

Kapitza thermal resistance between a metal and a nonmetal

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The thermal boundary conductance is derived for the heat flow between the electrons in a metal and the phonons in an ionic crystal. The image potential generated by the ion charges makes a regular pattern of surface charges on the surface of the metal. When the ions vibrate, these surface charges oscillate. Since the surface charges are the tails of the wave functions of the conduction electrons in the metal, the surface charges provide a matrix element between these electrons and the phonons in the insulator.

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I. INTRODUCTION

We derive a theory of how heat is transported through the interface between a metal and a nonmetal. The heat in a metal is carried primarily by electrons, while that in the insulator is carried by phonons. We propose that these two energy systems are linked at the interface by the image charges from the vibrating ions.

Kapitza¹ discovered the thermal boundary resistance between various metals and liquid helium. The first theory^{2,3} was based on elasticity, and considered only heat flow between the phonons of the two solids. This theory works well at very low temperatures, but does not explain the experimental data at room temperature.⁴⁻⁸ Two earlier theories of heat flow between a metal and an insulator used conventional electron-phonon coupling, such as deformation-potential interaction.^{9,10} Here we propose another mechanism that involves the image potential of an ion outside of a metal surface.

If the nonmetal is a polar material, with anions and cations, then an ion of charge Q has an image potential of

$$V(z) = -\frac{Q^2}{4z}. \quad (1)$$

The image potential is due to static charges on the metal surface. If a polar insulator is near the metal surface, the regular pattern of ion charges makes a regular pattern of charge density on the metal surface. When the ions vibrate, the charge density oscillates. The surface charge density consists of the tails of the electron wave functions. There is a direct coupling between the ion vibrations and the electron states in the metal. This direct coupling provides the matrix element for the interaction between the electrons in the metal and the phonons in the adjacent insulator.

The surface charge density is due to the polarization of the surface plasmons in the metal.¹¹⁻¹³ The electrons in the metal couple to the surface plasmon, and the surface plasmon couples to the ion charge. In the language of field theory, the electrons in the metal and the ions in the solid interact through the exchange of surface plasmons. This interaction can be used to construct the matrix element for energy transfer between the electrons in the metal and the phonons in the insulator.^{14,15} It is a type of electron-phonon interaction caused by the surface plasmon. The same inter-

action was used years ago to describe the vibrational excitation of molecules chemically bonded to the metal surface by the scattering of low-energy electrons.¹⁵ Schaich and Harris¹⁶ used it to calculate the friction coefficient between an atom or ion and a metal surface. We initially formulated the Kapitza problem using surface plasmons. However, this formalism proved to be unnecessarily cumbersome. The final theory, which is presented here, uses classical image theory and does not mention surface plasmons.

A neutral atom in the insulator, whether solid or fluid, has a van der Waals self-interaction with its image,¹⁴

$$V(z) = -\frac{C_3}{z^3}, \quad (2)$$

$$C_3 = \frac{\hbar}{4\pi} \int_0^\infty du \alpha_i(iu) \frac{\varepsilon(iu) - 1}{\varepsilon(iu) + 1}, \quad (3)$$

where $\alpha(iu)$ is the polarizability of the neutral atom, evaluated at imaginary frequencies, while $\varepsilon(iu)$ is the dielectric function of the metal, evaluated at long wavelength ($q \rightarrow 0$), and also at imaginary frequency. This formula applies if the metal has a planar surface. It can be used to construct a theory of Kapitza resistance between a metal and a nonionic solid such as argon. We do not provide this theory here, but will present it in a later publication.

In most calculations of the thermal boundary resistance between two insulators, the Lennard-Jones 6-12 potential is used between the atoms in the two solids or the liquid and the solid. The Lennard-Jones potential is also based on a van der Waals interaction. So in treating the case of a metal-nonmetal, we recognized that the van der Waals interaction has a different form, due to the feature that the metal is a conductor.

