In order to address these challenges, we develop in this paper a theory of boundary roughness scattering, based on the recently formulated atomistic S-matrix method \cite{22}, to determine the mode-resolved phonon coherence and specularity parameters for boundary models. Unlike existing approaches \cite{23,24}, our method is fully atomistic, not restricted to long-wavelength modes, and distinguishes coherent and incoherent scattering \cite{24,27} by treating boundary roughness in a statistical manner analogous to the theory of multiple scattering in disordered systems \cite{23,25,28} and conceptually similar to the approach in Ref. \cite{31}. We apply this theory to phonon scattering at the grain boundary (GB) between armchair- and zigzag-terminated graphene like in Fig. \ref{fig:fig1}(c), using realistic nonsymmetric low-energy GB models derived from \textit{ab initio} based structure predictions \cite{32}. We validate our method by comparing its predictions with the less precise Zhao-Frend method \cite{33} and analyze how the coherence and specularity parameters vary with phonon frequency, momentum and polarization/branch for the
I. THEORY AND MODEL

A. Grain boundary model and S matrix

To treat phonon scattering by the rough (32,32)|(56,0) graphene GB statistically, we need to generate the various possible GB configurations and their interatomic force constant (IFC) matrices. Each (32,32)|(56,0) graphene GB configuration, which consists of an undulating line of pentagon-heptagon defect pairs like in Fig. 1(c), is constructed from an 8-unit random sequence of the two lowest-energy (4,4)|(7,0) graphene GB configurations (GB-II and GB-III in Fig. 1(a)) in Ref. [32], with open-system and periodic boundary conditions in the $x$ and $y$ directions, respectively, to yield $2^8 = 256$ unique GB configurations. Given the large size of the GB models, we use the program GULP [34] and the empirical Tersoff potential [35], with parameters from Ref. [36], to model the C-C interatomic forces instead of more expensive ab initio methods and to compute the IFC matrices needed for the atomistic $S$-matrix calculations as described in Ref. [22, 37], with details of the GB structure generation and optimization given in Sec. S1 of the Supplemental Material [38]. The scheme of our calculations is shown in Fig. 2(b).

Using our code which implements the atomistic $S$-matrix method [22], we compute at each frequency $\omega = n\omega_0$, where $n = 1, \ldots, 25$ and $\omega_0 = 10^{13}$ rad/s, the unitary $N(\omega) \times N(\omega)$ matrix $S(\omega)$ which describes the mapping of the $N(\omega)$ incoming bulk phonon modes to the $N(\omega)$ outgoing bulk phonon modes on both sides of the boundary, for each GB configuration. Details of the $S$-matrix calculations are given in Sec. S2 of the Supplemental Material [38]. In the general scattering picture [22, 37], $S(\omega)$, which relates the incoming phonon state $\Phi_{in}$ to the outgoing phonon state $\Psi_{out}$ via the relation $\Psi_{out} = S(\omega)\Phi_{in}$, encodes the amplitude and phase changes. Numerically, $\Phi_{in}$ and $\Psi_{out}$, which represent a superposition of $N(\omega)$ bulk phonon modes, are column vectors with the $m$-th element of $\Phi_{in}$ ($\Psi_{out}$) equal to the complex flux amplitude of the $m$-th incoming (outgoing) phonon channel and represented by $[\Phi_{in}]_{m} = \Phi(k_{m})$ and $[\Psi_{out}]_{m} = \Psi(k_{m})$ for $m = 1, \ldots, N(\omega)$ with the momentum $k_{m}$ and branch $\nu_{m}$ associated with the $m$-th phonon channel. We can thus interpret $|\Phi(k')|^2$ and $|\Psi(k')|^2$ as the intensity of the incoming $k'$ and the outgoing $k$ phonon flux, respectively. Hence, the matrix element $[S(\omega)]_{mn} = S(k_{m}, k'_{n})$ is equal to the scattering amplitude from the $n$-th incoming to the $m$-th outgoing phonon channel, i.e.,

$$
\begin{pmatrix}
\Psi(k_{1}) \\
\vdots \\
\Psi(k_{N})
\end{pmatrix} =
\begin{pmatrix}
S(k_{1}, k'_{1}) & \ldots & S(k_{1}, k'_{N}) \\
\vdots & \ddots & \vdots \\
S(k_{N}, k'_{1}) & \ldots & S(k_{N}, k'_{N})
\end{pmatrix}
\begin{pmatrix}
\Phi(k'_{1}) \\
\vdots \\
\Phi(k'_{N})
\end{pmatrix}
$$

(1)

where $\{k_{1}, \ldots, k_{N(\omega)}\}$ and $\{k'_{1}, \ldots, k'_{N(\omega)}\}$ denote the momenta of the outgoing and incoming modes, respectively.

