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Calculation of the lattice thermal conductivity in granular crystals

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This paper provides a general model for the lattice thermal conductivity in granular crystals. The key development presented in this model is that the contribution of surface phonons to the thermal conductivity and the interplay between phonon anharmonic scattering and phonon scattering by boundaries are considered explicitly. Exact Boltzmann equation including spatial dependence of phonon distribution function is solved to yield expressions for the rates at which phonons scatter by the grain boundaries in the presence of intrinsic phonon scattering mechanisms. The intrinsic phonon scattering rates are calculated from Fermi's golden rule, and the vibration parameters of the model are derived as functions of temperature and crystallographic directions by using a lattice dynamics approach. The accuracy of the model is demonstrated with reference to experimental measurements regarding the effects of surface orientation and isotope composition on the thermal conductivity in single crystals, and the effect of grains size and shape on the thermal conductivity tensor in granular crystals. © *2014 AIP Publishing LLC*. [http://dx.doi.org/10.1063/1.4866362]

I. INTRODUCTION

The demand for increasing circuit density and power on chips makes heat dissipation a critical issue in circuit design. Heat dissipation through the substrate is a simple, yet convenient means of lowering circuit temperature (T). As a result, materials with high thermal conductivity (κ) are highly desirable for substrate applications. On the other hand, materials with low κ are extremely needed for power-generation through thermoelectric conversion.[1,2]

A granular crystal typically exhibits lower κ than the single crystal of the same material because of a high phonon scattering rate at grain boundaries. However, besides the phonon-boundary scattering mechanisms, the grains shape, size, and orientation are also important determinants of κ in a granular crystal over a wide T range.[3–9] A theory describing the dependence of κ on the characteristics of the constituent grains would therefore be of utmost importance for the control of heat transport and the design of materials for heat sink or thermoelectric applications. The usual approach to evaluate κ in granular crystals is based either on introducing in the expression of κ for an infinite crystal temperature-independent relaxation times associated with phonon scattering by grain boundaries, or averaging κ of a single crystal over the anisotropy directions. The results in this way agree with experimental data only when the boundaries are completely diffusive, or present no thermal resistance.[10]

Recently, attempts have been made to calculate κ in a granular crystal with considering the contribution of the interaction between microstructural components of the system.[11–15] Although the proposed approaches presented developments in the theory of phonon transport in systems where the phonon scattering rate is enhanced by the presence of boundaries, they are framed by expressions and assumptions valid for the specific class of granular crystals that are made up of randomly orientated grains giving rise to an isotropic κ.[16–20] The primary objective of this paper is to account for the contribution of phonons propagating on grains surfaces and the scattering of phonons by grains boundaries in the presence of temperature-dependent anharmonic phonon scattering rates to the lattice thermal conductivity of granular materials. A Boltzmann equation for phonons including terms describing the spatial dependence of the phonon distribution is solved to derive phonon-boundary scattering rates expressed in terms of the intrinsic phonon relaxation times and the strength of the interaction between surface phonons and volume phonons. Unlike the widely used Casimir's expression that describes low-temperature interactions between ballistic phonons and boundaries, the developed expressions for phonon-boundary scattering rates describe the interplay between intrinsic phonon scattering and phonon-boundary scattering in the full temperature range. Besides, they provide theoretical understanding of the widely used phonon specularity factor. They define the phonon specularity as the ratio of the strength of the interaction between surface phonons and volume phonons to the product of the phonon intrinsic relaxation time and the rate at which phonons are delivered to a unit volume of the reciprocal space. The derived formalism for the lattice thermal conductivity includes vibration parameters and relaxation times that describe anisotropic κ resulting from the grains shape and orientation. The paper is organized as follows. In Sec. II, we discuss the symmetry of κ and derive directional- and temperature-dependent κ in an infinite crystal using a lattice dynamical matrix and Fermi's golden rule for phonon-phonon interactions. In Sec. III, we describe the interplay between the intrinsic scattering of phonons and the scattering of phonons by the boundaries of a finite crystal. We present a solution for Boltzmann equation including a spatial dependence of the phonon distribution function arising from

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the presence of boundaries and derive expressions for the rates at which phonons scatter by the boundaries of a finite crystal in the presence of surface phonons and intrinsic phonon-phonon scattering mechanisms. In Sec. IV, we extend the expression of κ developed for a finite crystal to the case of a granular material by including probabilities for a phonon to transmit from grain to grain through the grain boundaries. We address the effect of grains shape and orientation tendency that may result in anisotropic κ. Finally, in Sec. V, we compare the results of the developed model to experimental data available in the literature.

II. LATTICE THERMAL CONDUCTIVITY IN AN INFINITE CRYSTAL

A. General theory

Let us begin with the investigation of the contribution of each high symmetry direction to the overall lattice thermal conductivity of the crystal. The phonon heat current $\mathbf{q}$ along any direction in any crystal can be considered as the sum of individual vector components $\mathbf{q}_{hkl}$ directed along the high-symmetry directions $[h,k,l]$ of the crystal. Thus, we may write

$$\mathbf{q} = \sum_{[hkl]} \mathbf{q}_{hkl}, \tag{1}$$

where the summation runs over all the high-symmetry directions of the crystal. On the other hand, the individual component $\mathbf{q}_{hkl}$ of the total heat current $\mathbf{q}$ is defined as the sum over all states k_{hkl} of the number of phonons with given frequency that are incident per unit time parallel to the high symmetry direction $[h,k,l]$, times the phonon energy $\hbar\omega(k_{hkl})$. This can be expressed as

$$\mathbf{q}_{hkl} = \sum_{k_{hkl}} \hbar\omega(k_{hkl}) N(k_{hkl}).\mathbf{v}_{hkl}. \tag{2}$$