II. INTERACTIONS AND MATRIX ELEMENTS

We derive the interaction between electrons in a metal and phonons in a polar crystal. We begin by writing the potential function $\phi(\mathbf{r})$ generated by an ion of charge e^* at $\mathbf{r}_0 = (0, 0, d)$ outside of the surface. The observer is at position $\mathbf{r} = (\rho, z > 0)$,

$$\phi(\mathbf{r}) = \frac{e^*}{\varepsilon_i} \left(\frac{1}{r} - \frac{\lambda}{r_I} \right), \quad (4)$$

$$r = \sqrt{\rho^2 + (z-d)^2}, \quad r_l = \sqrt{\rho^2 + (z+d)^2}, \quad \lambda \equiv \frac{\epsilon_m - \epsilon_i}{\epsilon_m + \epsilon_i}, \quad (5)$$

where (ϵ_m, ϵ_i) are the dielectric functions of the metal and insulator, respectively. Their precise form is discussed below. The interaction with ion displacements \mathbf{Q}_j in the insulator is

$$\delta\phi(\mathbf{r}) = - \sum_j \mathbf{Q}_j \cdot \vec{\nabla} \phi(\mathbf{r} - \mathbf{R}_j). \quad (6)$$

Equation (4) applies outside of the metal surface. Inside the metal the potential is

$$\phi(\mathbf{r}) = \frac{e^*}{\epsilon_i} (1 - \lambda) \frac{1}{r} = \frac{2e^*}{\epsilon_m + \epsilon_i} \frac{1}{r}. \quad (7)$$

The two-dimensional Fourier transform of Eqs. (4) and (7) is

$$\phi(\mathbf{r}) = \frac{2\pi e^*}{A\epsilon_i} \sum_{\mathbf{q}} \frac{1}{q} e^{i\mathbf{q}\cdot\rho} (e^{-q|z-d|} - \lambda e^{-q|z+d|}). \quad (8)$$

For values of z near the surface, we write the above expression as

$$\begin{aligned} \phi(\mathbf{r}) = & \frac{2\pi e^*}{\epsilon_i A} \sum_{\mathbf{q}} \frac{1}{q} e^{i\mathbf{q}\cdot\rho} e^{-qd} [(e^{qz} - \lambda e^{-qz})\Theta(z) \\ & + (1 - \lambda)e^{gz}\Theta(-z)]. \end{aligned} \quad (9)$$

If $\lambda=1$ the potential vanishes at the point $z=0$. The dielectric function ϵ_m is generally a function of wave vector and frequency. Phonon frequencies are small compared to plasmon frequencies, so the frequency dependence can be ignored. For three-dimensional bulk systems, the dielectric function $\epsilon(q)$ is given by random-phase approximation (RPA) or something similar. For surfaces, the dependence is more complicated. In the two-dimensional transform listed above, we employ the two-dimensional response of an electron gas, which is $\epsilon_m(q) = 1 + 2/(qa_0)$, where a_0 is the Bohr radius.

Since the electrons are confined to the space $z < 0$, the potential in this region is taken to be

$$\phi(\mathbf{r}) = \frac{2\pi a_0 e^*}{A} \sum_{\mathbf{q}} u(q) e^{i\mathbf{q}\cdot\rho} e^{-q(d-z)}, \quad (10)$$

$$u(q) = \frac{2}{2 + qa_0(\epsilon_i + 1)}. \quad (11)$$

Equation (9) has the image contribution to $\phi(r)$ changing at the surface $z=0$. This change is actually due to a surface charge, which is not centered precisely at $z=0$ nor is a point charge. The nature of the image potential and image charge has been investigated in numerous references. Some of the earliest are Refs. 17–25. Their results are usually given as an integral equation or a graph. The simple form we use above is an interpolation of these results.

For electrons in a metal, the potential energy for scattering the electron from (\mathbf{k}, k_i) to $(\mathbf{k} + \mathbf{q}, k_f)$ is¹³

$$V_e(\mathbf{q}) = e \int d^3r \psi^*(\mathbf{k} + \mathbf{q}, k_f; \mathbf{r}) \delta\phi(\mathbf{r}) \psi(\mathbf{k}, k_i; \mathbf{r}), \quad (12)$$

$$\psi(\mathbf{k}, k_i; \mathbf{r}) = \sqrt{\frac{2}{\Omega}} e^{i\mathbf{k}\cdot\rho} \phi(k_i, z), \quad (13)$$

where (\mathbf{k}, \mathbf{q}) are two-dimensional wave vectors parallel to the surface, and (k_i, k_f) are the z component of the electron's wave vector. The metal has a volume $\Omega = AL_m$. For the infinite-barrier model, the eigenfunction is

$$\phi(k_i, z) = \sin(k_i z). \quad (14)$$

However, finite-barrier models provide a better description of physical systems.²⁶ When using Eq. (14), the matrix element contains a factor of

$$I_{if} = \int_{-\infty}^0 dz e^{qz} \sin(k_i z) \sin(k_f z) \quad (15)$$

$$= \frac{2qk_i k_f}{[q^2 + (k_i - k_f)^2][q^2 + (k_i + k_f)^2]}. \quad (16)$$

The transverse integral $d^2\rho$ in matrix element (12) forces conservation of parallel wave vector. The transverse wave vector \mathbf{q} of the phonon changes the transverse wave vector of the electron by this amount.