The evaluation of Eq. (1) requires a configurational ensemble of $S$ matrices computed using the method described in Ref. [22], with each matrix describing a boundary configuration. For simplicity, we choose the (32,32)|(56,0) graphene GB as our boundary model which...
we construct from the two lowest-energy \((4,4)|(7,0)\) GB configurations \((\text{GB-II and GB-III in Fig. 2a})\) in Ref. \[32\] found using the \textit{ab initio} random structure searching method \[30\]. Each \((32,32)|(56,0)\) GB configuration comprises eight \((4,4)|(7,0)\) GB’s, a permutation of GB-II’s and GB-III’s, forming a continuous line of pentagon-heptagon defect pairs. This construction method yields \(2^8 = 256\) unique GB configurations. We set the direction of the phonon flux and the GB to be parallel to the \(x\)- and \(y\)-axis, respectively and impose periodic boundary conditions in the \(y\)-direction. Given the large size of the GB models, we use the empirical Tersoff potential \[35\], with parameters from Ref. \[36\], to model the C-C interatomic forces instead of more expensive \textit{ab initio} methods.

The program GULP \[33\] is used to optimize each GB configuration and to generate its force-constant matrices \(H_{\text{CL}}, H_c\) and \(H_{\text{CR}}\) needed for the \(S\)-matrix calculations. We also compute the force-constant matrices \(H_{\text{CL}}^{(0)}\) and \(H_{R}^{(0)}\) describing the armchair-edge (zigzag-edge) graphene in the left (right) lead. At each frequency \(\omega = n\omega_0\) \((n = 1, \ldots, 25)\) and \(\omega_0 = 10^{13}\) rad/s, we compute an \(N(\omega) \times N(\omega)\) matrix \(S_{\alpha}(\omega)\) for the \(\alpha\)-th GB configuration \((\alpha = 1, \ldots, 256)\).

### B. \(S\)-matrix theory of boundary roughness scattering

For a nonideal boundary that consists of a deterministic part corresponding to the smooth boundary and a stochastic part describing the boundary roughness, \(\Psi_{\text{out}}\) can be partitioned into its deterministic and stochastic components in a manner akin to the treatment of randomly scattered wave fields \[24\] [27], i.e.,

\[
[\Psi_{\text{out}}]_m = \langle [\Psi_{\text{out}}]_m \rangle + \delta [\Psi_{\text{out}}]_m \tag{2}\]

where \(\langle [\Psi_{\text{out}}]_m \rangle\) and \(\delta [\Psi_{\text{out}}]_m\) are its deterministic and stochastic components, respectively, and \(\langle \ldots \rangle\) represents the configurational average \[19\] assuming that every configuration is equally probable. Similarly, the deterministic and stochastic components of \(S(\omega)\) are defined via the expression \(S_m(\omega) = \langle S_m(\omega) \rangle + \delta S_m(\omega)\) where \(\langle S_m(\omega) \rangle = \sum_{n=1}^{N} \langle S_m(\omega) \rangle \langle \Phi_{\text{in}} \rangle_n\) and \(\delta S_m(\omega) = \sum_{n=1}^{N} \delta S_m(\omega) \langle \Phi_{\text{in}} \rangle_n\). For any given \(\langle \Phi_{\text{in}} \rangle_n\), the deterministic component \(\langle [\Psi_{\text{out}}]_m \rangle\) and hence \(\langle S_m(\omega) \rangle\) preserve the coherent amplitude and phase information from direct averaging.