Here, $\mathbf{v}_{hkl}$ is the phonon velocity in the high symmetry direction $[h,k,l]$, and $N(k_{hkl})$ is the phonon distribution in the state k_{hkl}, defined as the sum of the phonon distribution at equilibrium $\bar{N}(k_{hkl})$ and the deviation of the phonon distribution from equilibrium $\tilde{N}(k_{hkl})$ in the state k_{hkl}. Typically, in an infinite crystal, the change in the phonon distribution is due to the combined effects of temperature gradient together with phonon collisions with each other and defects. In the steady state regime, the total rate of change in the phonon distribution must vanish. Thus, Boltzmann equation, which describes this total rate of change in the phonon distribution, takes the form

$$-\mathbf{v}_{hkl}.\nabla N(k_{hkl}) + \frac{\partial N(k_{hkl})}{\partial t} = 0. \tag{3}$$

The usual way to solve Eq. (3) is to approximate its second term by $\frac{\partial N(k_{hkl})}{\partial t} = \frac{\bar{N}(k_{hkl}) - N(k_{hkl})}{\tau(k_{hkl})}$. With this approximation, it is assumed that in the absence of a temperature gradient, any deviation from equilibrium in the state k_{hkl} damps out rapidly in a time $\tau(k_{hkl})$. This approximation is valid in some circumstances, but it generally ignores the difference between the physical nature of the normal processes, which tend to displace the phonon distribution by a small vector $\mathbf{u}$ in the direction of the heat current, and the nature of the resistive processes, which tend to restore it back to its equilibrium value. Although the normal processes do not contribute to the thermal resistance, they must be taken into account when solving Boltzmann equation, because they cause the deviation of the phonon distribution function in a direction opposite to the resistance direction. The disregard of this effect often leads to inaccurate estimation of the magnitude of κ.[21] Therefore, a more accurate approximation to the second term in Eq. (3) would be given by

$$\frac{\partial N(k_{hkl})}{\partial t} = \frac{N_{\mathbf{u}}(k_{hkl}) - N(k_{hkl})}{\tau_N(k_{hkl})} + \frac{\bar{N}(k_{hkl}) - N(k_{hkl})}{\tau_R(k_{hkl})}, \tag{4}$$

where $N_{\mathbf{u}}(k_{hkl})$ is the displaced phonon distribution, which is stationary in the state k_{hkl} for the normal processes, and $\tau_{N(R)}(k_{hkl})$ the relaxation time associated with normal (resistive) processes.

In the case of an infinite crystal, the spatial dependence of the phonon distribution function can be ignored and Eq. (3) reduces to

$$-v_{z,hkl}\frac{d\bar{N}(k_{hkl})}{dT}\cdot\frac{\partial T}{\partial z} + \frac{\partial N}{\partial t} = 0. \tag{5}$$

In Eq. (5), it is assumed that the temperature gradient is directed along the z direction and is too weak to alter the deviation of the phonon distribution. By using Eq. (4) in Eq. (5) and following Callaway's mathematical arrangements,[22] the individual component of the total phonon heat current takes the form

$$\mathbf{q}_{hkl} = -\sum_{k_{hkl}} \tau(k_{hkl})\mathbf{v}_{hkl}.\nabla T_{hkl} \times \frac{(\hbar\omega(k_{hkl}))}{k_B T^2} \frac{\exp\left(\frac{\hbar\omega(k_{hkl})}{k_B T}\right)}{\left(\exp\left(\frac{\hbar\omega(k_{hkl})}{k_B T} - 1\right)\right)^2}\mathbf{v}_{hkl}, \tag{6}$$

where $\nabla T_{hkl} = \nabla T \cos\psi_{hkl}$ (the component of the temperature gradient aligned parallel to the high symmetry direction $[h,k,l]$), with ψ_{hkl} being the angle between the crystallographic direction along which the temperature gradient is directed and the high-symmetry direction $[h,k,l]$. In Eq. (6), $\tau(k_{hkl})$ is a total relaxation time defined as $\tau(k_{hkl}) = \tau_C(k_{hkl})\left[1 + \frac{\beta_{hkl}}{\tau_N(k_{hkl})}\right]$, with $\tau_C(k_{hkl})$ being a combined relaxation time for the state k_{hkl} defined as $\tau_C(k_{hkl}) = \frac{1}{\tau_N(k_{hkl})} + \frac{1}{\tau_R(k_{hkl})}$ and β_{hkl} a parameter with the dimension of a relaxation time given by

$$\beta_{hkl} = \frac{\int_0^{\theta_{D,hkl}/T} dx \frac{x^4 e^x}{(e^x-1)^2}\frac{\tau_C(k_{hkl})}{\tau_N(k_{hkl})}}{\int_0^{\theta_{D,hkl}/T} dx \frac{x^4 e^x}{(e^x-1)^2}\frac{1}{\tau_N(k_{hkl})}\left(1 - \frac{\tau_C(k_{hkl})}{\tau_N(k_{hkl})}\right)}, \tag{7}$$

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where $x = \frac{\hbar\omega(k_{hkl})}{k_B T}$ is a dimensionless parameter.[22] Thus, the thermal conductivity along the high-symmetry direction $[h,k,l]$ can be written as

$$\kappa_{hkl} = -\frac{\mathbf{q}_{hkl}}{\nabla T} = \sum_{k_{hkl}} \sum_{j} \tau_j(k_{hkl}) \bar{v}^2_{j,hkl} \frac{\left(\hbar\omega_j(k_{hkl})\right)}{k_B T^2} \times \frac{\exp\left(\frac{\hbar\omega_j(k_{hkl})}{k_B T}\right)}{\left(\exp\left(\frac{\hbar\omega_j(k_{hkl})}{k_B T} - 1\right)\right)^2} \cos\psi_{hkl}, \quad (8)$$

where the subscript j denotes the phonon polarization and $\bar{v}_{j,hkl}$ is a temperature-dependent phonon group velocity averaged over all k_{hkl} states. By combining this equation with Eq. (1), one can readily find that the thermal conductivity in an infinite crystal along a well-defined crystallographic direction takes the form

$$\kappa = \sum_{[hkl]} \sum_{k_{hkl}} \sum_{j} \tau_j(k_{hkl}) \bar{v}^2_{j,hkl} \frac{\left(\hbar\omega_j(k_{hkl})\right)}{k_B T^2} \times \frac{\exp\left(\frac{\hbar\omega_j(k_{hkl})}{k_B T}\right)}{\left(\exp\left(\frac{\hbar\omega_j(k_{hkl})}{k_B T} - 1\right)\right)^2} \cos\psi_{hkl}, \quad (9a)$$