III. PHONONS IN THE INSULATOR

Since the metal is bonded to the insulator, the phonon normal modes in equilibrium involve all of the atoms in both systems. However, during heat flow, there exists a temperature difference between the two solids. Then the phonons in the insulator are at a different temperature from those in the metal. This situation cannot be described by using the normal modes of the combined system. Instead, one must assume that the normal modes in the metal are independent of those in the insulator, with a small coupling between them at the interface. That raises the question of how we set up the vibrational modes in the insulator: what boundary condition is applied at the interface? The answer to this question is presently unknown. Here we made a simple assumption that the modes are those of a freestanding slab of material. This assumption is based upon the feature that the image potential has a long range, so the details of the surface bonding are unimportant.

The phonon eigenfunctions are

$$\mathbf{Q}_j = \frac{1}{\sqrt{N_{\lambda\mathbf{q}q_z}}} \sum_{\lambda} X_{\ell}(\lambda, \mathbf{q}, q_z) e^{i\mathbf{q}\cdot\rho} A_{\lambda, \mathbf{q}, q_z} \sin(q_z z) \hat{\xi}_{\ell}(\lambda, \mathbf{q}, q_z), \quad (17)$$

$$X_{\ell}(\lambda, \mathbf{q}, q_z) = \sqrt{\frac{\hbar}{M_{\ell} \omega_{\lambda}(\mathbf{q}, q_z)}}, \quad (18)$$

$$A_{\lambda, \mathbf{q}, q_z} = a_{\lambda\mathbf{q}q_z} + a_{\lambda, -\mathbf{q}, q_z}^{\dagger}. \quad (19)$$

The summation over λ is over polarizations. The index ℓ indicates which atom in the unit cell.

The most general eigenfunction in the z direction might contain a phase shift: $\sin(q_z z + \delta)$. We have used the theorem

of Ridley²⁷ that the optical-phonon amplitudes vanish at the surface, to set $\delta=0$.

The phonons in the insulator contribute the following potential, for $z < 0$ and $Z_j > 0$:

$$\delta\phi(\mathbf{r}) = -\frac{2\pi a_0}{A} \sum_{\mathbf{q},j} e_j u(\mathbf{q}) e^{i\mathbf{q}\cdot(\mathbf{r}-\mathbf{R}_j)} [i\mathbf{q}\cdot\mathbf{Q}_j + qQ_{jz}] e^{q(z-Z_j)}.$$

We use the above expression for the ion displacements \mathbf{Q}_j and find

$$\delta\phi(\mathbf{r}) = -\frac{\pi a_0}{A_0 \sqrt{N}} \sum_{\ell,\lambda,\mathbf{q},q_z} e_\ell e^{i\mathbf{q}\cdot\mathbf{r}+qz} u(\mathbf{q}) [i\mathbf{q}\cdot\hat{\xi}_\ell + q\xi_{\ell z}] X_\ell(\lambda, \mathbf{q}, q_z) \times \Lambda(\mathbf{q}, q_z) A_{\lambda,\mathbf{q},q_z} \Theta(z), \quad (20)$$

$$\Lambda(\mathbf{q}, q_z) = 2 \sum_{z_j} e^{-qZ_j} \sin(q_z Z_j) = \frac{\sin(q_z a_z)}{\cosh(q a_z) - \cos(q_z a_z)}, \quad (21)$$

where a_z is the lattice spacing in the z direction.

The interaction between the electrons and the phonons in Eq. (12) is

$$V = \frac{1}{L_m \sqrt{N}} \sum_{\mathbf{k}, \mathbf{q}, k_f, \sigma} C_{\mathbf{k}+\mathbf{q}, k_f, \sigma}^\dagger C_{\mathbf{k}, k_f, \sigma} A_{\lambda, \mathbf{q}, q_z} M_\lambda(\mathbf{q}, k_f, k_i, q_z),$$

$$M_\lambda(\mathbf{q}, k_f, k_i, q_z) = -\frac{2\pi e a_0}{A_0} \sum_{\ell} e_\ell u(\mathbf{q}) X_\ell(\lambda, \mathbf{q}, q_z) \Lambda(\mathbf{q}, q_z) I_{if} \times (q, k_i, k_f) [i\mathbf{q}\cdot\hat{\xi}_\ell + q\xi_{\ell z}].$$

Transverse wave vector is conserved: the parallel wave vector \mathbf{q} of the phonon is transferred to the parallel wave vector of the electron.