It follows from Eq. \[2\] that \(\langle [\delta \Psi_{\text{out}}]_m \rangle = 0\), i.e., the amplitude fluctuations of the outgoing phonon state average to zero, and thus \(\langle [\delta S_m(\omega) \rangle_n = 0\). However, the configurational average of \(\langle [\Psi_{\text{out}}]_m^n \rangle\), the probability of the phonon being scattered to the \(m\)-th outgoing phonon channel, is \(\langle [\Psi_{\text{out}}]_m^n \rangle^2 \geq \langle [\Psi_{\text{out}}]_m^n \rangle^2 + \langle [\delta \Psi_{\text{out}}]_m^n \rangle^2\), implying that the transition probability fluctuations associated with boundary roughness are not necessarily zero since \(\langle [\Psi_{\text{out}}]_m^n \rangle^2 \geq \langle [\Psi_{\text{out}}]_m^n \rangle^2\). Hence, the configurational average of the transition probability is given by \(\langle [S_m(\omega)]_m^n \rangle = \langle [S_m(\omega)]_m^n \rangle^2 + \langle [\delta S_m(\omega)]_m^n \rangle^2\), which we rewrite as \(W_{\text{total}}(\omega)_{mn} = W_{\text{coh}}(\omega)_{mn} + W_{\text{incoh}}(\omega)_{mn}\) where \(W_{\text{total}}\), \(W_{\text{coh}}\) and \(W_{\text{incoh}}\) are the total, coherent and incoherent transition probability matrices, respectively, with their matrix elements given by \(W_{\text{total}}(\omega)_{mn} = \langle [S_m(\omega)]_m^n \rangle \tag{3a}\)

\(W_{\text{coh}}(\omega)_{mn} = \langle [S_m(\omega)]_m^n \rangle^2 \tag{3b}\)

\(W_{\text{incoh}}(\omega)_{mn} = \langle [S_m(\omega)]_m^n \rangle^2 - \| [S_m(\omega)]_m^n \|^2 \tag{3c}\)

\(W_{\text{total}}(\omega)_{mn}\) represents the total transition probability between the \(n\)-th incoming and the \(m\)-th outgoing channel while \(W_{\text{coh}}(\omega)_{mn}\) and \(W_{\text{incoh}}(\omega)_{mn}\) correspond to its coherent and incoherent components.

### C. Definition of mode-resolved phonon coherence and specularity

To characterize the coherence and specularity of the \(n\)-th incoming phonon channel, we use the transition probabilities from Eq. \[3\] to define the phonon coherence \(C_n(\omega)\),

\[
C_n(\omega) = \sum_{m=1}^{N(\omega)} W_{\text{coh}}(\omega)_{mn} , \tag{4}\]

the sum of the coherent transition probabilities, as its probability of being coherently scattered. Equation \[4\] satisfies \(0 < C_n \leq 1\) and can be interpreted as the proportion of the incoming phonon flux redistributed to the outgoing phonon channels after coherent scattering. We recall that the specularity parameter is the probability that the incident phonon is scattered into the outgoing phonon channels associated with specular scattering by an ideal boundary. Given that the structural randomness of the rough boundary results in both coherent and incoherent scattering, we can characterize the specularity of each type of scattering independently. To estimate the specularity parameter associated with each type of out-scattering from the \(n\)-th incoming phonon channel at frequency \(\omega\), we propose a statistical characterization of the ‘spread’ in the transition probabilities, given by

\[
P^\text{total}_n(\omega) = \sqrt{\frac{\sum_{m=1}^{N(\omega)} |W_{\text{total}}(\omega)_{mn}|^2}{\sum_{m=1}^{N(\omega)} |W_{\text{total}}(\omega)_{mn}|^2}} \tag{5a}\]

\[
P^\text{coh}_n(\omega) = \sqrt{\frac{\sum_{m=1}^{N(\omega)} |W_{\text{coh}}(\omega)_{mn}|^2}{\sum_{m=1}^{N(\omega)} |W_{\text{coh}}(\omega)_{mn}|^2}} \tag{5b}\]

\[
P^\text{incoh}_n(\omega) = \sqrt{\frac{\sum_{m=1}^{N(\omega)} |W_{\text{incoh}}(\omega)_{mn}|^2}{\sum_{m=1}^{N(\omega)} |W_{\text{incoh}}(\omega)_{mn}|^2}} \tag{5c}\]
where \( P^\text{coh}_n, P^\text{incoh}_n \) and \( P^\text{total}_n \) represent the coherent, incoherent and total specularity, respectively. Equation (5) corresponds to the normalized second moment of the transition probabilities, satisfying \( 0 < P^\text{total}_n, P^\text{coh}_n, P^\text{incoh}_n \leq 1 \), and is related to the inverse participation ratio used to characterize disordered eigenstates in Anderson localization theory [41]. The numerator in Eq. (6) counts the effective number of outgoing channels over which the scattered energy is distributed and measures how evenly it is spread across the outgoing (transmitted and reflected) channels in different branches. The specularity parameters are related to the coherence from Eq. (4) through the compact expression

\[
(P^\text{total}_n)^2 = C_n^2 (P^\text{coh}_n)^2 + (1 - C_n)^2 (P^\text{incoh}_n)^2. \tag{6}
\]

