]. This is primarily because the relatively short spacing between two interfaces means that the phonon wave packet does not undergo significant attenuation or amplitude modulation during propagation. Consequently, the wave packet preserves a shape and amplitude profile similar to that of a plane wave at both interfaces, making the TMM prediction equivalent to the MSTM result.

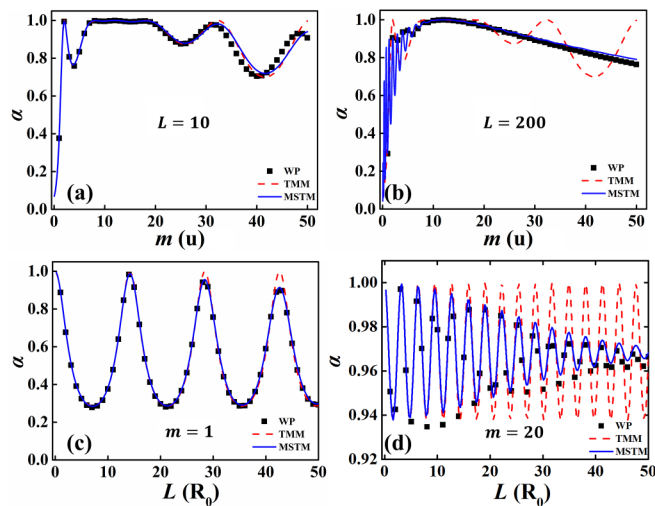


FIG. 3. The transmission coefficients α obtained through WP simulations, the TMM and MSTM versus the atomic mass m in the interfacial layer with a fixed length of (a) $L = 10R_0$ and (b) $L = 200R_0$. The transmission coefficients obtained through WP simulation, the TMM and MSTM versus the length L with a fixed atomic mass of (c) $m = 1$ u and (d) $m = 20$ u. An incident wave vector $k_1 = 0.177$ ($1/\text{\AA}$) is used for the WP simulations, TMM and MSTM calculations, and the wave-packet width of $173 \text{ \AA}$ is used for the WP simulations and MSTM calculations.

This scenario effectively serves as a reference case, validating the consistency between different approaches when the spatial coherence effect can be neglected.

However, when the interfacial layer is sufficiently long ($L = 200R_0$), the TMM results deviate substantially from the wave-packet simulations with the variation of the interfacial layer mass, whereas the MSTM continues to yield consistent results [Fig. 3(b)]. This is because when the interfacial spacing is sufficiently large, the spatial coherence effect can no longer be neglected at multiple interfaces, which leads to strong distortion and spreading of wave packet across the interfaces [see Fig. 2(c)] and thus causes significant deviations from the plane-wave assumption used in TMM.

After investigating the impact of interfacial layer length L , we then discuss the influence of the atomic mass m of interfacial layer on phonon transmission. This variation effectively mimics the scenario of phonon transport across different materials. We further compare the phonon transmission for two representative cases: $m = 1$ and 20 , as shown in Figs. 3(c) and 3(d), respectively. For the case of $m = 1$, the results from the MSTM show excellent agreement with the wave-packet simulations, while the TMM result exhibits a gradual deviation from the wave-packet simulations with the increase of interfacial layer length L [Fig. 3(c)]. This deviation primarily arises from wave-packet broadening over longer propagation distances, which leads to a non-negligible difference in phonon amplitudes at the two interfaces, an effect not considered by the TMM due to its underlying plane-wave assumption. Furthermore, the phonon group velocity in the interfacial layer is relatively high in this case, resulting in a broader wave-packet envelope as described by Eq. (9). The high group velocity allows the wave packet to maintain a slowly varying amplitude over longer distances, thereby delaying the onset of significant discrepancies. As a result, noticeable differences between the TMM and wave-packet simulations emerge only when L becomes sufficiently large.

In contrast, when the atomic mass of interfacial layer is increased ($m = 20$), the phonon group velocity becomes significantly lower, leading to the reduced spatial broadening of the phonon wave packet. This causes the amplitude to vary more rapidly across the interfacial layer, resulting in a more pronounced difference at two interfaces. As evident in Fig. 3(d), the MSTM continues to provide consistent results with the wave-packet simulations because it explicitly accounts for the spatial broadening of the phonon wave packet. However, the TMM results deviate significantly from the wave-packet simulations for large L values due to its intrinsic plane-wave assumption. This deviation in Fig. 3(d) is particularly pronounced compared to the lighter mass case in Fig. 3(c).

