Mode-Resolved Continuum Mechanics Model of Phonon Scattering from Embedded Cylinders

Vineet Unni and Joseph P Feser*

Department of Mechanical Engineering, University of Delaware, 19716
(Dated: January 14, 2016)

Abstract

Phonon scattering from media with embedded spherical nanoparticles has been studied extensively over the last decade due to its application to reducing the thermal conductivity of thermoelectric materials. However, similar studies of thermal transport in fiber-embedded media have received little attention. Calculating the thermal conductivity tensor from microscopic principles requires knowledge of the scattering cross section spanning all possible incident elastic wave orientations, polarizations and wavelengths including the transition from Rayleigh to geometric scattering regimes. In this paper, we use continuum mechanics to develop an analytic treatment of elastic wave scattering for an embedded cylinder and show that a classic treatise on the subject contains important errors for oblique angles of incidence, which we correct. We also develop missing equations for the scattering cross section at oblique angles and study the sensitivity of the scattering cross section as a function of elastodynamic contrast mechanisms. In particular, we find that for oblique angles of incidence, both elastic and density contrast are important mechanisms by which scattering can be controlled, but that their affects can offset one another, similar to the theory of reflection at flat interfaces. The solution developed captures the scattering physics for all possible incident elastic wave orientations, polarizations and wavelengths including the transition from Rayleigh to geometric scattering regimes, thus enabling its incorporation into calculations of the thermal conductivity tensor for media with embedded nanofibers.

* jpfeser@udel.edu
INTRODUCTION

Phonons are the dominant carriers of heat in most non-metallic crystalline solids. Deviations from perfect crystal structure and perfect harmonic bonding give rise to phonon scattering which determines a materials thermal conductivity. In the absence of nanostructures, such phonon scattering events usually include phonon-phonon scattering, point defect scattering in alloys, boundary scattering, and phonon-electron scattering in heavily doped materials. Advances in materials synthesis now also permit the intentional embedding of nanocrystalline particulates in a variety of dielectric, metallic, and semiconducting matrix materials. Embedded nanocrystals are capable of dramatically reducing the thermal conductivity of alloy semiconductors through increased phonon scattering. Depending on the application, this may be a desirable or undesirable feature.

One important application where it is desirable is in energy conversion by thermoelectric devices, where the performance characteristics are strongly enhanced by reducing the lattice thermal conductivity. In particular in thermoelectric materials, there is window of interparticle spacings available above 10nm in which nanoscatervers can scatter phonons without significantly harming electronic transport, due to the fact that the electron/hole mean-free-path is typically 10nm in degenerate conductors,[1] while more than 50% of the lattice thermal conductivity is carried by phonons with mean-free-path above 40nm for traditional thermoelectric materials like PbTe [2]; the difference is even more stark in some good electronic materials like Si, where the intrinsic phonon mean-free-path is as high as 1000nm [3]. On the other hand, in emerging technologies such as electro-optic devices employing quantum confinement, maintaining low temperatures in the presence of nanostructures is integral to device performance and impeded phonon transport may not be desirable. In either scenario, understanding which factors determine the scattering rate of thermal wavelength phonons in solids with embedded nanostructures is an important goal.

Significant attention has been given to theoretical understanding of phonon scattering in embedded spherical nanoinclusions and their affect on thermal transport properties [4–6]. However, apparently no similar investigations have been performed for pseudo-random arrangements of embedded nanocylinders. In contrast, changes in phonon dispersion relations caused by periodic arrangements of nanocylinders (i.e. phononic crystals) have been studied quite extensively. Many known or conceivable methods of producing embedded fiber
nanocomposites involve either pseudo-random fiber orientation or aligned cylinders with random placement in 2D. For example, the former case would result from short fibers dispersed 3 dimensionally in a matrix or from filled fiber mats; the latter would result from vapor-liquid-solid growth from a substrate. For such random arrangements, the composites are not phononic crystals and the effect of embedded fibers would be more appropriately considered as an alteration of the scattering behavior of an effective medium.

A necessary precondition for calculating thermal properties using Boltzmann transport theory in the relaxation time approximation is the ability to calculate the scattering rate of phonons for all phonon polarizations and for all possible angles of incidence. Unlike scattering from embedded spheres where there is a high degree of symmetry, scattering due to cylinders is not expected to be independent of incident angle, nor are the scattering rates of the two transverse modes expected be equivalent for the same angle of incidence.

For simple geometries like cylinders and spheres where the embedded scatterer conforms to the coordinate axes, continuum mechanics is capable of obtaining exact solutions to elastic wave scattering from isolated embedded particles. Such solutions can give polarization-specific scattering cross sections, take into account all sources of elastodynamic scattering contrast, do not rely on perturbation theory, and give results for arbitrary wavevector, which is especially important in the intermediate scattering parameter range \((k^*R = 0.1 \ 10)\) where optimized nanocomposites are likely to operate \([4, 5, 7]\). White has reported an approach to calculate the scattered wave displacements for obliquely incident elastic waves from 3 dimensional embedded cylinders \([8]\), and has experimentally validated the model in 2D (i.e. for wavevectors perpendicular to a cylinder axis). However, we will demonstrate that there are important errors when applying the equations developed by White to oblique angles of incidence. In addition, this classic treatise is missing the necessary equations to calculate the scattering cross section at oblique angles of incidence.

The objective of this manuscript is to redevelop the equations governing the scattered field such that they are corrected, to provide additional equations which allow the calculation of scattering cross section at oblique angles of incidence, and to study the polarization-depandannt sensitivity of the scattering cross section as a function of elastodynamic contrast mechanisms and angle of incidence. This information is to provide the basis for incorporation of nanocylinder scattering in calculations of the anisotropic thermal conductivity tensor.
PROBLEM DEFINITION

Consider the scattering of a plane compressional or shear wave of a single frequency obliquely incident on an infinitely long isotropically elastic cylindrical discontinuity (medium 2) embedded in a different isotropic elastic medium (medium 1). Figure 1 shows the orientation of the cylinder and the incident wave with coordinate axes. The incident wave approaches with propagation direction in the x-z plane, defined by a wavevector along unit vector $\hat{a}$, which has an oblique incidence relative to the x-y plane. The angle between $\hat{a}$ and the x-y plane is denoted by $\phi_2$, for incident compressional waves or by $\psi_2$ for shear waves. The incident wave encounters a cylindrical scattering medium with radius $a$ from the z-axis denoted as region 1. This both produces a scattered wave in medium 2 and excites an internal wave in region 1. The total wave displacement in region 2 is a superposition of the incident and scattered waves. For continuity, both the displacements and the traction must be continuous at the interface between regions 1 and 2. If both mediums are linearly elastic with isotropic elastic tensors, then the equations of motion inside each medium are

$$
\rho \frac{\partial^2 \vec{u}}{\partial t^2} = (\lambda + 2\mu) \nabla (\nabla \cdot \vec{u}) - \mu (\nabla \times \nabla \times \vec{u})
$$