We motivate Eq. (5) from the advantages and consistency of its asymptotic \((N \to \infty)\) behavior with expected \( P \) values under well-localized conditions [31]. In the Casimir \((P = 0)\) limit where the incoming phonon energy is diffused uniformly over all \( N \) outgoing phonon channels, we have \( P^\text{total}_n = N^{-1/2} \) so that \( \lim_{N \to \infty} P^\text{total}_n = 0 \). For perfectly specular reflection \((P = 1)\), there is only one outgoing phonon channel with a transition probability of unity (i.e. \( |W_{\text{total}}(\omega)|_{mn} = 1 \) for some \( m \)) and \( P^\text{total}_n = 1 \) as expected. For partially specular scattering \((P = p)\) where there is one dominant outgoing phonon channel with transition probability \( p \) and the transition probability to each remaining channel is \( \frac{1-p}{N-1} \), we obtain \( \lim_{N \to \infty} P^\text{total}_n = p \).

II. RESULTS AND DISCUSSION

A. Comparison with Zhao-Freund specularity parameter

In addition to its consistency under well-defined conditions, we also validate Eq. (5) by comparing its predictions to the lattice dynamics-based approach from Ref. [33] in which Zhao and Freund define a frequency-dependent specularity parameter \( p(\omega) \), which lacks modal resolution and we may consider as the specularity parameter averaged over all the modes in all phonon branches at the frequency \( \omega \), based on the relative value of the actual phonon transmission to the transmission functions predicted from the acoustic mismatch model (AMM) and diffuse mismatch model (DMM). As we can resolve the phonon branch, we generalize the Zhao-Freund estimate to define the more precise frequency- and branch-dependent specularity parameter [33] for the left-lead \( \alpha \)-branch phonons as

\[
p_{\alpha,L}(\omega) = \frac{\Xi_{\alpha,L}(\omega) - \Xi^{(\text{DMM})}_{\alpha,L}(\omega)}{\Xi^{(\text{AMM})}_{\alpha,L}(\omega) - \Xi^{(\text{DMM})}_{\alpha,L}(\omega)} \tag{7}
\]

where \( \alpha = \text{LA} \) (longitudinal acoustic), TA (transverse acoustic), ZA (flexural acoustic), LO (longitudinal optical), TO (transverse optical) or ZO (flexural optical), and \( \Xi_{\alpha,L}, \Xi^{(\text{AMM})}_{\alpha,L} \) and \( \Xi^{(\text{DMM})}_{\alpha,L} \) are the transmission functions calculated with the atomistic S-matrix, AMM and DMM method, respectively, as described in Sec. S3 of the Supplemental Material [33]. We also define the analogous branch-averaged, frequency-dependent total specularity parameter

\[
\mathcal{P}_{\alpha,L}(\omega) = \frac{\sum_{n=1}^{N} P^\text{total}_n(\omega) \Theta(v'_{x,n}) \delta v'_{x,n,\alpha}}{\sum_{n=1}^{N} \Theta(v'_{x,n}) \delta v'_{x,n,\alpha}}, \tag{8}
\]

by averaging \( P^\text{total}_n \) from Eq. (5) over all the incoming left-lead \( \alpha \)-branch phonon channels. The comparison between Eqs. (7) and (8) is made over the frequency range in which we have long-wavelength phonons with momentum \( k \) satisfying \( |k| < k_{\text{cutoff}} \) where the cutoff momentum \( k_{\text{cutoff}} \) is set as half of the distance between the \( \Gamma \) and \( K \)-point in the first Brillouin zone (BZ).