When considering the spatial coherence, it is important to note that the transmission coefficient α gradually converges as the distance between the two interfaces increases. This convergence occurs over a length scale closely related

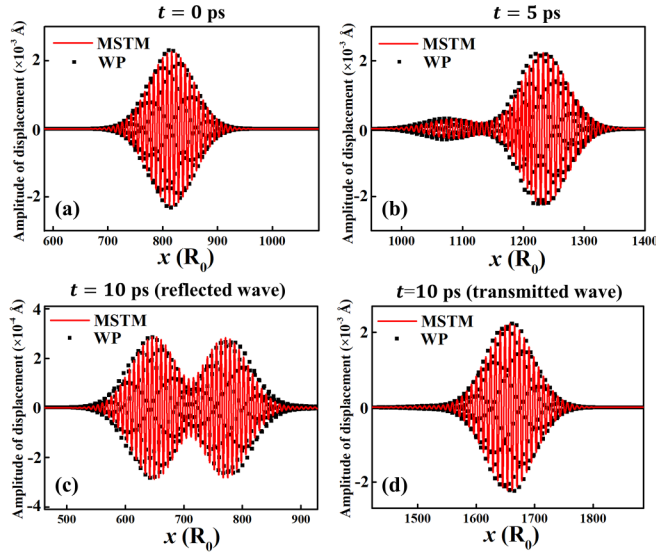


FIG. 4. Wave-packet propagation process in the two-interface graphene system obtained from the inverse Fourier transform of the MSTM solution (solid line) and from the time-domain wave-packet simulation (square) at (a) $t = 0$ ps, (b) $t = 5$ ps, (c) $t = 10$ ps for the reflected wave, and (d) $t = 10$ ps for the transmitted wave. The system parameters are $L = 50R_0$ and $m = 20$ u, and the incident wave-packet width and wave vector are set as 173 Å and $k_1 = 0.177$ ($1/\text{Å}$), respectively.

lated to wave-packet broadening in the interfacial layer. When the transmission converges, it indicates that the wave packet has completely lost coherence between two interfaces. Consequently, different interfaces behave independently, and interference between multiple reflected components of the wave packet is suppressed.

Moreover, the application of MSTM is not limited just to the evaluation of transmission coefficient. Its key advantage is that it retains the full inter- k phase correlations and provides a closed-form k -space representation for a multi-interface stack, which is directly equivalent to the time-domain wave-packet simulations. In particular, MSTM yields analytic terms [e.g., $g_{1,i}(k')$, $g_{1,r}(k')$, $g_{2,t}(k')$, $g_{2,r}(k')$, $g_{3,t}(k')$], which encode all multiple reflections and interference inside the stack. With this information, we can reconstruct the real-space wave packet via an inverse Fourier transform at arbitrary times. This allows us to resolve not only the integrated transmission, but also the time-dependent evolution and distortion of the reflected and transmitted wave packets in each region of the real space (i.e., the wave-packet dynamics in coordinate space), which cannot be obtained from a simple spectrum-weighted plane-wave model.

To demonstrate the above points, we take the two-interface system with $L = 50R_0$ and $m = 20$ u as an example. Here we consider an incident wave packet with width of 173 Å and wave vector $k_1 = 0.177$ ($1/\text{Å}$). Figure 4 shows the reconstructed wave packet from MSTM (solid line) at the initial time ($t = 0$ ps), at the time snapshot when the packet encounters the interfaces ($t = 5$ ps), and at the time snapshot when the transmission process is completed ($t = 10$ ps), in comparison with the corresponding time-domain wave-packet simulation results (squares). These three sets of results are

almost indistinguishable, demonstrating that MSTM faithfully reproduces the real-space wave-packet evolution and wave-form distortion at arbitrary time snapshots. This agreement highlights the fact that MSTM has advantages over the simple spectrum-weighted plane-wave model, as MSTM retains the complete phase information required to fully describe the coherent phonon wave-packet transport dynamics in multi-interface heterostructures.

To further validate the accuracy and practical applicability of the MSTM in realistic materials with different dimensionalities, we use the two-interface system as an example and construct realistic two-dimensional (2D) (graphene/*h*-BN/graphene) and three-dimensional (3D) (Si/Ge/Si) heterostructures. After structure relaxation, both the MSTM and wave-packet simulations are used to calculate the transmission coefficient in these realistic heterostructures for comparison. For the 2D (graphene/*h*-BN/graphene) heterostructure, we employ the optimized Tersoff potential [67] to describe the interatomic interactions, and vary the thickness of the *h*-BN layer for validation. The incident wave packet with width of 173 Å and wave vector $k_1 = 0.177$ ($1/\text{Å}$) is used in the simulation. As shown in Fig. 5(a), the results from the MSTM are in excellent agreement with those from the wave-packet simulation. Similarly, for the 3D (Si/Ge/Si) structure, we use the original Tersoff potential [68] to model the interaction, with the incident wave vector set as $k_1 = 0.057$ ($1/\text{Å}$) and the wave-packet width of 173 Å . Figure 5(b) shows that the MSTM also provides accurate predictions of the transmission coefficient in excellent agreement with those obtained from the wave-packet simulation methods for 3D (Si/Ge/Si) heterostructures. These results demonstrate the versatility and accuracy of the MSTM for realistic materials with different dimensionalities.