Where $\rho$ is the density of the material, and $\lambda$ and $\mu$ are the Lamé constants. The Lamé constants are easily connected to the elastic constants: $C_{11} = \lambda + 2\mu$ and $C_{44} = \mu$. Considering displacements that are temporally sinusoidal ($\vec{u} = \vec{U}(x, y, z)e^{-i\omega t}$), any spatial portion

FIG. 1. COORDINATE AXES AND ANGLE DEFINITIONS FOR THE SCATTERING PROBLEM. VECTOR $\hat{a}$ LIES IN PLANE x-z
of the displacement field which satisfies Eq. 1 can be expressed as the superposition of
displacements derived from scalar functions (Ψ, Θ, and χ) which satisfy scalar Helmholtz
equations. In particular (1) if \((\nabla^2 + k^2)\Psi = 0\) then \(\tilde{L} = \nabla \Psi\) is a solution representing a
longitudinal wave, (2) if \((\nabla^2 + k_S^2)\Theta = 0\) then \(\tilde{M} = \nabla \times (\hat{z} \Theta)\) is a solution representing a
transverse wave with displacements polarized along the \(\hat{z} \times \hat{a}\) direction, which is coincident
with \(\hat{y}\) and thus referred to a \(y\)-transverse wave from here on. (3) if \((\nabla^2 + k_S^2)\chi = 0\) then
\(\tilde{N} = (1/k_S)\nabla \times \nabla \times (\hat{z} \chi)\) is a transverse wave with displacements polarized along \(\hat{z} \times \hat{a} \times \hat{a}\).
These displacements are orthogonal to both \(\tilde{L}\) and \(\tilde{M}\)-type waves and will be referred to as quasi-\(z\) transverse waves because the displacements are in the \(\hat{z}\) direction for waves at \(\psi_2 = 0\) (normal incidence).

**Incident Wave Expressions**

The displacement of an incident compressional plane wave is of the form

\[
\tilde{L}_{inc} = \hat{a}u_0 e^{-i\omega t} e^{ik_2(x \cos \phi_2 + z \sin \phi_2)}
\]  

which can be derived from the scalar potential \(\tilde{L}_{inc} = \nabla \Psi_{inc}\) where

\[
\Psi_{inc} = \frac{u_0}{ik_2} e^{ik_2(x \cos \phi_2 + z \sin \phi_2)}
\]  

where \(k_2 = \omega/c_2\) and \(c_2 = \sqrt{(\lambda_2 + 2\mu_2)/\rho_2}\) is the sound speed of the compressional wave
through region 2. This can be expressed in cylindrical coordinates as

\[
\Psi_{inc} = \frac{u_0}{ik_2} \sum_{n=0}^{\infty} e^{iKz} e_n(i)^n J_n(k_2' r) \cos(n\theta)
\]  

where

\[
e_n = \begin{cases} 
1 & : \ n = 0 \\
2 & : \ n > 0 
\end{cases}
\]  

and \(K \equiv k_2 \sin(\phi_2)\), and \(k_2' \equiv k_2 \cos(\phi_2)\).

The displacements due to transverse incident plane waves can be derived from scalar
potentials in a similar manner. The potential

\[
\Theta_{inc} = \frac{u_0}{ik_{II}} \sum_{n=0}^{\infty} e^{iKz} e_n(i)^n J_n(k_{II}' r) \cos(n\theta)
\]  

generates a plane y-transverse incidence wave via the operation \( \tilde{M}_{inc} = \nabla \times (\hat{z} \Theta_{inc}) \). Here, \( k_\Pi = \omega/c_\Pi \) and \( c_\Pi = \sqrt{\mu_2/\rho_2} \) is the velocity of propagation of a shear wave through the region 2. The scalar potential

\[
\chi_{inc} = -\frac{u_0}{k_\Pi} \sum_{n=0}^{\infty} e^{ikz} e_n(i)^n J_n(k_\Pi' r) \cos(n\theta)
\]  

(7)
generates a plane a quasi-z-transverse incidence wave with displacements along the direction \( \hat{z} \times \hat{a} \times \hat{a} \) via the operation \( \tilde{N}_{inc} = \frac{1}{k_\Pi}[\nabla \times \nabla \times (\hat{z} \chi_{inc})] \).

Given the potential functions, both the incident wave displacement and stress fields can be calculated. In particular, the radial components of the stress tensor can be obtained in cylindrical coordinates from the displacements using

\[
T_{rr} = \lambda (\nabla \cdot \tilde{U}) + 2\mu \frac{\partial U_r}{\partial r}
\]  

(8)

\[
T_{r\theta} = \mu \left( r \frac{\partial}{\partial r} \left( \frac{U_{\theta}}{r} \right) + \frac{1}{r} \frac{\partial U_r}{\partial \theta} \right)
\]  

(9)

\[
T_{rz} = \mu \left( \frac{\partial U_z}{\partial r} + \frac{\partial U_r}{\partial z} \right)
\]  

(10)

The calculated displacement and stress fields are given in Tables II-IV for the three possible polarizations of incident waves. Table I gives the definition of \( \beta_n \), used in Tables II-IV, for each of the three incident polarizations. For convenience we define several non-dimensional parameters in Eqns 11-14.

\[
x_2 = k_2 r
\]  

(11)

\[
x_2' = k_2 r \cos(\phi_2)
\]  

(12)

\[
x_\Pi = k_\Pi r
\]  

(13)

\[
x_\Pi' = k_\Pi r \cos(\psi_2)
\]  

(14)

**Scattered Wave Expressions**

The scattered wave displacement fields in both region 1 and region 2 can be constructed as the superposition of compressional and shear waves. In region 2, the displacement field can be expressed as

\[
\tilde{U}_{scat,2} = \tilde{L}_2 + \tilde{M}_2 + \tilde{N}_2
\]  

(15)
where
\[ \tilde{L}_2 = \sum_{n=0}^{\infty} A_n (\nabla \Phi_n) \]
(16)
\[ \tilde{M}_2 = \sum_{n=0}^{\infty} B_n (\nabla \times (\hat{z} \Theta_n)) \]
(17)
\[ \tilde{N}_2 = \frac{1}{k_{\|}} \sum_{n=0}^{\infty} C_n (\nabla \times \nabla \times (\hat{z} \chi_n)) \]
(18)