and the average thermal conductivity of the same crystal is

$$\bar{\kappa} = \frac{1}{m} \sum_{[hkl]} \sum_{k_{hkl}} \sum_{j} \tau_j(k_{hkl}) \bar{v}^2_{j,hkl} \frac{\left(\hbar\omega_j(k_{hkl})\right)}{k_B T^2} \times \frac{\exp\left(\frac{\hbar\omega_j(k_{hkl})}{k_B T}\right)}{\left(\exp\left(\frac{\hbar\omega_j(k_{hkl})}{k_B T} - 1\right)\right)^2}, \quad (9b)$$

where m is the number of high-symmetry directions in the crystal structure under consideration. We note here that the number of high-symmetry directions in a given crystalline structure equals the number of independent elastic constants.[23] The major importance of Eqs. (9a) and (9b) stems in that they can be used to describe κ either for a specific surface orientation or as an average over all crystallographic directions, with taking into account the various intrinsic phonon processes that may influence the heat transport mechanism. We will see in the Secs. III–V that with including appropriate boundary conditions, Eqs. (9a) and (9b) can be tuned to predict the dependence of grain size and shape on κ in a granular crystal of random or preferred grains orientation.

B. Calculation details

For the implementation of Eqs. (9a) and (9b), we derive the phonon eigenfrequencies $\omega_j(k_{hkl})$ from the adiabatic bond charge model.[24] The phonon group velocities in thin films and wires have been intensively investigated by using continuum medium approximations.[25–29] However, since, in this work, we adopt a discrete lattice model, we write the temperature-dependent average group velocity for the j-polarized acoustic phonon in the direction $[h,k,l]$ as given in Ref. 30

$$\bar{v}_{j,hkl} = \frac{\sum_{k_{hkl}} v_{j,k_{hkl}} . \bar{N}_j(k_{hkl})}{\sum_{k_{hkl}} \bar{N}_j(k_{hkl})}. \quad (10)$$

As described in Ref. 22, the introduction of the parameter β facilitates the solution of Boltzmann equation when the effects of the normal processes, which drag the crystal momentum back and forth between the normal modes, are accounted for. Nevertheless, the elegance and physical reasonableness of such a solution is somewhat abused by the use of Debye-like phonon dispersion relations that are reliable at low temperatures only. In order to overcome this issue and widen the temperature range in which the model is applicable, we calculate the Debye temperature, which is involved in the expression of β (see Eq. (7), as a function of temperature. By equating the specific heat C calculated with the exact phonon dispersion relations to the Debye approximation of the specific heat

$$C_{j,hkl} = k_B \sum_{k_{hkl}} \frac{\left(\frac{\hbar\omega_j(k_{hkl})}{2k_B T}\right)^2}{\sinh\left(\frac{\hbar\omega_j(k_{hkl})}{2k_B T}\right)} = 3rN_c k_B \left(\frac{T}{\theta_{D(j,hkl)}}\right)^3 \int_0^{\theta_{D(j,hkl)}/T} \frac{x^4 e^x}{(e^x - 1)^2} dx, \quad (11)$$

and considering the resulting equation as an expression for the Debye temperature, we obtain the theoretical dependence of the Debye temperature on temperature. In Eq. (11), r is the number of atoms per unit cell and N_c the number of unit cells in the crystal. The temperature-dependent Debye temperature of diamond, as calculated from Eq. (11), is shown in Fig. 1 for longitudinal and transverse phonon polarizations in the three high-symmetry directions of the diamond structure.

The relaxation times τ_N and τ_R associated with the normal and resistive processes that are invoked in the model need to be evaluated to describe the exact magnitude of κ over a wide temperature range. In order to determine these relaxation times, we consider that the overall resistive processes are due to phonon scattering by point-defects and three-phonon Umklapp processes. This is commonly described by Matthiessen's rule $\frac{1}{\tau_R} = \frac{1}{\tau_I} + \frac{1}{\tau_U}$. Here τ_I is the relaxation time associated with phonon scattering by point-defects, and τ_U is the relaxation time associated with phonon scattering through Umklapp processes. To calculate τ_I, we use Klemen's theory,[31,32] and to calculate $\tau_N(k_{hkl})$ and $\tau_U(k_{hkl})$, we employ Fermi's golden rule formula, based on the cubic anharmonic part of the crystal Hamiltonian as perturbation.[33] We express the cubic anharmonic part of the Hamiltonian within the anharmonic elastic continuum scheme.[30] Then, with assuming a single mode relaxation time and employing Fermi's golden rule formula, the relaxation rate of the j-polarized phonon in the state k_{hkl} takes the form[30]

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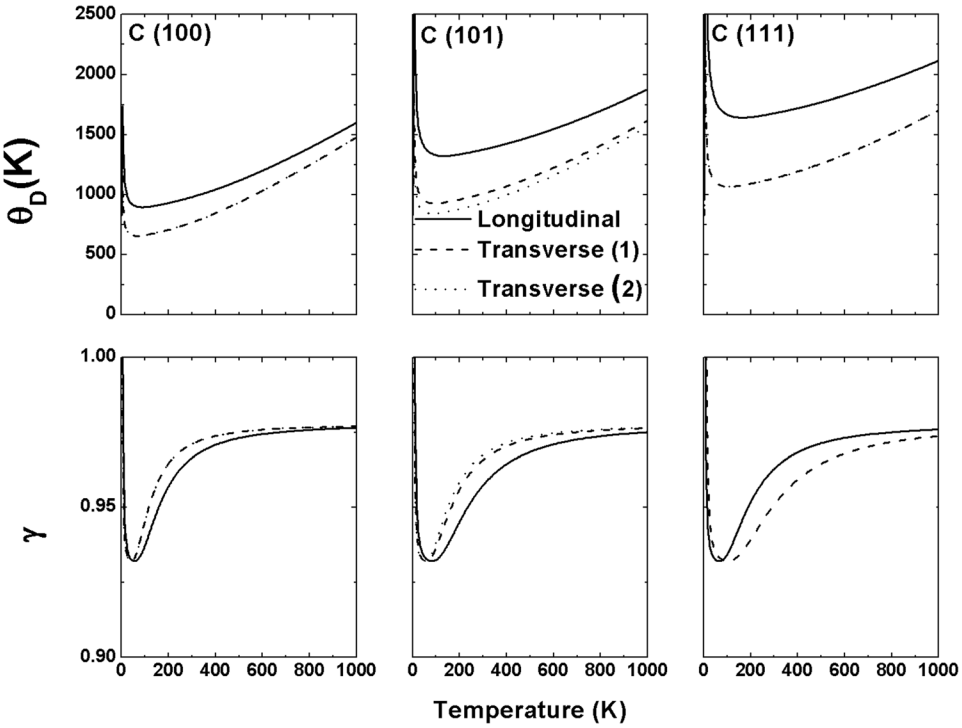