We observe excellent agreement between \( \mathcal{P}_{\text{TAL}} \) and \( P_{\text{LA,L}} \) over the entire frequency range in Fig. 6. The agreement between \( \mathcal{P}_{\text{TAL}} \) and \( P_{\text{TA,L}} \) is also remarkably good although the two quantities diverge at higher frequencies, possibly because of the deviation of the TA phonon frequencies from the linear dispersion implicitly assumed in \( \Xi^{(\text{AMM})}_{\alpha,L} \) in Eq. (7) for estimating \( P_{\alpha,L} \). The sensitivity of the agreement between Eqs. (7) and (8) to the phonon dispersion linearity is also reflected in the poor agreement between \( \mathcal{P}_{\text{ZAL}} \) and \( P_{\text{ZA,L}} \) for ZA phonons, which have a quadratic phonon dispersion in
the long-wavelength limit in graphene,

although the general trend of the ZA phonon specularity increasing with frequency is captured. The close agreement between Eqs. (6) and (8) for long-wavelength LA and TA phonons supports our approach for estimating the specularity parameters in Eq. (9).

B. Specularity and coherence of graphene phonons

In Fig. 4 we analyze the reciprocal-space distribution of the phonon coherence ($C_n$) and the total, coherent and incoherent specularity parameters ($P_n^{\text{total}}$, $P_n^{\text{coh}}$ and $P_n^{\text{incoh}}$) for the ZA, TA and LA phonon modes over the entire first BZ in armchair-edge graphene, computed from Eqs. (5) and (11) over the frequency range of $\omega = \omega_0$ to $25\omega_0$ rad/s in intervals of $\omega_0 = 10^{13}$ rad/s, using the method described in Ref. [22]. The mode-resolved data over the entire BZ is obtained by plotting the mode-resolved data at each frequency and then sweeping over the aforementioned frequency range. The corresponding results for zigzag-edge graphene are omitted here but given in Sec. S4 of the Supplemental Material [38]. The convergence of $C_n$ and $P_n^{\text{total}}$ with respect to GB width is also discussed in Sec. S5 of the Supplemental Material [38].

In Fig. 4(d), we observe that $C_n$ for ZA phonons increases as $k_n$ decreases, suggesting that long-wavelength ZA phonons are more sensitive to GB roughness, against conventional expectations that boundary roughness scatters short-wavelength phonons more strongly [3]. In contrast, Figs. 4(c) and (f) show that $C_n$ for LA and TA phonons decreases as $k_n$ increases, indicating that long-wavelength LA and TA phonons are less incoherently scattered. The trend in Fig. 4(d) is consistent with the $P_n^{\text{total}}$ distribution in Figs. 4(g) to (i), which show $P_n^{\text{total}}$ decreasing for LA and TA phonons but increasing for ZA phonons as $k_n$ increases. We speculate that this is related to the significantly higher point-defect scattering rates of ZA phonons in graphene [13]. The greater GB scattering of ZA phonons implies that in suspended polycrystalline graphene, the in-plane LA and TA phonons play a more significant role in heat conduction than the out-of-plane ZA phonons which are said to dominate thermal transport in pristine graphene [12]. It has also been proposed by Soffer [14, 15] that the specularity parameter should vary anisotropically as $P = \exp[-(2\eta k_n)^2]$, where $\eta$ is the root-mean-square surface roughness, and has no $k_n$-dependence. However, we do not observe such anisotropy for $P_n^{\text{total}}$ in Figs. 4(g) to (i), indicating a disagreement with Soffer’s formula. Furthermore, in the long-wavelength limit, the $P_n^{\text{total}}$ for ZA phonons does not converge to unity as suggested by the formula.

C. Coherent vs. incoherent specularity parameters

It is widely assumed [19, 22, 24] that coherent (incoherent) scattering is perfectly specular (diffuse), i.e., $P_n^{\text{coh}} = 1$ ($P_n^{\text{incoh}} = 0$), although there is no direct evidence for this relationship. Underlying this assumption is the idea that the perfect interface is smooth although at the atomistic level, lattice imperfections must occur because of the crystallographic discontinuity. Given this assumption, it follows from Eq. (6) that coherence is equivalent to specularity ($C_n = P_n^{\text{total}}$). We exploit our ability to distinguish coherent from incoherent scattering to analyze how specularity actually depends on coherence, by comparing the $P_n^{\text{coh}}$ and $P_n^{\text{incoh}}$ distributions generally have similar $k_n$-dependence, with $P_n^{\text{coh}} < P_n^{\text{total}}$ because incoherent scattering is strongly diffuse ($P_n^{\text{incoh}} \ll 1$) with no significant $k_n$-dependence for ZA, TA and LA phonons, as can be seen in Figs. 4(m) to (o), and Eq. (6) implies that $P_n^{\text{total}} = \max\{P_n^{\text{coh}}, P_n^{\text{incoh}}\}$. The near uniform small value of $P_n^{\text{incoh}}$ over the entire BZ in Figs. 4(m) to (o) also suggests that the diffuse character of incoherent scattering is captured by Eq. (6).