The permitted scalar functions \( \Phi_n, \Theta_n, \) and \( \chi_n \) satisfy the scalar Helmholtz equation, and must be chosen to be compatible with the incident wavevector/polarization at the interface of the cylindrical discontinuity. In region 2, the relevant potentials are

\[ \Phi_n(r, \theta, z) = e^{iK_z} H_n(k_2 \cos(\phi_2) r) \frac{\cos(n\theta)}{\sin(n\theta)} \]
(19)
\[ \Theta_n(r, \theta, z) = e^{iK_z} H_n(k_{\|} \cos(\psi_2) r) \frac{\sin(n\theta)}{\cos(n\theta)} \]
(20)
\[ \chi_n(r, \theta, z) = e^{iK_z} H_n(k_{\|} \cos(\psi_2) r) \frac{\cos(n\theta)}{\sin(n\theta)} \]
(21)

The choice of upper or lower trigonometric function depends on whether the incident wave is longitudinal (upper function) or transverse (lower function). The wavenumbers must be chosen to have the same frequency as the incident wave, \( \omega = c_2 k_2 = c_{\|} k_{\|} \). In region 2, the Hankel function of the first kind, \( H_n \equiv J_n + iY_n \), is chosen because it represents a traveling wave carrying energy away from the cylinder as opposed to \( H_n^{(2)} \equiv J_n - iY_n \) which carries energy toward the cylinder, or \( J_n \) and \( Y_n \) which individually represent standing waves. Analogous arguments can be made to construct the scattered displacement field in

<table>
<thead>
<tr>
<th>Polarization Vector</th>
<th>Mode Name</th>
<th>( \beta_n )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \hat{a} )</td>
<td>longitudinal</td>
<td>( u_0 e_n i^{n-1} / (k_2) )</td>
</tr>
<tr>
<td>( \hat{z} \times \hat{a} )</td>
<td>y-transverse</td>
<td>( u_0 e_n i^{n-1} / (k_{|}) )</td>
</tr>
<tr>
<td>( \hat{z} \times \hat{a} \times \hat{a} )</td>
<td>quasi-z-transverse</td>
<td>( u_0 e_n i^{n-2} / (k_{|}) )</td>
</tr>
</tbody>
</table>
### TABLE II. Displacement and stress components for an incident longitudinal wave

<table>
<thead>
<tr>
<th>Component</th>
<th>Expression</th>
</tr>
</thead>
<tbody>
<tr>
<td>$U_r/(1/r)$</td>
<td>$\sum_{n=0}^{\infty} \beta_n e^{iKz} \left[ -x_2' J_n'(x_2') \right] \cos (n\theta)$</td>
</tr>
<tr>
<td>$U_\theta/(1/r)$</td>
<td>$\sum_{n=0}^{\infty} \beta_n e^{iKz} \left[ \pm n J_n(x_2') \right] \sin (n\theta)$</td>
</tr>
<tr>
<td>$U_z/(1/r)$</td>
<td>$\sum_{n=0}^{\infty} \beta_n e^{iKz} \left[ -i (K r) J_n(x_2') \right] \cos (n\theta)$</td>
</tr>
<tr>
<td>$T_{rr}/(\mu_2/r^2)$</td>
<td>$\sum_{n=0}^{\infty} \beta_n e^{iKz} \left[ -2 \left( x_2' \right)^2 \left( J_n''(x_2') - \left( \frac{x_2'}{r^2} \right)^2 \left( \frac{\lambda^2}{2\mu_2} \right) J_n(x_2') \right) \right] \cos (n\theta)$</td>
</tr>
<tr>
<td>$T_{r\theta}/(\mu_2/r^2)$</td>
<td>$\sum_{n=0}^{\infty} \beta_n e^{iKz} \left[ \pm 2 n \left( \left( x_2' \right) J_n'(x_2') - J_n(x_2') \right) \right] \sin (n\theta)$</td>
</tr>
<tr>
<td>$T_{rz}/(\mu_2/r^2)$</td>
<td>$\sum_{n=0}^{\infty} \beta_n e^{iKz} \left[ -2 i \left( x_2' \right) (K r) J_n'(x_2') \right] \cos (n\theta)$</td>
</tr>
</tbody>
</table>

### TABLE III. Displacement and stress components for a y-transverse incident wave

<table>
<thead>
<tr>
<th>Component</th>
<th>Expression</th>
</tr>
</thead>
<tbody>
<tr>
<td>$U_r/(1/r)$</td>
<td>$\sum_{n=0}^{\infty} \beta_n e^{iKz} \left[ \pm n J_n \left( x_{II}' \right) \right] \cos (n\theta)$</td>
</tr>
<tr>
<td>$U_\theta/(1/r)$</td>
<td>$\sum_{n=0}^{\infty} \beta_n e^{iKz} \left[ - (k_{II}' r) J_n'(x_{II}') \right] \sin (n\theta)$</td>
</tr>
<tr>
<td>$U_z/(1/r)$</td>
<td>0</td>
</tr>
<tr>
<td>$T_{rr}/(\mu_2/r^2)$</td>
<td>$\sum_{n=0}^{\infty} \beta_n e^{iKz} \left[ \pm 2 n \left( x_{II}' J_n'(x_{II}') - J_n(x_{II}') \right) \right] \cos (n\theta)$</td>
</tr>
<tr>
<td>$T_{r\theta}/(\mu_2/r^2)$</td>
<td>$\sum_{n=0}^{\infty} \beta_n e^{iKz} \left[ - (x_{II}')^2 \left( 2 J_n''(x_{II}') + J_n(x_{II}') \right) \right] \sin (n\theta)$</td>
</tr>
<tr>
<td>$T_{rz}/(\mu_2/r^2)$</td>
<td>$\sum_{n=0}^{\infty} \beta_n e^{iKz} \left( K r \right) \left[ \pm i n J_n (x_{II}') \right] \cos (n\theta)$</td>
</tr>
</tbody>
</table>

region 1, however in region 1 the displacement field must be finite at the origin. The relevant expansion can be obtained using Eqs. 15-21, but with a different set of expansion coefficients, using Bessel functions of the first kind, and by using wavenumber/angles that correspond to region 1. These substitutions are summarized in Table V and yield the following generating potentials for region 1.
TABLE IV. Displacement and stress components for a quasi-z transverse incident wave