FIG. 1. Longitudinal and transverse Debye temperatures and Grüneisen parameters for different crystallographic directions in diamond structure.

$$\tau^{-1}_{N(U)}(k_{hkl}) = \frac{\pi\hbar\gamma^2_{j,hkl}}{\rho\bar{N}_j(k_{hkl})\Omega\bar{v}^2_{j,hkl}}\omega_j(k_{hkl})\omega_{j'}(\mathbf{k}')\omega_{j''}(\mathbf{k}'')$$

$$\times\sum_{\mathbf{k}'j',\mathbf{k}''j'',\mathbf{G}}\times\left[\begin{array}{l}\dfrac{\bar{N}_{j'}(\mathbf{k}')\left(\bar{N}_{j''}(\mathbf{k}'')+1\right)}{\bar{N}_j(k_{hkl})+1}\delta\left(\omega_j(k_{hkl})+\omega_{j'}(\mathbf{k}')-\omega_{j''}(\mathbf{k}'')\right)\delta_{k_{hkl}\hat{\mathbf{k}}_{hkl}+\mathbf{k}',\mathbf{k}''+\mathbf{G}}\\ \\ +\dfrac{1}{2}\dfrac{\bar{N}_{j'}(\mathbf{k}')\bar{N}_{j''}(\mathbf{k}'')}{\bar{N}_j(k_{hkl})}\delta\left(\omega_j(k_{hkl})-\omega_{j'}(\mathbf{k}')-\omega_{j''}(\mathbf{k}'')\right)\delta_{k_{hkl}\hat{\mathbf{k}}_{hkl}+\mathbf{G},\mathbf{k}'+\mathbf{k}''}\end{array}\right], \quad (12)$$

where ρ is the crystal density, Ω the crystal volume, $\gamma_{j,hkl}$ the temperature-dependent Grüneisen parameter for j-polarized phonon of $[h,k,l]$ symmetry, $\hat{\mathbf{k}}_{hkl}$ a unit wavevector pointing in the high symmetry direction $[h,k,l]$, $\mathbf{G}$ a reciprocal lattice vector, and δ either the Dirac delta function or Kronecker delta symbol. The method for the summation over the phonon wavevectors and reciprocal lattice vectors is detailed in Ref. 30. The derivation of $\gamma_{j,hkl}$ as a function of temperature is carried out by assuming that the contribution from each single mode Grüneisen parameter $\gamma_j(k_{hkl})$ to the overall Grüneisen parameter $\gamma_{j,hkl}$ is set by its contribution to the specific heat $C_{j,hkl}$ as

$$\gamma_{j,hkl} = \frac{\sum\limits_{k_{hkl}}\gamma_j(k_{hkl})\times C_{j,hkl}}{\sum\limits_{k_{hkl}} C_{j,hkl}}, \quad (13)$$

then calculating the single mode Grüneisen parameter $\gamma_j(k_{hkl})$ from its definition $\gamma_j(k_{hkl}) = \frac{-\Omega}{\omega_j(k_{hkl})}\frac{\partial\omega_j(k_{hkl})}{\partial\Omega}$. The temperature-dependent Grüneisen parameter of diamond, as calculated from Eq. (13), is shown in Fig. 1 for longitudinal and transverse phonon polarizations in the three high-symmetry directions of the diamond structure.

III. LATTICE THERMAL CONDUCTIVITY IN A ROD OF RANDOM SHAPE

So far, Boltzmann equation is solved with disregarding the spatial dependence of the phonon distribution function N. Such a treatment, while mathematically convenient, eliminates the possibility of studying the effect of the scattering of the phonons by the boundaries of a real crystal, and the contribution of the crystal surface to κ. In order to draw a theoretical understanding of the effects of the size and surface on κ, let us consider the geometry of a rod of random shape, with a temperature gradient aligned parallel to the rod axis in the z direction. In such a configuration, the thermal gradient pumps phonons in the z direction to every point of the cross section of the rod at a rate independent of location in the cross section. In the volume of the rod, these phonons lose their momenta at a rate described by the resistive relaxation time τ. However, the phonons in the vicinity of the boundary tend to be absorbed, giving rise to a dependence of the phonon heat flux on the distance from the boundary. Hence, the variation of N with respect to position can no longer be ignored in Boltzmann equation. For small deviations from equilibrium, we can assume that the temperature gradient depends on z only. Therefore, the distribution function N

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has an explicit x and y dependence, with an implicit dependence on z through the temperature gradient. The corresponding Boltzmann equation (Eq. (3)) for the state k_{hkl} takes the form

$$v_z \frac{d\bar{N}}{dT}\frac{\partial T}{\partial z} + v_x \frac{\partial \tilde{N}}{\partial x} + v_y \frac{\partial \tilde{N}}{\partial y} + \frac{\tilde{N}}{\tau} = 0. \tag{14}$$