It should be pointed out that the application of MSTM is not limited only to the two-interface system. To illustrate this point, we extend to examine the validity of the MSTM in a three-interface system composed of 2D materials as graphene/*h*-BN/graphene/*h*-BN, by varying the thickness of the third layer (the second graphene sheet) and calculating the corresponding phonon transmission. As shown in Fig. 5(c), the MSTM results consistently reproduce the interference trends and show excellent agreement with the wave-packet simulations, confirming that the MSTM can reliably describe the phonon transmission in multi-interface heterostructures.

Finally, we discuss the shapes of the transmitted and reflected wave packets predicted by the MSTM in the momentum space, after passing through a two-interface model with fixed parameters ($m = 50$ and $L = 200R_0$). As shown in Fig. 6(a), although the reflected and transmitted waves in momentum space retain a Gaussian shape in general, the envelope exhibits small oscillations arising from the wavelength-dependent scattering at multiple interfaces, thereby distinguishing them from the original Gaussian wave packet.

Since phonons may exhibit different spectral line shapes depending on their excitation conditions or the nature of the system, other broadened profiles than Gaussian are also commonly encountered [69,70]. Therefore, we study the impact of the line profile of phonon wave packet in order to verify the applicability of the proposed method. In this regard, we apply

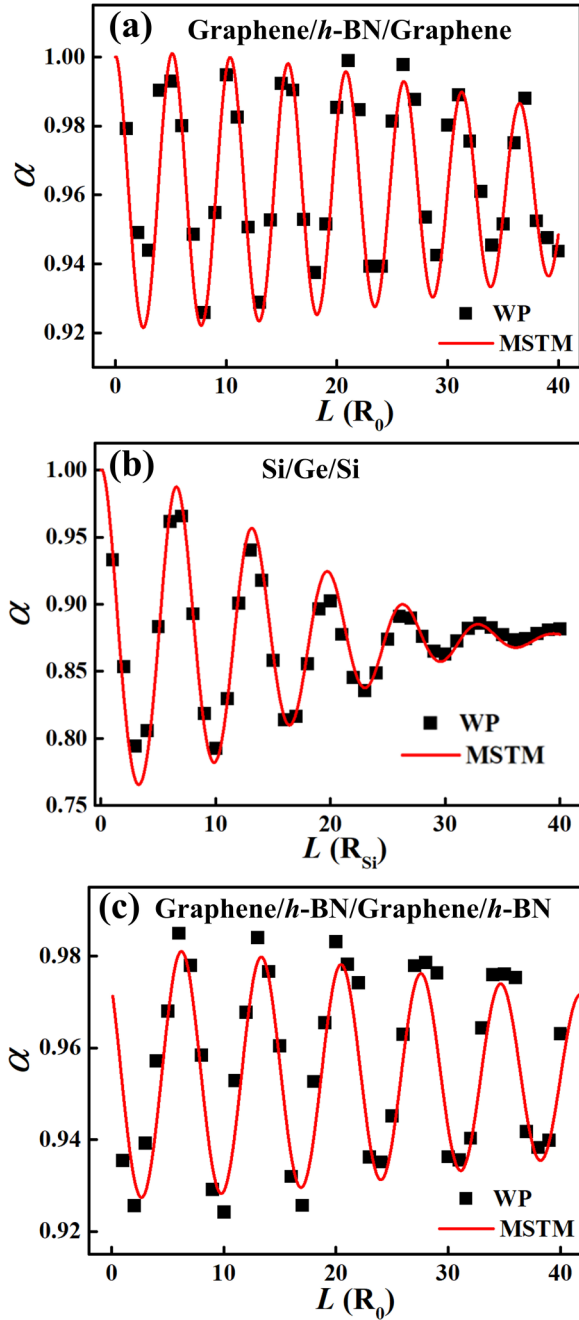


FIG. 5. (a) The transmission coefficient α obtained from the wave-packet simulation and MSTM for 2D graphene/h-BN/graphene heterostructure with varying interfacial layer length L . The incident wave packet with width of $173 \text{ \AA}$ and wave vector $k_1 = 0.177 \text{ (1/\AA)}$ is used in the simulation. (b) The transmission coefficient obtained from the wave-packet simulation and MSTM for 3D Si/Ge/Si heterostructure with varying interfacial layer length L . The incident wave packet with width of $173 \text{ \AA}$ and wave vector $k_1 = 0.0575 \text{ (1/\AA)}$ is used in the simulation. (c) The transmission coefficient obtained from the wave-packet simulation and MSTM for 2D graphene/h-BN/graphene/h-BN heterostructure with varying length of the third layer. The incident wave packet with width of $173 \text{ \AA}$ and wave vector $k_1 = 0.177 \text{ (1/\AA)}$ is used in the simulation. Here R_0 and R_{Si} denote the lattice constant of graphene and silicon, respectively.