\[
\begin{align*}
    U_r/(1/r) &= \sum_{n=0}^{\infty} \beta_ne^{iKz} \left[ i(Kr) \frac{x_{II}'}{x_{II}} J_n(x_{II}') \right] \cos(n\theta) \\
    U_\theta/(1/r) &= \sum_{n=0}^{\infty} \beta_ne^{iKz} \left[ \mp in \left( \frac{Kr}{x_{II}} \right) J_n(x_{II}') \right] \sin(n\theta) \\
    U_z/(1/r) &= \sum_{n=0}^{\infty} \beta_ne^{iKz} \left[ \frac{(x_{II}')^2 J_n(x_{II}')}{x_{II}} \right] \cos(n\theta) \\
    T_{rr}/(\mu_2/r^2) &= \sum_{n=0}^{\infty} \beta_ne^{iKz} \left[ 2i(x_{II}')^2 \left( \frac{Kr}{x_{II}} \right) J_n''(x_{II}') \right] \cos (n\theta) \\
    T_{r\theta}/(\mu_2/r^2) &= \sum_{n=0}^{\infty} \beta_ne^{iKz} \left[ \mp 2i n \frac{Kr}{x_{II}} (x_{II}'J_n(x_{II}') - J_n'(x_{II}')) \right] \sin(n\theta) \\
    T_{rz}/(\mu_2/r^2) &= \sum_{n=0}^{\infty} \beta_ne^{iKz} \left[ \frac{2(x_{II}')^3 J_n'(x_{II}')}{x_{II}} \left( 1 - \frac{1}{2\cos^2\psi_2} \right) \right] \cos (n\theta)
\end{align*}
\]

\[
\Phi_n(r, \theta, z) = e^{iKz} J_n(k_1 \cos(\phi_1)r) \frac{\cos(n\theta)}{\sin(n\theta)} \tag{22}
\]

\[
\Theta_n(r, \theta, z) = e^{iKz} J_n(k_1 \cos(\psi_1)r) \frac{\sin(n\theta)}{\cos(n\theta)} \tag{23}
\]

TABLE V. To obtain the scattered wave field in region 1, the following substitutions are needed in Eqs. 15-21.

\[
\begin{align*}
    A_n & \quad D_n \\
    B_n & \quad E_n \\
    C_n & \quad F_n \\
    H_n(z) & \quad J_n(z)
\end{align*}
\]

Subscript II Subscript I

Subscript II Subscript I

9
\[ \chi_n(r, \theta, z) = e^{iKz} J_n(k_1 \cos(\psi_1)r) \frac{\cos(n\theta)}{\sin(n\theta)} \]  

(24)

where again the wavenumbers are choosen to allow temporal phase-matching with the incident wave, so that the frequency, \( \omega = c_1 k_1 = c_I k_I \). The values of \( K = k_2 \sin(\phi_2) = k_II \sin(\psi_2) = k_1 \sin(\phi_1) = k_I \sin(\psi_1) \) must be the same in Eqs. 19-24 in order for the spatial phase of waves to be matched at the interface of the cylinder, which gives rise to an elastic analog to Snell’s law.

\[
\frac{\sin \phi_1}{c_1} = \frac{\sin \psi_1}{c_1} = \frac{\sin \phi_2}{c_2} = \frac{\sin \psi_2}{c_II}
\]  

(25)

Thus, one uses the known angle of incidence (either \( \phi_2 \) or \( \psi_2 \)) to calculate the the remaining three angles from Eqns. 25.

**Matching Conditions**

The displacement and stress tensor fields at the boundary of the cylinder must be continuous at the interface between region 1 and region 2. This gives the closure necessary to solve for the unknown expansion coefficients \( A_n, B_n, C_n, D_n, E_n, \) and \( F_n \) defining the scattered waves. At each value \( n \) of the summation \( (n = 0, 1, 2, \ldots, \infty) \), the matching conditions define a set of 6 linear algebraic equations to be solved. These can be summarized as

\[
(U_i)_n^{L} + (U_i)_n^{M2} + (U_i)_n^{N2} + \cdots - (U_i)_n^{L1} - (U_i)_n^{M1} - (U_i)_n^{N1} = -(U_i)^{\text{inc}}_n \]  

(26)

and

\[
(T_{ir})_n^{L} + (T_{ir})_n^{M2} + (T_{ir})_n^{N2} + \cdots - (T_{ir})_n^{L1} - (T_{ir})_n^{M1} - (T_{ir})_n^{N1} = -(T_{ir})^{\text{inc}}_n \]  

(27)

where in both Eq. 26 and 27 the index, \( i = r, \theta, \text{or} \ z \) refers to the cylindrical directional component evaluated at the cylinder surface, and \( n \) refers to the index of the summand (not an algebraic power). The displacement expressions for each term can be obtained by performing the operations in Eq. 16-18 on the potential functions 19-21. The resulting expressions for the displacements and stresses are given in Tables VI-VIII for the scattered wave in region 2. To save space, the expressions associated with region 1 are not explicitly shown but are easily obtained by the substitutions in Table V.
TABLE VI. Displacement and Stress Tensor Components associated with scattered wave $L_2$; to obtain the analogous expressions in medium 1, make the substitutions in Table V

<table>
<thead>
<tr>
<th>Component</th>
<th>Expression</th>
</tr>
</thead>
<tbody>
<tr>
<td>$(U_r)_{L_2}$</td>
<td>$\sum_{n=0}^{\infty} A_n e^{iKz} \left[ -x_2' H_n'(x_2') \right] \cos(n\theta)$</td>
</tr>
<tr>
<td>$(U_\theta)_{L_2}$</td>
<td>$\sum_{n=0}^{\infty} A_n e^{iKz} \left[ \pm n H_n(x_2') \right] \sin(n\theta)$</td>
</tr>
<tr>
<td>$(U_z)_{L_2}$</td>
<td>$\sum_{n=0}^{\infty} A_n e^{iKz} \left[ -i \left( Kr \right) H_n(x_2') \right] \cos(n\theta)$</td>
</tr>
<tr>
<td>$(T_{rr})_{L_2}$</td>
<td>$\sum_{n=0}^{\infty} A_n e^{iKz} \left[ -2 (x_2')^2 \left( H_n''(x_2') - \left( \frac{x_2}{x_2'} \right)^2 \left( \frac{\lambda_2}{2\mu_2} \right) H_n(x_2') \right) \right] \cos(n\theta)$</td>
</tr>
<tr>
<td>$(T_{r\theta})_{L_2}$</td>
<td>$\sum_{n=0}^{\infty} A_n e^{iKz} \left[ \pm 2n \left( (x_2') H_n'(x_2') - H_n(x_2') \right) \right] \sin(n\theta)$</td>
</tr>
<tr>
<td>$(T_{rz})_{L_2}$</td>
<td>$\sum_{n=0}^{\infty} A_n e^{iKz} \left[ -2 i (x_2') \left( Kr \right) H_n'(x_2') \right] \cos(n\theta)$</td>
</tr>
</tbody>
</table>

Importantly, a number of non-trivial discrepancies are found when the expressions in Tables VI-VIII are compared with those given in Ref [8] at non-zero angles of incidence. In particular, the expression given for $T_{rr}$ in Table I.A. of Ref [8], as well as all six expressions associated with $C_n$ for the stress and displacement components in Table I.B. of that reference are given incorrectly. In spite of these errors, the expressions in Ref [8] will still give correct results in the special case where the angle of incidence is zero. However, in the more general case of oblique incidence, the expressions in the current manuscript must be used.