Like in Fig. 4(g), the $P_n^{\text{coh}}$ distribution for ZA phonons in Fig. 4(j) is significantly smaller than unity, indicating that even coherent scattering is not fully specular for out-of-plane polarized phonons. The $P_n^{\text{coh}}$ distribution for LA and TA phonons in Fig. 4(k) and (l) show that the coherent specularity diverges from unity as we move away from the BZ center. To explain the reduced ZA phonon specularity ($P_n^{\text{total}}$), we compare the main scattering transitions for an incoming armchair-edge graphene (a) ZA and (b) TA phonon at normal incidence ($k_y = 0$) to the boundary at a single frequency of $\omega = 5\omega_0$ rad/s in Fig. 5. The incoming ZA phonon is forward-scattered to several outgoing channels while the incoming TA phonon is forward-scattered to a single outgoing channel on the zigzag-edge side. The distinctive periodic arrangement in the distribution of the main outgoing ZA phonon channels, separated by an interval of $\Delta k_y$, is due to diffraction by the smooth part of the boundary which has a periodicity equal to $W_{\text{GB}}$ the width of the constituent (4,4)/(7,0) GB such that $\Delta k_y = 2\pi/W_{\text{GB}}$. For a clear representation of diffraction by the ‘smooth’ boundary with the aforementioned transverse periodicity, we plot the equivalent scattering transitions for the pure GB-II and GB-III boundaries in Sec. S6 of the Supplemental Material [38]. A similar effect has also been reported for molecular dynamics simulations of symmetric graphene GB’s [47]. This diffractive scattering is seen for other ZA phonon channels but none of the in-plane LA and TA phonons.
We have formulated an $S$ matrix-based theory of boundary roughness scattering to predict the mode-resolved coherence and specularity parameters and applied it to the (32,32)/(56,0) graphene GB. The predicted specularity parameters are shown to be consistent with those of Zhao and Freund [23]. We find that phonon scattering is predominantly coherent for graphene GB’s although contrary to expectations, coherence and specularity are lowest for long-wavelength ZA phonons because of diffractive scattering by the GB, while the opposite trend is seen for LA and TA phonons. Our results also demonstrate that incoherent scattering is much more diffuse than coherent scattering and that coherence and specularity are not necessarily equivalent. Given its generality, our method can be applied in a straightforward manner to analyze phonon coherence and specularity in other atomistic boundary models.

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Figure 4. (a-c) Phonon dispersion, (d-f) coherence ($C_n$) and the estimated (g-i) total, (j-l) coherent and (m-o) incoherent mode-resolved specularity parameters ($P_n^{\text{total}}$, $P_n^{\text{coh}}$, and $P_n^{\text{inccoh}}$) for the ZA, TA and LA phonons in armchair-edge graphene impinging on the grain boundary. The modes in the incoming phonon flux are filled circles colored according to their numerical value while the modes in the outgoing flux are hollow squares. The frequency range is $\omega = \omega_0$ to $5\omega_0$ where $\omega_0 = 10^3$ rad/s, with the maximum frequency ($\omega_{\text{max}}$) for the ZA, TA and LA phonons equal $12\omega_0$, $21\omega_0$ and $25\omega_0$, respectively. The iso-frequency contours are indicated in intervals of $\Delta\omega = \omega_0$ in (d-o) using solid gray lines. The phonon dispersions in (a-c) are indicated with color contours in intervals of $\Delta\omega = \omega_0/2$.

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III. SUMMARY

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Figure 5. Main scattering transitions for an incoming (a) ZA and (b) TA phonon, labeled $\Psi_{in}$, at normal incidence to the grain boundary from the armchair-edge graphene on the left at $\omega = 5 \times 10^{13}$ rad/s. The bulk LA, TA and ZA phonon channels on the armchair-edge (left subpanel) and zigzag-edge (right subpanel) graphene side are displayed within their respective first Brillouin zones. The color scales indicate the transition probability from $W_{\text{total}}(\omega)$ for the dominant outgoing channels, with the transitions indicated by dotted lines and transition probabilities written in Italic font.

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