The solution of Eq. (14) is somewhat simplified by noting that in the very vicinity of a crystal boundary parallel to the heat current, phonons are either at thermal equilibrium with the boundary, or out of equilibrium due to interactions with surface phonons propagating on that boundary. At the opposite boundary, all the phonons of wavevector k_{hkl} are absorbed then reemitted back, or reflected with momentum $-k_{hkl}$ and equilibrium distribution $\bar{N}(k_{hkl})$. With these considerations, the solution of Eq. (14) for any cross section dimensions and shape is given by

$$\tilde{N} = \frac{R\tau}{2}\left[\left(1-\exp\left(\frac{-x(y)}{\tau v_x}\right)\right)+\left(1-\exp\left(\frac{-y(x)}{\tau v_y}\right)\right)\right] + \sigma_z \exp\left(\frac{-x(y)}{\tau v_x}\right) + \sigma_z \exp\left(\frac{-y(x)}{\tau v_y}\right), \tag{15}$$

where $R = -v_z \frac{d\bar{N}}{dT}\frac{\partial T}{\partial z}$ is the negative of the rate at which phonons are delivered to a unit volume of the reciprocal space, $x(y)$ is the y-dependent distance from a boundary parallel to the x axis, measured in a direction normal to the rod axis, and $y(x)$ the x-dependent distance from a boundary parallel to the y axis, measured in a direction normal to the rod axis, and σ_z the deviation of the phonon distribution due to interactions with surface phonons propagating in the direction of the phonon heat current. Upon substituting Eq. (15) in Eq. (14) we find

$$R = \left(\frac{1}{\tau_{B,x}} + \frac{1}{\tau_{B,y}} + \frac{1}{\tau}\right)\langle \tilde{N} \rangle, \tag{16}$$

with,

$$\frac{1}{\tau_{B,\alpha}} = \frac{\int\int v_\alpha \frac{\partial \tilde{N}}{\partial \alpha} dxdy}{\int\int \tilde{N} dxdy}, \tag{17}$$

where $\alpha = x$ or y, and

$$\langle \tilde{N} \rangle = \frac{\int\int \tilde{N} dxdy}{\int\int dxdy}. \tag{18}$$

By comparing Eq. (16) with Eq. (5), we find that in order to account for the interplay between the phonon-phonon interaction and phonon-boundary scattering in a finite crystal over a wide temperature range, one has to add to the phonon-phonon scattering rates calculated in Sec. II additional temperature-dependent scattering rates $\frac{1}{\tau_{B,\alpha}}$ associated with phonon-boundary scattering in the x and y directions whose expressions are given by Eqs. (17) and (18).

IV. LATTICE THERMAL CONDUCTIVITY IN A GRANULAR CRYSTAL

A. Lattice thermal conductivity of a single columnar grain

Let us now consider that a phonon heat current is directed along the axis of a columnar single grain of rectangular cross section oriented along the z axis. By using Eqs. (15)–(18), we find that the rates at which phonons scatter by the boundaries of this grain are given by

$$\frac{1}{\tau_{B,x}} = \frac{v_x}{l_x} \cdot \frac{\left(1-2\frac{\sigma_z}{\tau R}\right)\left(1-\exp\left(\frac{-l_x}{\tau v_x}\right)\right)}{2-\left[\sum_\alpha \frac{\tau v_\alpha}{l_\alpha}\left(1-\exp\left(\frac{-l_\alpha}{\tau v_\alpha}\right)\right)\left(1-2\frac{\sigma_z}{\tau R}\right)\right]}, \tag{19a}$$

and

$$\frac{1}{\tau_{B,y}} = \frac{v_y}{l_y} \cdot \frac{\left(1-2\frac{\sigma_z}{\tau R}\right)\left(1-\exp\left(\frac{-l_y}{\tau v_y}\right)\right)}{2-\left[\sum_\alpha \frac{\tau v_\alpha}{l_\alpha}\left(1-\exp\left(\frac{-l_\alpha}{\tau v_\alpha}\right)\right)\left(1-2\frac{\sigma_z}{\tau R}\right)\right]}, \tag{19b}$$

where l_x and l_y label the dimensions of the grain cross section along the x- and y-axis, respectively. To evaluate these rates, we need to estimate a magnitude for the term $\frac{2\sigma_z}{\tau R}$ in Eqs. (19a) and (19b). This can be made possible by examining the general solution of $\tilde{N}$ in Eq. (15). It is clear from Eq. (15) that, in the case of completely diffusive boundaries, σ_z equals zero. However, in the case of total specular phonon reflections at grain boundaries, $\frac{R\tau}{2}$ must remain equal to σ_z for all values of z to insure that $\tilde{N}$ reduces to τR (which is the same as without boundary scattering) at any position in the crystal. In the intermediate case (partial specular phonon reflections at grain boundaries), the ratio of σ_z to $\frac{R\tau}{2}$ must be equal to a positive constant smaller than one for any value of z to insure that $\tilde{N}$ reduces very fast to τR (the value for an infinite crystal) as phonons move away from the boundaries. Thus, the term $\frac{2\sigma_z}{\tau R}$ is always independent of the position in the crystal and has a magnitude between zero and one. This term also has the effect of increasing the cross section dimensions l_x and l_y (see Eqs. (19a) and (19b)). Furthermore, one would expect that irregularities at the grain boundaries reduce the surface phonon lifetime, and consequently reduce σ_z. Thus, the term $\frac{2\sigma_z}{\tau R}$ in Eqs. (19a) and (19b) has all the characteristics of the so-called phonon specularity factor.[34–37] Therefore, we will refer to it in what follows as the phonon specularity factor t. For partially diffusive boundaries, it has been shown that the specularity factor t depends on the characteristics of the incident phonon and surface asperities according to $t = \exp\left(\frac{-16\pi^2\lambda^2\omega^2}{v^2}\right)$, where λ is the root mean square (*rms*) surface irregularity.[38,39]

The normalized rate at which phonons scatter by one of the boundaries is calculated as a function of normalized

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intrinsic relaxation time, with considering $l_x = l_y$ and assuming an isotropic crystal $(v_x = v_y = v_z)$ for several specularity factors. The results are shown in Fig. 2. As can be noticed, for the case of a total specular phonon reflection $(t = 1)$, $\frac{1}{\tau_{B,\alpha}} = 0$ (as if there is no boundary). However, in the case of a completely diffusive boundary $(t = 0)$, $\frac{1}{\tau_{B,\alpha}} \underset{\tau \to \infty}{\to} \frac{v}{l_\alpha}$, which is the well-known Casimir limit established for the lifetime of ballistic phonons at low temperatures, and $\frac{1}{\tau_{B,\alpha}} \underset{\tau \to 0}{\to} \frac{v}{2l_\alpha}$.