CALCULATION OF SCATTERING CROSS SECTION

The expansion coefficients of the scattered waves $A_n$, $B_n$, $C_n$, $D_n$, $E_n$, and $F_n$, corresponding to any incident wave of arbitrary polarization and angle of incidence, by applying the matching conditions, Eqns. 26 and 27, at each value of summand. However, the displace-
TABLE VII. Displacement and Stress Tensor Components associated with scattered wave \( M_2 \); to obtain the analogous expressions in medium 1, make the substitutions in Table V

<table>
<thead>
<tr>
<th>Component</th>
<th>Expression</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \langle U_r \rangle_{M_2} ) ( \frac{(1/a)}{ } )</td>
<td>( \sum_{n=0}^{\infty} B_n e^{iKz} (\pm nH_n (k_{II}'r)) \frac{\cos(n\theta)}{\sin(n\theta)} )</td>
</tr>
<tr>
<td>( \langle U_\theta \rangle_{M_2} ) ( \frac{(1/a)}{ } )</td>
<td>( \sum_{n=0}^{\infty} B_n e^{iKz} (- (k_{II}'r) H_n' (k_{II}'r)) \frac{\sin(n\theta)}{\cos(n\theta)} )</td>
</tr>
<tr>
<td>( \langle U_z \rangle_{M_2} ) ( \frac{(1/a)}{ } )</td>
<td>0</td>
</tr>
<tr>
<td>( \langle T_{rr} \rangle_{M_2} ) ( \frac{(\mu_2/a^2)}{ } )</td>
<td>( \sum_{n=0}^{\infty} B_n e^{iKz} \left[ \pm 2n (x_{II}' H_n' (x_{II}') - H_n (x_{II}')) \right] \frac{\cos(n\theta)}{\sin(n\theta)} )</td>
</tr>
<tr>
<td>( \langle T_{r\theta} \rangle_{M_2} ) ( \frac{(\mu_2/a^2)}{ } )</td>
<td>( \sum_{n=0}^{\infty} B_n e^{iKz} \left[ -(x_{II}')^2 (2H_n'' (x_{II}') + H_n (x_{II}')) \right] \frac{\sin(n\theta)}{\cos(n\theta)} )</td>
</tr>
<tr>
<td>( \langle T_{r\phi} \rangle_{M_2} ) ( \frac{(\mu_2/a^2)}{ } )</td>
<td>( \sum_{n=0}^{\infty} B_n e^{iKz} (Kr) \left[ \pm inH_n(x_{II}') \right] \frac{\cos(n\theta)}{\sin(n\theta)} )</td>
</tr>
</tbody>
</table>

The time-averaged energy flux passing through a surface can be calculated from the time
TABLE VIII. Displacement and Stress Tensor Components associated with scattered wave $N_2$; to obtain the analogous expressions in medium 1, make the substitutions in Table V

<table>
<thead>
<tr>
<th>Component</th>
<th>Expression</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\langle U_r \rangle_{N_2}$</td>
<td>$\frac{(1/a)}{z}$ $\sum_{n=0}^{\infty} C_n e^{iKz} \left[ i(Kr) \left( \frac{x_{II}'}{x_{II}} \right) H_{n'}(x_{II}) \right] \frac{\cos(n\theta)}{\sin(n\theta)}$</td>
</tr>
<tr>
<td>$\langle U_\theta \rangle_{N_2}$</td>
<td>$\frac{(1/a)}{z}$ $\sum_{n=0}^{\infty} C_n e^{iKz} \left[ \mp i n \left( \frac{Kr}{x_{II}} \right) H_n(x_{II}) \right] \frac{\sin(n\theta)}{\cos(n\theta)}$</td>
</tr>
<tr>
<td>$\langle U_z \rangle_{N_2}$</td>
<td>$\frac{(1/a)}{z}$ $\sum_{n=0}^{\infty} C_n e^{iKz} \left[ \left( \frac{(x_{II}')}^2}{x_{II}} \right) H_n(x_{II}) \right] \frac{\cos(n\theta)}{\sin(n \theta)}$</td>
</tr>
<tr>
<td>$\langle T_{rr} \rangle_{N_2}$</td>
<td>$\frac{(1/\mu_2/a^2)}{z}$ $\sum_{n=0}^{\infty} C_n e^{iKz} \left[ 2i(x_{II}')(2) \left( \frac{Kr}{x_{II}} \right) H_n''(x_{II}) \right] \frac{\cos(n\theta)}{\sin(n \theta)}$</td>
</tr>
<tr>
<td>$\langle T_{r\theta} \rangle_{N_2}$</td>
<td>$\frac{(1/\mu_2/a^2)}{z}$ $\sum_{n=0}^{\infty} C_n e^{iKz} \left[ \mp 2i n \frac{Kr}{x_{II}} (x'<em>{II} H_n'(x</em>{II}) H_{n'}(x_{II}) - H_n(x_{II})) \right] \frac{\sin(n\theta)}{\cos(n \theta)}$</td>
</tr>
<tr>
<td>$\langle T_{rz} \rangle_{N_2}$</td>
<td>$\frac{(1/\mu_2/a^2)}{z}$ $\sum_{n=0}^{\infty} C_n e^{iKz} \left[ 2(x_{II}')^3 H_n'(x_{II}) \left( 1 - \frac{1}{2 \cos^2 \psi_2} \right) \right] \frac{\cos(n\theta)}{\sin(n \theta)}$</td>
</tr>
</tbody>
</table>

dependencies of the displacements ($s_j(t)$) and stress components ($\sigma_{ij}(t)$) as

$$F = \left\langle \int \int \left[ \sigma_{ij}(r, \theta, z, t) \cdot \frac{\partial u_j(r, \theta, z, t)}{\partial t} \right] \cdot dA_i \right\rangle_t$$