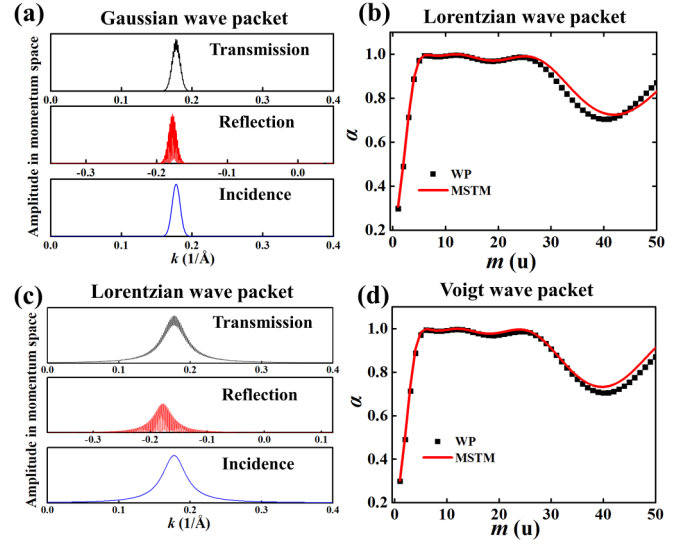


FIG. 6. (a) The shapes of the transmitted, reflected, and incident phonon wave packets in momentum space ($m = 50 \text{ u}$, $L = 200R_0$). The transmitted and reflected wave packets exhibit substantial departures from this initial Gaussian shape. (b) The transmission coefficient of Lorentzian phonon wave packet passing through a two-interface system with $L = 5R_0$ versus the atomic mass m . (c) The shapes of the transmitted, reflected, and incident Lorentzian phonon wave packets in momentum space ($m = 50 \text{ u}$, $L = 200R_0$). The transmitted and reflected wave packets also exhibit substantial departures from initial Lorentzian shape. (d) The transmission coefficients of Voigt phonon wave packet passing through a two-interface graphene system with $L = 5R_0$ versus the atomic mass m . The Voigt phonon wave-packet parameters are set as $\chi = 0.3$, $\gamma_1 = 100 \text{ \AA}$ and $\sigma_1 = 173 \text{ \AA}$ and $k_1 = 0.177 \text{ (1/\AA)}$.

Lorentzian wave packets in real space for both numerical simulations and analytical calculations. Similar to the Gaussian wave packet, the phonon wave packet with Lorentzian line shape in real space can be expressed as

$$u_{j\lambda\beta}(x, t) = A\epsilon_{j\lambda\beta} e^{ik_1(x-x_c)} e^{-\frac{|x-x_c|}{\gamma_1}} e^{-i\omega t}, \quad (30)$$

where the parameter γ_1 determines the linewidth of the Lorentzian phonon wave packet in material 1. In our simulations, the parameter γ_1 is set as $\gamma_1 = 100 \text{ \AA}$ and the other parameters are identical to those of the Gaussian wave packet. As shown in Fig. 6(b), the wave-packet simulation results are in agreement with the predictions by Eq. (29), further validating the universality of MSTM among different line shapes. Additionally, similar to the case of Gaussian wave packets, the transmitted and reflected waves obtained based on the Lorentzian wave packets also exhibit significantly different shapes compared to the original incident wave in momentum space, as shown in Fig. 6(c).

In addition, we also adopt the Voigt function to further validate that the MSTM is applicable to different waveforms. The Voigt function, which combines Gaussian and Lorentzian profiles, can be expressed as [71]

$$u_{j\lambda\beta}(x, t) = \chi A\epsilon_{j\lambda\beta} e^{ik_1(x-x_c)} e^{-\frac{|x-x_c|}{\gamma_1}} e^{-i\omega t} + (1 - \chi) A\epsilon_{j\lambda\beta} e^{ik_1(x-x_c)} e^{-\frac{(x-x_c)^2}{2\sigma_1^2}}, \quad (31)$$

where χ controls the relative weight of the Gaussian and Lorentzian components. In this work, the Voigt phonon wave-packet parameters are set as $\chi = 0.3$, $\gamma_1 = 100 \text{ \AA}$ and $\sigma_1 = 173 \text{ \AA}$ and $k_1 = 0.177 (1/\text{\AA})$. As shown in the Fig. 6(d), the results from the MSTM are consistent with those obtained from the wave-packet simulation. This agreement further validates the applicability of MSTM in modeling phonon transport with various line shapes, demonstrating its generality in capturing the key features observed in the wave-packet approach.