B. Lattice thermal conductivity of granular crystals made up of columnar grains

When several columnar grains are assembled parallel to each other to form a granular crystal, and a thermal gradient is aligned parallel to the grains axes, phonons may transmit specularly from grain to grain. Such a phonon mechanism increases the phonon free path between two successive phonon-boundary scattering events. Therefore, for the case of a granular crystal made up of columnar grains, the calculation of κ along the grains axes can be carried out with considering the granular crystal as a single columnar grain of effective cross section dimensions larger than the actual cross section dimensions of the constituent grains (l_x and l_y). The use of Eq. (9a) with the phonon-boundary scattering rates expressed in Eqs. (19a) and (19b) modified with effective cross section dimensions yield κ of a granular crystal made up of columnar grains grown with a preferred orientation, whereas the use of Eq. (9b) with the same phonon-boundary scattering rates modified with effective cross section dimensions yield κ of a granular crystal made up of columnar grains oriented randomly.

We express the effective cross section dimension along the α direction (x or y direction) as

$$l_{eff,\alpha} = l_{1,\alpha} + \mu_{12} l_{2,\alpha} + \mu_{12}\mu_{23} l_{3,\alpha} + \cdots + \prod_{i=2}^{n_\alpha} \mu_{(i-1)i} l_{n,\alpha}, \tag{20}$$

where, $l_{i,\alpha}$ is the dimension of the *ith* grain in the α direction, n the number of grains in the α direction, and $\mu_{(i-1)i}$ the probability for a phonon incident from grain $(i-1)$ to transmit specularly to the *ith* grain. For normal incidence, this transmission probability is given by[40,41]

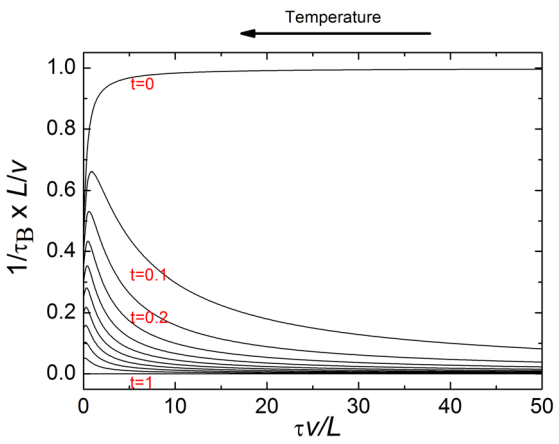

FIG. 2. Normalized Phonon-boundary scattering rate versus normalized intrinsic phonon relaxation time for several phonon specularity factors.

$$\mu_{(i-1)i} = t\frac{4Z_{i-1}Z_i}{(Z_{i-1}+Z_i)^2}, \tag{21}$$

where t is the specularity factor defined previously and Z_i the acoustic impedance of the *ith* grain defined as $Z_i = \rho v_i$. Let $\bar{l}_\alpha$ be the average grain size in theαdirection and $\bar{\mu}$the average specular transmission probability, the effective cross section dimension along theαdirection takes the form

$$\bar{l}_{eff,\alpha} = \bar{l}_\alpha \sum_{i=0}^{\bar{n}_\alpha - 1} \bar{\mu}^i, \tag{22}$$

where $\bar{n}_\alpha$ equals $\frac{L_\alpha}{\bar{l}_\alpha}$ rounded to the nearest integer, with L_α being the dimension of the sample in the α direction. For the case of well oriented columnar grains, $\bar{\mu}$obviously reduces to t. In order to deduce $\bar{\mu}$ for randomly oriented columnar grains, we average Eq. (21) over all possible combinations of orientations. This averaging procedure leads to $\bar{\mu} = \frac{4t}{2m}\left(\frac{m}{4} + \sum_{\substack{[hkl] \\ [h'l'k'] \neq [hkl]}} \frac{\bar{v}_{hkl}\bar{v}_{h'k'l'}}{(\bar{v}_{hkl}+\bar{v}_{h'k'l'})^2}\right)$. Here m is the number of high symmetry directions in the crystal structure under consideration, and $\bar{v}_{hkl}$ is the speed given by Eq. (10) averaged over the three phonon polarizations. It is clear that with these expressions for $\bar{\mu}$, we neglect possible phonon polarization conversion. However, it has been demonstrated that the error introduced by such an approximation does not alter the conclusion of a calculation involving specular phonon transmission.[34]

C. Lattice thermal conductivity of granular crystals made up of non-columnar grains

Additional complications arise in the calculation of κ of a granular crystal made up of non-columnar grains as one has to account for the existence of boundaries along the z direction (the direction along which the phonon heat current is directed). However, the problem is simplified by noting that in such a case, every grain in the direction of the phonon heat current experiences the same heat flux, but different temperature gradient due to the thermal resistances of the boundaries. Thus, the effect of grain boundaries in the z direction can be accounted for by simply considering that these boundaries add resistances to the intrinsic resistance of a columnar grain without boundaries in the z direction. Therefore, the thermal resistance in the z direction can be expressed as

$$R_z = \sum_{i=2}^{n_z} R_1 + R_i + R_{B,(i-1)i}, \tag{23}$$

where R_1 is the resistance of the first grain, $R_i$the resistance of the *ith* grain, $R_{B,(i-1)i}$ the resistance of the boundary between the grain $(i-1)$ and the *ith* grain, and $n_z$the average number of grains in the z direction. Considering L_z the sample dimension in the z direction, $\bar{l}_z$ the average grain size in the z direction, $\bar{R}_B$ an average boundary thermal resistance, and $\bar{n}_z$ equals $\frac{L_z}{\bar{l}_z}$ rounded to the nearest integer, κ for a granular crystal made up of non-columnar grains can be written as

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$$\kappa = \frac{L_z}{\bar{n}_z\left[\frac{\bar{l}_z}{\kappa_{col}} + \bar{R}_B\right] - \bar{R}_B}, \tag{24}$$

where κ_{col} is the thermal conductivity of the granular crystal without boundaries in the z direction.