(28)

where the outer bracket denotes a time-averaging of the flux. Up until now displacement and stress have been treated as complex quantities, but for calculation of energy fluxes, we are interested in real displacements leading to real stresses. To obtain results in their real form, complex conjugates of the solutions are added.

$$\sigma_{ij}(r, \theta, z, t) = \frac{1}{2} \left[ (T_{ij} e^{-i\omega t}) + (T_{ij} e^{-i\omega t})^* \right]$$

(29)

$$u_j(r, \theta, z, t) = \frac{1}{2} \left[ (U_{ij} e^{-i\omega t}) + (U_{ij} e^{-i\omega t})^* \right]$$

(30)

Carrying out the time-averaging operation gives an average energy flux

$$F = \frac{i\omega}{4} \int \int \left[ (T_{ij}^* U_j) - (T_{ij} U_j^*) \right] \cdot dA_i$$

(31)
The energy intensity \([W/m^2]\) carried by an incident plane wave, \(W\), can be obtained from this by considering an planer area perpendicular to the direction of travel, in which case the incident power/area is just the integrand

\[
W = \frac{i\omega}{4} \left[ (T^*_i U_j)(T_{ij} U^*_j) \right] \cdot \hat{a}_i \tag{32}
\]

After some manipulation it can be shown that the energy intensities for incident longitudinal and both transverse polarization are respectively given by

\[
W_{\text{long}} = \left( \frac{\lambda_2}{2} + 2\mu_2 \right) u_0^2 \left( k_2^2 \omega \right) \tag{33}
\]

\[
W_{\text{trans}} = \left( \frac{\mu_2 u_0^2}{2} \right) \left( k_{II} \omega \right) \tag{34}
\]

Simple expressions for the scattered energy can be obtained by applying Eq. 31 on an imaginary cylinder of radius \(b \gg a\). In that case the Hankel function takes on the limiting behavior

\[
H_n(x') \to \left( \frac{2}{\pi x'} \right)^{1/2} e^{i(x'-(n+1/2)\pi/2}). \tag{35}
\]

Using \(H_n'(x') \to iH_n\) and \(H_n''(x') \to -H_n\) and taking \(b \to \infty\), gives the limiting behavior of wave energy carried by the L, M, N scattered waves as

\[
P_L = \sum_{n=0}^{\infty} A_n A^*_n \left( 2\mu_2 + \lambda_2 \right) \left( \omega k_2^2 \right) \tag{36}
\]

\[
P_M = \sum_{n=0}^{\infty} B_n B^*_n \left( \mu \cos^2 \psi_2 \right) \left( \omega k_{II}^2 \right) \tag{37}
\]

\[
P_N = \sum_{n=0}^{\infty} C_n C^*_n \left( \mu \cos^2 \psi_2 \right) \left( \omega k_{II}^2 \right) \tag{38}
\]

Equations 36-38 are correct regardless of the polarization of incident energy. The scattering cross section for incident waves of type \(j\) into scattered waves of polarization \(i\) is then

\[
Q_{ij} = \frac{P_j}{W_i} \tag{39}
\]

For incident compression waves, these become

\[
Q_{CC} = \frac{2}{k_2} \left[ 2\|A_0\|^2 + \sum_{n=1}^{\infty} \|A_n\|^2 \right] \tag{40}
\]

\[
Q_{CS} = \frac{2}{k_2 \cos^2 \psi_2} \left[ 2\|B_0\|^2 + \sum_{n=1}^{\infty} \|B_n\|^2 \right] \tag{41}
\]
\[ Q_{CS_z} = \frac{2}{k_2} \cos^2 \psi_2 \left( 2\|C_0\|^2 + \sum_{n=1}^{\infty} \|C_n\|^2 \right) \] (42)

For incident shear waves of either polarization, these become

\[ Q_{SC} = \frac{2}{k_{II}} \left( 2\|A_0\|^2 + \sum_{n=1}^{\infty} \|A_n\|^2 \right) \] (43)

\[ Q_{SS_y} = \frac{2}{k_{II}} \cos^2 \psi_2 \left( 2\|B_0\|^2 + \sum_{n=1}^{\infty} \|B_n\|^2 \right) \] (44)

\[ Q_{SS_z} = \frac{2}{k_{II}} \cos^2 \psi_2 \left( 2\|C_0\|^2 + \sum_{n=1}^{\infty} \|C_n\|^2 \right) \] (45)

In the case of obliquely incident shear waves, these expressions differ by a factor of \( \cos^2(\psi_2) \) from those derived in Ref [8].

One other important physical aspect of calculating the scattering cross section is that due to Snell’s Law (Eq. 25) some of the internal and external scattered modes may be evanescent waves. In the case of external scattered modes, this always happens when a transverse phonon with angle, \( \psi > \sin^{-1}(c_T/c_L) \), is incident on a cylinder, producing an evanescent compressional mode. Evanescent modes should carry no energy, yet in our formulation, the complex scattering coefficients, \( \|A_n\| \), are generally still non-zero. This is because the expansion in Eqn. 35 is not the correct one for imaginary arguments and does not lead to the form given in Eq. 43, but rather \( Q_{SC} = 0 \) in that case. Therefore, we set \( Q_{SC} = 0 \) if \( \text{Im}(\phi) < 0 \). Otherwise, the math in the preceding sections is correct and requires no special considerations to account for evanescent modes.

One final practical consideration is the number of terms to be evaluated. In principle, there are an infinite number of expansion coefficients, \( A_n, B_n, C_n, D_n, E_n, \) and \( F_n \) since \( n = 0, 1, 2, \cdots, \infty \). In the Rayleigh regime, usually only one or two of the lowest order terms are required for accurate results. However, in the Geometric regime a large number of terms (often hundreds or thousands) are required for convergence and accuracy. Thus, we continue the calculation of expansion coefficients until a relative convergence tolerance for the scattering cross section is met.