Using a simplified model, this work only focused on the finite broadening effect of wave-packet evolution and its implications for phonon transmission across interfaces under normal incidence. More specifically, the present MSTM is designed to describe the transmission of coherent phonon wave packets with finite width in regimes where the preservation of phase coherence remains essential. Therefore, the current formulation is most applicable to relatively low temperatures, at which the dephasing anharmonic effect remains weak. At high temperatures, however, anharmonic phonon-phonon interactions and inelastic interfacial scattering become increasingly important [72–75], which can reduce the phase coherence and introduce energy redistribution or mode conversion processes beyond the scope of the present model. In this sense, the current MSTM should be targeted for resolving coherent or near-coherent wave-packet transmission physics. Moreover, a comprehensive evaluation of interfacial thermal conductance should take into account phonon incidence from various angles and polarizations, which introduces considerable computational complexity. Future effort is required for extending this approach to include multiangle and multipolarization effects. Additionally, a deeper understanding of phonon transport across complex interfaces can be achieved by further considering realistic material characteristics, such as anisotropy, anharmonicity, interface roughness, as well as incorporating multibranch effects and inelastic scattering.

IV. CONCLUSION

In summary, we have developed an analytical method named MSTM to calculate the phonon transmission coefficient across the interfaces taking into account the spatial coherence of phonons. The validity of developed MSTM is examined against the phonon wave-packet simulations that can explicitly monitor the propagation of phonons with finite spatial broadening across various types of interfaces. It is found

that phonon spatial coherence has negligible impact on the transmission coefficient across a single interface. However, in the multi-interface system, such spatial coherence effect significantly influences the phonon transmission coefficient and distorts the phonon waveform. In this case, the MSTM can provide consistent transmission with the phonon wave-packet simulations, while the conventional theory breaks down due to the use of plane-wave assumption. More importantly, MSTM faithfully resolves the wave-packet dynamics at arbitrary times during propagation, showing excellent agreement with time-domain wave-packet simulations. This makes MSTM an efficient surrogate for wave-packet simulations, which can substantially reduce computational cost without sacrificing accuracy. In addition, consistent MSTM predictions across different wave-packet line shapes further confirm the broad applicability of the developed framework. Our findings offer physical insights and a valuable tool for investigating phonon transmission across multilayered materials, which is highly pertinent to the structural design of phononic metamaterials and thermal interface materials.

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DATA AVAILABILITY

The data that support the findings of this article are not publicly available upon publication because it is not technically feasible and/or the cost of preparing, depositing, and hosting the data would be prohibitive within the terms of this research project. The data are available from the authors upon reasonable request.

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- [1] M. Maldovan, Sound and heat revolutions in phononics, *Nature (London)* **503**, 209 (2013).
 - [2] S. Huberman, R. A. Duncan, K. Chen, B. Song, V. Chiloyan, Z. Ding, A. A. Maznev, G. Chen, and K. A. Nelson, Observation of second sound in graphite at temperatures above 100 K, *Science* **364**, 375 (2019).
 - [3] J. Chen, J. He, D. Pan, X. Wang, N. Yang, J. Zhu, S. A. Yang, and G. Zhang, Emerging theory and phenomena in thermal conduction: A selective review, *Sci. China Phys. Mech. Astron.* **65**, 117002 (2022).
 - [4] Z. Zhang, Y. Guo, M. Bescond, J. Chen, M. Nomura, and S. Volz, Coherent thermal transport in nano-phononic crystals: An overview, *APL Mater.* **9**, 081102 (2021).
 - [5] M. N. Luckyanova *et al.*, Coherent phonon heat conduction in superlattices, *Science* **338**, 936 (2012).
 - [6] J. Ravichandran *et al.*, Crossover from incoherent to coherent phonon scattering in epitaxial oxide superlattices, *Nat. Mater.* **13**, 168 (2014).
 - [7] G. Chen, Non-Fourier phonon heat conduction at the microscale and nanoscale, *Nat. Rev. Phys.* **3**, 555 (2021).
 - [8] M. Simoncelli, N. Marzari, and F. Mauri, Unified theory of thermal transport in crystals and glasses, *Nat. Phys.* **15**, 809 (2019).
 - [9] L. Isaeva, G. Barbalinardo, D. Donadio, and S. Baroni, Modeling heat transport in crystals and glasses from a unified lattice-dynamical approach, *Nat. Commun.* **10**, 3853 (2019).