The thermal resistance of a boundary between two different materials is the inverse of the boundary thermal conductance TC, which is defined as[42]

$$TC = \frac{1}{2(2\pi)^3}\sum_j \int \frac{1}{k_B T^2}\hbar^2\omega_j^2(\mathbf{k})v_j(\mathbf{k}_z) \times \frac{\exp\left(\frac{\hbar\omega_j(\mathbf{k})}{k_B T}\right)}{\left[\exp\left(\frac{\hbar\omega_j(\mathbf{k})}{k_B T}\right) - 1\right]^2}\Gamma_j(\mathbf{k})d\mathbf{k}. \tag{25}$$

Here, $v_j(\mathbf{k}_z)$ is the speed of the j-polarized phonon along the z direction, and $\Gamma_j(\mathbf{k})$ is the probability for a phonon of polarization j and wavevector $\mathbf{k}$to transmit specularly or diffusively across the boundary. However, it can be shown that the transmission probability across a boundary between two grains of the same material is independent of the orientations of the grains at both sides of the boundary,[43] and of magnitude given by

$$\Gamma_j(\mathbf{k}) = \Gamma = \bar{\mu} + \frac{1-t}{2}. \tag{26}$$

Thus, κ in a granular material made up of non-columnar grains can be derived by inserting Eq. (26) in Eq. (25), and then using the resulting equation in Eq. (24).

D. Anisotropic lattice thermal conductivity in granular crystals

Let us now define a Cartesian coordinate system (x, y, z), with the z-axis aligned parallel to the direction along which the grains are grown and the x- and y-axes aligned parallel to the basal planes of the grains. Since the grains dimensions $(\bar{l}_x, \bar{l}_y, \bar{l}_z)$ and the sample dimensions $(\bar{L}_x, \bar{L}_y, \bar{L}_z)$ are the determinants of the thermal conductivity of a granular crystal, the principal axes of the thermal conductivity tensor $\mathbf{K}$ of a granular crystal will always be aligned to x, y, zdirections. Therefore, $\mathbf{K}$ with respect to the Cartesian coordinate system (x, y, z) is given by

$$\mathbf{K} = \begin{pmatrix} \kappa_x & 0 & 0 \\ 0 & \kappa_y & 0 \\ 0 & 0 & \kappa_z \end{pmatrix}, \tag{27}$$

where the components $\kappa_x, \kappa_y, \kappa_z$ can be calculated from Eq. (24) with assuming a phonon heat current in the x, y, and z directions, respectively.

If we consider that the direction of a phonon heat current with respect to (x, y, z) is defined by

$$\hat{\mathbf{s}} = \begin{pmatrix} \sin\theta\cos\varphi \\ \sin\theta\sin\varphi \\ \cos\theta \end{pmatrix}, \tag{28}$$

where θ is the angle between the phonon heat current and z, and φ the azimuthal angle, the phonon heat current in (x, y, z) can be written as

$$\mathbf{q} = -\mathbf{K}\hat{\mathbf{s}}\|\nabla T\|, \tag{29}$$

where $\|\nabla T\|$ is the magnitude of ∇T. However, only the component of $\mathbf{q}$ that is aligned with ∇T contributes to the heat flux. The magnitude of this component in (x, y, z) is given by

$$q_{net} = \mathbf{q}\hat{\mathbf{s}}. \tag{30}$$

Upon substituting Eq. (29) in Eq. (30) and comparing the result to $q_{net} = -\kappa_{eff}\|\nabla T\|$, we find that the effective thermal conductivity κ_{eff} of the granular crystal for a phonon heat current in a direction defined by the angles θ and φ is given by

$$\kappa_{eff} = -\left(\kappa_x \sin^2\theta\cos^2\varphi + \kappa_y \sin^2\theta\sin^2\varphi + \kappa_z\cos^2\theta\right). \tag{31}$$

Anisotropic κ in a granular crystal is clearly demonstrated in Eq. (31). For columnar grains grown along the crystal optical axis and have cubic, hexagonal, tetragonal, or trigonal symmetry, κ_x and κ_y, to some extent, can be assumed equivalent, and consequently the terms $\cos^2\varphi$ and $\sin^2\varphi$ cancel out of Eq. (31). In the case of randomly oriented non-columnar grains, $\mathbf{K}$obviously reduces to a scalar.

V. COMPARISON WITH EXPERIMENTS

In order to verify its accuracy, the model described above has been used to reproduce experimentally measured κ in single and granular crystals containing negligible amount of defects. For the calculation of κ in single crystals, the actual dimensions of the samples were used as input parameters. However, for the calculation of κ in granular crystals, the actual dimensions of the samples and constituent grains were used as input parameters, and the *rms* irregularity λ at the grains boundaries was slightly adjusted until best agreement was obtained between the theoretical and experimental curves.

The model was applied to calculate κ in enriched and natural silicon (Si) and diamond single crystals of well-defined surface orientation. The theoretical results are compared in Fig. 3 with the measurements of Ruf *et al.* on Si[44] and the measurements of Oslon *et al.* on diamond.[45] The agreement between calculated and measured κ demonstrates the accuracy of the calculation method used to account for the dependence of surface orientation on κ.