15
RESULTS AND DISCUSSION

Using the results of the previous section, we now investigate the scattering behavior of elastically embedded cylinders. In general the scattering cross section of an embedded cylinder is a function of up to 9 geometric and materials parameters:

\[ Q = \frac{Q(a, k_2 \text{ or } k_{l1}, \phi_2 \text{ or } \psi_2, \lambda_1, \lambda_2, \rho_1, \rho_2, \mu_1, \mu_2)}{} \]  

(46)

Dimensional analysis can reduce the dependence to 6 non-dimensional variables. A convenient choice in the case of incident compressional waves is

\[ \gamma = \gamma \left( k_2 a, \phi_2, \frac{\rho_1 - \rho_2}{\rho_2}, \frac{C_{11,1} - C_{11,2}}{C_{11,2}}, \frac{C_{44,1} - C_{44,2}}{C_{44,2}}, \frac{C_{11,2}}{C_{44,2}} \right). \]  

(47)

A similarly convenient choice in the case of either polarization of incident transverse waves is

\[ \gamma = \gamma \left( k_{l1} a, \psi_2, \frac{\rho_1 - \rho_2}{\rho_2}, \frac{C_{11,1} - C_{11,2}}{C_{11,2}}, \frac{C_{44,1} - C_{44,2}}{C_{44,2}}, \frac{C_{11,2}}{C_{44,2}} \right). \]  

(48)

Here \( \gamma \equiv \frac{Q}{ka} \) is the dimensionless scattering efficiency in 2D, representing the ratio of the scattering cross section relative to the cylinder’s geometric cross section. \( ka \) is called the scattering parameter. The 3rd term is the fractional density contrast and the 4th and 5th terms are the fractional longitudinal an shear elastic contrast of the two mediums respectively. The final terms is the ratio of the longitudinal to shear elastic constants \( C_{11}/C_{44} = (\lambda + 2\mu)/\mu \); For group IV and III-V semiconductors this spans a small range (1.8 < \( C_{11}/C_{44} < 2.2 \) for Si, Ge, GaP, GaAs, InAs, GaSb, InSb, InP). However, most other classes of cubic materials have higher \( C_{11}/C_{44} \), with some as high as 9 (PbTe = 8.2, PbSe = 7.8, Nb = 8.6). Thus, when embedding particles with similar crystal structure and bonding chemistry, \( \Delta C_{11}/C_{11} \approx \Delta C_{44}/C_{44} \), but this is generally not true otherwise. At this point, we should caution that the model developed in the preceding sections is strictly valid only for isotropic mediums, which is not the case for single crystals regardless of whether they have cubic crystal structure. However, the degree of anisotropy is not large in many cubic crystals (in Si for example the longitudinal sound speed in the [111] direction differs from [100] by about 10%), so it is hoped that the insights from the present model will still prove useful.

To understand some general predictions of the model, we will now explore the scattering efficiency, \( \gamma \), for some illuminating cases.

In Figure 2, scattering efficiency for phonons at normal incidence angle (\( \Psi_2 = 0 \)) is plotted for a NiSi\(_2\) cylindrical discontinuity embedded in a Si\(_{0.5}\)Ge\(_{0.5}\) matrix for size parameters.
ranging from the Rayleigh regime up to the geometric regime. The properties for these materials are given in Table IX. Some basic features are evident: (1) in the Rayleigh regime, scattering efficiency scales as $\gamma \sim (ka)^3$. Note that this is a different behavior than scattering from embedded spheres, where $\gamma_{sph} \sim (ka)^4$. (2) In the geometric regime, $\gamma$ oscillates about 2. (3) In the intermediate regime, Mie oscillations exist and these may persist for several orders of magnitude before and after $ka = 1$. For oblique angles of incidence, the behavior is more complicated. Intuitively, based on a geometric thinking, one expects that scattering might be weaker for waves traveling parallel to the cylinder axis. While this intuition is confirmed in the geometric limit, it fails for long wavelength compressional waves which are strongly scattered into transverse waves even for parallel travel; in fact, in the Rayleigh regime compressional waves traveling parallel to the cylinder scatter more strongly than waves with normal incidence. Similar behavior is not observed for incident transverse waves, in part because compressional scattered modes are evanescent and carry no energy, while according to Snell’s law, transverse waves scattering into transverse waves would carry energy along the axis of the cylinder. Thus no energy is scattered away from the cylinder for transverse waves coincident with the cylinder axis for any wavelength.

The limits of continuum limit as applied to scattering of thermal wavelength phonons warrant further discussion. Kakodkar [9] has recently compared the exact continuum model developed in this manuscript to an atomistically resolved computational model of phonon scattering for embedded cylinders with diameters between 2nm-9nm and for incident phonon wavelengths spanning the entire Brillouin zone. Kakodkar found excellent agreement between continuum and atomistically resolved theory for acoustic phonons in the first quarter of the Brillouin zone, which in the case of Ge embedded in Si was sufficient to capture the

<table>
<thead>
<tr>
<th>Parameter Si$<em>{0.5}$Ge$</em>{0.5}$ NiSi$_2$</th>
<th>$\rho$ [kg/m$^3$]</th>
<th>3826</th>
<th>4803</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$C_{11}$ [GPa]</td>
<td>146</td>
<td>199</td>
</tr>
<tr>
<td></td>
<td>$C_{44}$ [GPa]</td>
<td>74</td>
<td>53</td>
</tr>
</tbody>
</table>

TABLE IX. PARAMETERS USED TO GENERATE FIGURES 2 AND 3
first Mie scattering oscillation in the toughest case of 2nm cylinder diameters or about 8 atoms wide [9]. However, we should note that in weaker scatterers, the first peak in the Mie oscillations generally occurs at higher wavenumber (see the longitudinal case in Fig. 2, for example), in which case the continuum model will correctly predict the hump before the first Mie peak, but will inaccurately describe physics near and above the first Mie oscillation. For wavevectors \( k \gtrsim 0.25k_{\text{max}} \) continuum theory will fail, and in particular will miss important physical effects such as phonon dispersion, evanescent modes associated with phonon band gaps or maximum frequencies in the scattering medium, optical vibration modes, and the edge of the first Brillouin zone [9]. However, for the purposes of calculating thermal transport properties, continuum theory may still be sufficient since embedded nanostructures are typically designed to scatter long wavelength acoustic phonons, while other mechanisms such as phonon-phonon and point defect scattering are dominant at high wavevector and for optical modes. This warrants further investigation but is beyond the scope of this paper.

**Contrast Mechanisms in the Mie and Rayleigh Regimes**

The goal of this section is to determine which materials parameters or combinations have the greatest influence on the scattering efficiency. In geometric limit, geometry alone determines the scattering efficiency, and thus the materials parameters are expected to have no influence. However, as shown in Fig. 2, transition to the geometric limit sometimes requires very large scattering parameter. On the other hand, in the Mie and Rayleigh regimes the materials properties have great influence on the scattering cross section.

Mie oscillations occur due to wave interference, the degree of which is determined both by geometry and phase speed. The later depends on materials properties such as the speed of sound. For the application of controlling phonon scattering, it is particularly important to understand how the first scattering efficiency peak (at low scattering parameter) is related to the matrix/particle materials properties, since nanoparticles are primarily designed to control scattering of long-wavelength phonons.