- [10] Z. Zhang, Y. Guo, M. Bescond, J. Chen, M. Nomura, and S. Volz, Heat conduction theory including phonon coherence, *Phys. Rev. Lett.* **128**, 015901 (2022).
- [11] Z. Zhang, Y. Guo, M. Bescond, J. Chen, M. Nomura, and S. Volz, How coherence is governing diffuson heat transfer in amorphous solids, *npj Comput. Mater.* **8**, 96 (2022).
- [12] M. S. Kushwaha, P. Halevi, L. Dobrzynski, and B. Djafari-Rouhani, Acoustic band structure of periodic elastic composites, *Phys. Rev. Lett.* **71**, 2022 (1993).
- [13] M. Maldovan, Phonon wave interference and thermal bandgap materials, *Nat. Mater.* **14**, 667 (2015).
- [14] S. Q. Hu, L. Feng, C. Shao, I. A. Strelnikov, Y. A. Kosevich, and J. Shiomi, Two-path phonon interference resonance induces a stop band in a silicon crystal matrix with a multilayer array of embedded nanoparticles, *Phys. Rev. B* **102**, 024301 (2020).
- [15] L. Feng, T. Shiga, H. Han, S. Ju, Y. A. Kosevich, and J. Shiomi, Phonon-interference resonance effects by nanoparticles embedded in a matrix, *Phys. Rev. B* **96**, 220301(R) (2017).
- [16] Y. Qiu, M. Nomura, Z. Zhang, *et al.*, Roadmap on thermodynamics and thermal metamaterials, *Front. Phys.* **20**, 65500 (2025).
- [17] S. Lu, Z. Zhang, Y. Li, P. Hänggi, and J. Chen, Phononic metagrating for lattice wave manipulation, *Phys. Rev. B* **109**, 075404 (2024).
- [18] B. L. Davis and M. I. Hussein, Nanophononic metamaterial: Thermal conductivity reduction by local resonance, *Phys. Rev. Lett.* **112**, 055505 (2014).
- [19] Z. Zhang, Y. Ouyang, J. Chen, and S. Volz, A phononic rectifier based on carbon schwarzite host-guest system, *Chin. Phys. B* **29**, 124402 (2020).
- [20] W. Ren, S. Lu, C. Yu, J. He, Z. Zhang, J. Chen, and G. Zhang, Impact of moiré superlattice on atomic stress and thermal transport in van der Waals heterostructures, *Appl. Phys. Rev.* **10**, 041404 (2023).
- [21] K. Saaskilahti, J. Oksanen, J. Tulkki, and S. Volz, Spectral mapping of heat transfer mechanisms at liquid-solid interfaces, *Phys. Rev. E* **93**, 052141 (2016).
- [22] Z.-Y. Ong and C. H. Lee, Transport and localization in a topological phononic lattice with correlated disorder, *Phys. Rev. B* **94**, 134203 (2016).
- [23] R. Cheaito, C. A. Polanco, S. Addamane, J. Zhang, A. W. Ghosh, G. Balakrishnan, and P. E. Hopkins, Interplay between total thickness and period thickness in the phonon thermal conductivity of superlattices from the nanoscale to the microscale: Coherent versus incoherent phonon transport, *Phys. Rev. B* **97**, 085306 (2018).
- [24] S. Lu, Z. Zhang, Y. Li, P. Hänggi, and J. Chen, Single phonon diode operating on a metagrating surface, *Phys. Rev. B* **112**, 075407 (2025).
- [25] W. Zhang, T. S. Fisher, and N. Mingo, Simulation of interfacial phonon transport in Si-Ge heterostructures using an atomistic Green's function method, *J. Heat Transfer* **129**, 483 (2007).
- [26] Z. Tian, K. Esfarjani, and G. Chen, Enhancing phonon transmission across a Si/Ge interface by atomic roughness: First-principles study with the Green's function method, *Phys. Rev. B* **86**, 235304 (2012).
- [27] J. S. Wang, J. Wang, and J. T. Lü, Quantum thermal transport in nanostructures, *Eur. Phys. J. B* **62**, 381 (2008).