The model was also applied to reproduce κ measurements of Uma *et al.* on polycrystalline Si films made up of non-columnar randomly oriented grains,[46] and those of Belay *et al.* on polycrystalline chemical vapor deposited (CVD) diamond films made up of non-columnar randomly oriented grains of natural abundance composition (98.9% ^{12}C and 1.1% ^{13}C), and of 50% of each carbon isotope.[47] The theoretical and experimental results are shown together in Fig. 4. The agreement of the model results with the experimental measurements further demonstrates the physical

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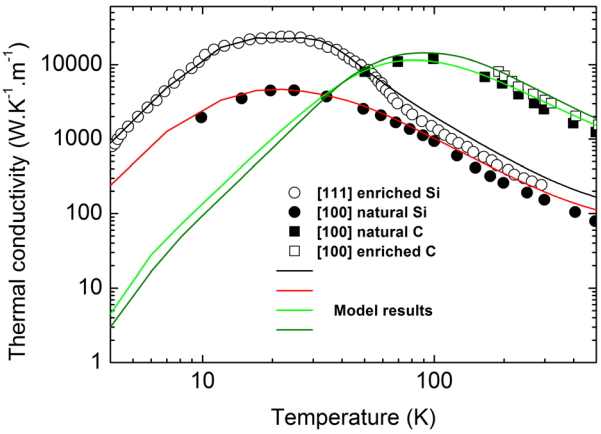

FIG. 3. Effects of surface orientation and isotope composition on the thermal conductivity of silicon and diamond single crystals. The symbols present experimental data from Refs. 38 and 39. The solid lines present theoretical results obtained from the model described in the present work.

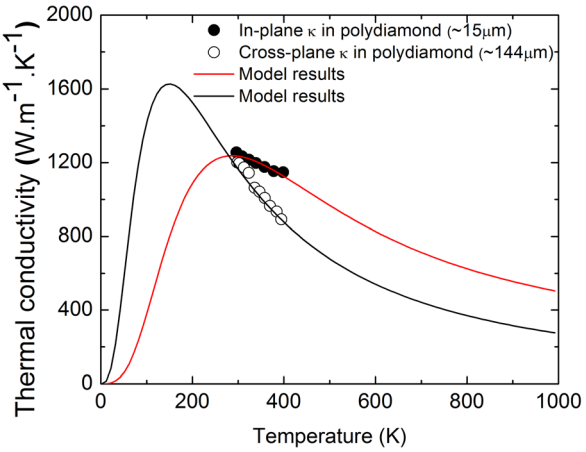

FIG. 5. Temperature-dependent anisotropic thermal conductivity in a diamond crystal made up of columnar grains. The symbols present experimental data from Ref. 42. The solid lines present theoretical results obtained from the model described in the present work.

reasonableness of the assumptions used for the description of the phonon transport across boundaries parallel and perpendicular to temperature gradient.

To verify its accuracy in describing anisotropic κ, the model was compared to the measurements of Graebner *et al.* on polycrystalline CVD diamond films made up of columnar grains.[48] Graebner *et al.* measured κin both directions parallel (in-plane) and perpendicular (cross-plane) to the plane of the films, and reported on temperature-dependent anisotropic κ. While cross-plane κtends to be greater than in-plane κ at low temperatures, in-plane κ exceeds cross-plane κat high temperatures, and the anisotropy in κincreases as the temperature increases. These experimental results are shown in Fig. 5 together with the model results. The good agreement between the experimental and theoretical curves highlights the importance of considering temperature-dependent phonon-boundary scattering rates to accurately describe anisotropic κ over a wide temperature range. The experimentally observed temperature-dependent anisotropic κ can be understood if we realize that the rate at which phonons scatter by partially diffusive grain boundaries parallel to the temperature gradient direction increases with temperature (see Fig. 3). While boundaries perpendicular to the temperature gradient give rise to a temperature-independent boundary resistance above Debye temperature, boundaries parallel to the temperature gradient yield low phonon-boundary scattering rate at low temperatures resulting in cross-plane κ higher than in-plane κ at low temperatures, and high phonon-boundary scattering rate at high temperatures resulting in cross-plane κ lower than in-plane κ at high temperatures.

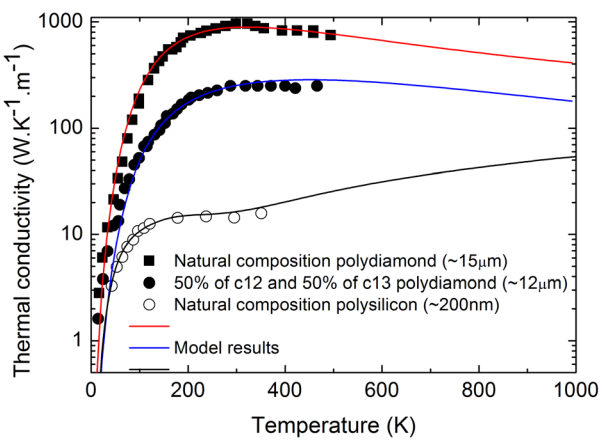

FIG. 4. Effects of isotope composition on the thermal conductivity of polycrystalline silicon and diamond films made up of non-columnar randomly oriented grains. The symbols present experimental data from Refs. 40 and 41. The solid lines present theoretical results obtained from the model described in the present work.

VI. CONCLUSION

Boltzmann transport equation that accounts for the physical natures of the intrinsic phonon mechanisms and involves spatial dependence of phonon distribution function has been solved to derive formalism for the lattice thermal conductivity in a finite crystal. The anharmonic phonon scattering rates have been derived from Fermi's golden rule, based on the cubic anharmonic part of the crystal Hamiltonian as perturbation, and the lattice vibration parameters for each phonon polarization have been derived as functions of temperature and crystallographic direction by using exact phonon dispersion curves. The derived formalism has been extended to provide a theoretical description of the contribution of surface phonons to the lattice thermal conductivity and the interplay between the anharmonic phonon scattering rate and the rate at which phonons scatter by grain boundaries in a granular crystal. The developed model differs from the existing models in that it precisely describes the phonon-boundary scattering rates (which is the dominant phonon scattering rate in granular crystals) as a function of temperature and clearly demonstrates the role of surface phonons to the lattice thermal conductivity. Furthermore, it provides a physical definition for the widely used phonon specularity factor. The accuracy and wide scope of the developed model have been demonstrated with reference to reported data regarding the effects of surface orientation and isotope composition on the thermal conductivity of single crystals and

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the effects of grains size and shape on the thermal conductivity of granular materials. The experimentally measured thermal conductivity, for all cases could be well described over a wide temperature range.

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