Figure 4 shows a psuedocolor image of the scattering efficiency as a function of both the relative elastic contrast and density contrast in the Mie regime, using either \( k_2a = 2 \) or \( k_{\Pi}a = 2 \) for longitudinal or transverse waves respectively. The evaluation is done at an angle of incidence of either \( \phi_2 = 35^\circ \) (longitudinal) or \( \psi_2 = 35^\circ \) (transverse) rather than normal
incidence because phonons at this angle have the maximum differential contribution to heat flow perpendicular to the axis of the cylinder in the BTE-derived thermal conductivity integral \( k = \int k(\phi) d\phi \) where \( k(\phi) \sim \sin(\phi) \cos^2(\phi) \). Figure 4 shows that the scattering efficiency is highly dependent on both density contrast, \( \Delta \rho/\rho \) and elastic contrast \( \Delta C_{11}/C_{11} \) or \( \Delta C_{44}/C_{44} \) in the early Mie regime, and in particular, it shows that if the sound speed of the embedded cylinder is the same as that of the matrix, then the scattering efficiency is greatly suppressed, regardless of whether there is large density and/or elastic contrast. Fig. 4 also shows that large density contrast (in the absence of increased stiffness) is generally more effective at increasing scattering cross section than similar levels of elastic contrast. Alternatively, embedding a lower elastic constant material in the absence of density contrast is nearly as effective. Note that the scattering cross section does not monotonically rise with increasing contrast, though. This is in stark contrast to behavior in the Rayleigh regime \((ka \ll 1)\).

In the Rayleigh regime, the scattering efficiency scales as \( Q/2a = \alpha(ka)^3 \). The scaling factor, \( \alpha \), depends on elastodynamic contrast mechanisms as well as the incidence angle.

\[
\alpha = \alpha \left( \phi_2, \frac{\rho_2 - \rho_1}{\rho_2}, \frac{C_{11,1} - C_{11,2}}{C_{11,2}}, \frac{C_{44,1} - C_{44,2}}{C_{44,2}}, \frac{C_{11,2}}{C_{44,2}} \right).
\]  

(49)

For a given matrix material (i.e. fixed \( C_{11,2}/C_{44,2} \)), we can than therefore more universally capture results in the Rayleigh regime by plotting \( \alpha \). If there is no contrast (i.e. \( \frac{C_{11,2}}{C_{11,1}} = \frac{C_{44,2}}{C_{44,1}} = \frac{\rho_2 - \rho_1}{\rho_2} \)) then \( \alpha = 0 \) must be zero, and since \( Q > 0 \), the function \( \alpha \) must also be a local minimum.

Fig. 5 shows a contour plot of \( \alpha \) as a function of elastic and density contrast for a group IV matrix material \( (C_{11,2}/C_{44,2} = 2) \) such as Si\(_{1-x}\)Ge\(_x\) subject to obliquely incident waves \( (\phi_2 = 35^\circ \text{ (longitudinal)} \text{ or } \psi_2 = 35^\circ \text{ (transverse)} \text{.}) \). In the Rayleigh limit, \( \alpha \) and, by extension, the scattering cross section show sensitivity to both density and elastic contrast for weak levels of contrast. However, for longitudinal and y-transverse incidence polarizations, the scattering cross-section becomes nearly independent of elastic contrast once the density contrast is sufficiently large \( (\Delta \rho/\rho_2 \gtrsim 1) \); The scattering cross section of z-transverse polarization waves is co-dependent on density and elastic contrast over the entire range studied.
CONCLUSIONS

In summary, we have developed a continuum model for scattering of plane elastic waves of arbitrary angle of incidence and polarization from an elastic cylindrical discontinuity in isotropic mediums. The model fixes several deficiencies that were present in a classic treatise on the subject [8] that enable it to make accurate predictions at oblique angles of incidence.

This manuscript provides insights as to which mechanisms of contrast are responsible control of the scattering cross section in both the Mie and Rayleigh scattering regimes. In particular we find that in the early Mie regime, scattering efficiency is strongly influenced both elastic and density contrast. While either mechanisms can be used to raise the scattering cross section, choosing matrix/embedded materials with similar sound speed effectively suppresses scattering cross section. In the Rayleigh regime, density contrast is found to be the most effective mechanism of scattering contrast for longitudinal waves and for transverse waves polarized perpendicular to the cylinder axis (y-transverse). For quasi-z transverse waves at oblique angles of incidence, elastic and density contrast mechanisms have similar effectiveness.

Thus, the current model predicts the mode-resolved scattering cross section for all acoustic waves in isotropic elastic mediums with embedded elastic cylinders, over all scattering regimes without resorting to perturbation theory. While the model is quite general and can to be applied to a diverse set of engineering applications, we envision that it will be particularly useful in supporting rapid calculations of the anisotropic thermal conductivity tensor for composites with embedded cylinders using Boltzmann transport theory, which requires mode resolved scattering cross section information at all angle of incidence.

The author would like to thank the University of Delaware Research Foundation for financial support.


domain thermoreflectance for measuring thermal conductivity accumulation functions”. *Review of Scientific Instruments*, 84(6), pp. –.


FIG. 2. Scattering efficiency of NiSi$_2$ cylinders in Si$_{0.5}$Ge$_{0.5}$ as a function of scattering parameter at normal angle-of-incidence for different incident polarizations. Black lines indicate the total scattering efficiency while symbols indicate the portion scattered into compressional (blue box), y-transverse (green circle), and quasi-z transverse modes (red cross).
FIG. 3. Scattering efficiency of NiSi$_2$ cylinders in Si$_{0.5}$Ge$_{0.5}$ as a function of scattering parameter at normal angle-of-incidence for different incident polarizations. Black lines indicate the total scattering efficiency while symbols indicate the portion scattered into compressional (blue box), y-transverse (green circle), and quasi-z transverse modes (red cross).
FIG. 4. Scattering efficiency as a function of relative elastic and density contrast in the Mie regime ($ka = 2$) at an oblique angle of incidence, $\phi_2 = 35^\circ$ (longitudinal) or $\psi_2 = 35^\circ$ (transverse).
FIG. 5. $\alpha \equiv Q/(2k^3a^4)$ as a function of relative elastic and density contrast in the Rayleigh regime ($ka \ll 1$) at an oblique angle of incidence, $\phi_2 = 35^\circ$ (longitudinal) or $\psi_2 = 35^\circ$ (transverse).