- [28] B. Latour and Y. Chalopin, Distinguishing between spatial coherence and temporal coherence of phonons, *Phys. Rev. B* **95**, 214310 (2017).
- [29] P. Jiang, Y. Ouyang, W. Ren, C. Yu, J. He, and J. Chen, Total-transmission and total-reflection of individual phonons in phononic crystal nanostructures, *APL Mater.* **9**, 040703 (2021).
- [30] T. Maranets and Y. Wang, Prominent phonon transmission across aperiodic superlattice through coherent mode-conversion, *Appl. Phys. Lett.* **125**, 042205 (2024).
- [31] T. Maranets, M. Nasiri, and Y. Wang, Influence of spatial coherence on phonon transmission across aperiodically arranged interfaces, *Phys. Lett. A* **512**, 129572 (2024).
- [32] T. Yoshihiro and N. Nishiguchi, Mode-conversion effects of phonons on Anderson localization, *Phys. Rev. B* **100**, 235441 (2019).
- [33] A. M. Shaarawi, I. M. Besieris, A. M. Attiya, and E. El-Diwany, Acoustic X-wave reflection and transmission at a planar interface: Spectral analysis, *J. Acoust. Soc. Am.* **107**, 70 (2000).
- [34] E. T. Swartz and R. O. Pohl, Thermal boundary resistance, *Rev. Mod. Phys.* **61**, 605 (1989).
- [35] T. Beechem, S. Graham, P. Hopkins, and P. Norris, Role of interface disorder on thermal boundary conductance using a virtual crystal approach, *Appl. Phys. Lett.* **90**, 054104 (2007).
- [36] J.-H. Jiang, S. Lu, and J. Chen, Phonon focusing effect in an atomic level triangular structure, *Chin. Phys. Lett.* **40**, 096301 (2023).
- [37] S. Tamura, D. C. Hurley, and J. P. Wolfe, Acoustic-phonon propagation in superlattices, *Phys. Rev. B* **38**, 1427 (1988).
- [38] P. K. Schelling, S. R. Phillpot, and P. Keblinski, Phonon wave-packet dynamics at semiconductor interfaces by molecular-dynamics simulation, *Appl. Phys. Lett.* **80**, 2484 (2002).
- [39] Z. T. Tian, B. E. White, and Y. Sun, Phonon wave-packet interference and phonon tunneling based energy transport across nanostructured thin films, *Appl. Phys. Lett.* **96**, 263113 (2010).
- [40] A. A. Maznev, Boundary scattering of phonons: Specularity of a randomly rough surface in the small-perturbation limit, *Phys. Rev. B* **91**, 134306 (2015).
- [41] S. Plimpton, Fast parallel algorithms for short-range molecular dynamics, *J. Comput. Phys.* **117**, 1 (1995).
- [42] L. Lindsay and D. A. Broido, Optimized Tersoff and Brenner empirical potential parameters for lattice dynamics and phonon thermal transport in carbon nanotubes and graphene, *Phys. Rev. B* **81**, 205441 (2010).
- [43] S. Chen, Q. Wu, C. Mishra, J. Kang, H. Zhang, K. Cho, W. Cai, A. A. Balandin, and R. S. Ruoff, Thermal conductivity of isotopically modified graphene, *Nat. Mater.* **11**, 203 (2012).
- [44] Y. Gu, Phonon thermal transport in semi-disordered isotopic-superlattice graphene nanoribbons, *Numer. Heat Transf. A: Appl.* **73**, 115 (2018).
- [45] S. Bernard, E. Whiteway, V. Yu, D. G. Austing, and M. Hilke, Probing the experimental phonon dispersion of graphene using ^{12}C and ^{13}C isotopes, *Phys. Rev. B* **86**, 085409 (2012).
- [46] J.-H. Zou and B.-Y. Cao, Phonon thermal properties of graphene on *h*-BN from molecular dynamics simulations, *Appl. Phys. Lett.* **110**, 103106 (2017).
- [47] H. T. T. Nguyen, Structural evolution of in-plane hybrid graphene/hexagonal boron nitride heterostructure upon heating, *J. Mol. Graph. Model.* **125**, 108579 (2023).

- [48] J. Chen, G. Zhang, and B. Li, Thermal contact resistance across nanoscale silicon dioxide and silicon interface, *J. Appl. Phys.* **112**, 064319 (2012).
- [49] S. Hu, Z. Zhang, P. Jiang, J. Chen, S. Volz, M. Nomura, and B. Li, Randomness-induced phonon localization in graphene heat conduction, *J. Phys. Chem. Lett.* **9**, 3959 (2018).
- [50] X. Tu, J. Li, J. Yan, S. Wang, L. Li, C. Li, and Z. Wang, Picosecond ultrasonics for studying elastic modulus of polycrystalline chromium nanofilms: Thickness dependence and stiffness enhancement, *Coatings* **13**, 438 (2023).
- [51] T. Dehoux *et al.*, Optical tracking of picosecond coherent phonon pulse focusing inside a sub-micron object, *Light Sci. Appl.* **5**, e16082 (2016).
- [52] Y. Ezzahri *et al.*, Coherent phonons in Si/SiGe superlattices, *Phys. Rev. B* **75**, 195309 (2007).
- [53] Y. Ezzahri, S. Dilhaire, S. Grauby, J. M. Rampnoux, W. Claeys, Y. Zhang, G. Zeng, and A. Shakouri, Study of thermomechanical properties of Si/SiGe superlattices using femtosecond transient thermoreflectance technique, *Appl. Phys. Lett.* **87**, 103506 (2005).
- [54] Y. Huang *et al.*, Nanometer-scale acoustic wave packets generated by stochastic core-level photoionization events, *Phys. Rev. X* **14**, 041010 (2024).
- [55] R. Qi *et al.*, Measuring phonon dispersion at an interface, *Nature (London)* **599**, 399 (2021).
- [56] S. Shan, Z. Zhang, S. Lu, S. Volz, and J. Chen, Generation of interfacial phonon modes and their contribution to thermal transport across the GaN/ZnO interface, *Phys. Rev. B* **112**, 155302 (2025).
- [57] T. Feng, Y. Zhong, J. Shi, and X. Ruan, Unexpected high inelastic phonon transport across solid-solid interface: Modal nonequilibrium molecular dynamics simulations and Landauer analysis, *Phys. Rev. B* **99**, 045301 (2019).
- [58] S. Shan, Z. Zhang, S. Volz, and J. Chen, Phonon mode at interface and its impact on interfacial thermal transport, *J. Phys.: Condens. Matter* **36**, 423001 (2024).
- [59] L. Yang, B. Latour, and A. J. Minnich, Phonon transmission at crystalline-amorphous interfaces studied using mode-resolved atomistic Green's functions, *Phys. Rev. B* **97**, 205306 (2018).
- [60] K. Gordiz and A. Henry, Phonon transport at crystalline Si/Ge interfaces: The role of interfacial modes of vibration, *Sci. Rep.* **6**, 23139 (2016).
- [61] F. Liu, R. Mao, Z. Liu, J. Du, and P. Gao, Probing phonon transport dynamics across an interface by electron microscopy, *Nature (London)* **642**, 941 (2025).
- [62] Y. Xu, B.-Y. Cao, and Y. Zhou, Near-interface effects on interfacial phonon transport: Competition between phonon-phonon interference and phonon-phonon scattering, *Int. J. Heat Mass Transf.* **232**, 125943 (2024).
- [63] Y. Kurman *et al.*, Spatiotemporal imaging of 2D polariton wave packet dynamics using free electrons, *Science* **372**, 1181 (2021).
- [64] A. L. P. r. Prieto, S. Brouard, and J. G. Muga, Explicit solution for a Gaussian wave packet impinging on a square barrier, *J. Phys. A: Math. Gen.* **36**, 2371 (2003).
- [65] P. Soven, Coherent-potential model of substitutional disordered alloys, *Phys. Rev.* **156**, 809 (1967).
- [66] P. N. Sen and G. Lucovsky, Study of the optic phonons in the III-V quaternary alloy system: $\text{Ga}_{1-x}\text{Al}_x\text{As}_{1-y}\text{P}_y$ by the average t -matrix approximation, *Phys. Rev. B* **12**, 2998 (1975).
- [67] A. Kınacı, J. B. Haskins, C. Sevik, and T. Çağın, Thermal conductivity of BN-C nanostructures, *Phys. Rev. B* **86**, 115410 (2012).
- [68] J. Tersoff, Modeling solid-state chemistry: Interatomic potentials for multicomponent systems, *Phys. Rev. B* **39**, 5566(R) (1989).
- [69] T. Q. P. Vuong, G. Cassaboais, P. Valvin, S. Liu, J. H. Edgar, and B. Gil, Exciton-phonon interaction in the strong-coupling regime in hexagonal boron nitride, *Phys. Rev. B* **95**, 201202(R) (2017).
- [70] Đ. Dangić, L. Monacelli, R. Bianco, F. Mauri, and I. Errea, Large impact of phonon lineshapes on the superconductivity of solid hydrogen, *Commun. Phys.* **7**, 150 (2024).
- [71] T. Ida, M. Ando, and H. Toraya, Extended pseudo-Voigt function for approximating the Voigt profile, *J. Appl. Crystallogr.* **33**, 1311 (2000).
- [72] Y. Zhou and M. Hu, Full quantification of frequency-dependent interfacial thermal conductance contributed by two- and three-phonon scattering processes from nonequilibrium molecular dynamics simulations, *Phys. Rev. B* **95**, 115313 (2017).
- [73] Y. Xu and Y. Zhou, Metric for quantifying elastic and inelastic thermal transport at interfaces, *Phys. Rev. B* **110**, 115305 (2024).
- [74] Y. Xu, L. Yang, and Y. Zhou, The interfacial thermal conductance spectrum in nonequilibrium molecular dynamics simulations considering anharmonicity, asymmetry and quantum effects, *Phys. Chem. Chem. Phys.* **24**, 24503 (2022).
- [75] Y. Zhou, X. Zhang, and M. Hu, Nonmonotonic diameter dependence of thermal conductivity of extremely thin Si nanowires: Competition between hydrodynamic phonon flow and boundary scattering, *Nano Lett.* **17**, 1269 (2017).