IV. ENERGY TRANSFER

The energy transfer through the surface, in watts per area, is

$$J_Q = \frac{2\pi}{\hbar A L_m^2 N} \sum_{\lambda, \mathbf{k}, \mathbf{q}, k_i, k_f, q_z} |M_\lambda|^2 \hbar \omega_\lambda(\mathbf{q}, q_z) \Xi,$$

$$\Xi = \delta[\varepsilon(\mathbf{k}, k_i) - \varepsilon(\mathbf{k} + \mathbf{q}, k_f) - \hbar \omega(\mathbf{q}, q_z)] [f_k(1 - f_{k+q})(N_q + 1) - f_{k+q}(1 - f_k)N_q] - \delta[\varepsilon(\mathbf{k}, k_i) - \varepsilon(\mathbf{k} + \mathbf{q}, k_f) + \hbar \omega(\mathbf{q}, q_z)] \times [f_k(1 - f_{k+q})N_q - f_{k+q}(1 - f_k)(N_q + 1)], \quad (22)$$

where f_k are the electron occupation number, N_q is the phonon occupation number, and $\varepsilon(\mathbf{k}, k_i)$ is the band dispersion of the electrons. The expression for Ξ is familiar from earlier discussions of energy transfer between electron and phonon systems: see Ref. 28 for metals, Ref. 29 for semiconductors, and Ref. 10. The summations over states give

$$\sum_{\mathbf{k}, \mathbf{q}, k_i, k_f, q_z} = \frac{A L_m^2 \Omega}{2^4 \pi^7} \int d^2 k \int d^2 q \int dk_i \int dk_f \int dq_z. \quad (23)$$

The prefactor of $A L_m^2 \Omega$ cancel similar factors in the matrix elements, and the final energy current density is independent of these factors. The final expression is

$$J_Q = \frac{\Omega_0}{\hbar \pi^6 2^3} \int d^2 k \int d^2 q \int dk_i \int dk_f \int dq_z \sum_{\lambda} |M_\lambda|^2 \Xi, \quad (24)$$

where Ω_0 is the volume per ion in the polar material.

V. ELECTRONIC INTEGRAL

Expression (24) contains a seven-dimension integral. Four ($d^2 k dk_i dk_f$) are related to the electronic properties of the metal, and three ($d^2 q dq_z$) are related to phonons in the insulator. Here we evaluate the four integrals relating to the electronic model. We use the infinite-barrier model for the boundary condition. We assume a free-electron metal with a spherical Fermi surface, where k_F is the Fermi wave vector. Consider the following function $P(q)$:

$$P(q) = \int d^2 k \int dk_i \int dk_f |I_{if}|^2 \Xi. \quad (25)$$

Examine just the first term in Ξ . Let $W = \hbar \omega_\lambda(\mathbf{q}, q_z)$. The argument of the delta function of energy is

$$0 = \frac{\hbar^2}{2m} [k^2 + k_i^2 - (\mathbf{k} + \mathbf{q})^2 - k_f^2] - W \quad (26)$$

$$= -\frac{\hbar^2}{2m} [q^2 + 2qk \cos(\theta) + k_f^2 - k_i^2 + Q^2], \quad Q^2 = \frac{2m}{\hbar^2} W. \quad (27)$$

Write $d^2 k = k dk d\theta$ and the angular integral gives

$$\int_0^{2\pi} d\theta \delta(E) = \frac{4m}{\hbar^2} \frac{1}{[4q^2 k^2 - (q^2 + k_f^2 + Q^2 - k_i^2)^2]^{1/2}}. \quad (28)$$

Next do the integral $k dk = (m/\hbar^2) d\varepsilon(k)$. This integral is dominated by the occupation factors in the region near the Fermi surface, where

$$\int dE_i f(E_i) [1 - f(E_i - W)] = \frac{W}{e^{W/\beta_e} - 1} = W n_e(W). \quad (29)$$

For the rest of the integrand we set $k^2 = k_F^2 - k_i^2$. A similar derivation applies to the other three factors in Ξ . These steps bring us to the expression

$$P(q) = 2 \left(\frac{2m}{\hbar^2} \right)^2 W [n_p(W) - n_e(W)] \Phi, \quad (30)$$

$$\Phi = \int_0^{k_F} dk_i \int_0^{k_F} dk_f \frac{|I_{if}|^2}{[4q^2(k_F^2 - k_i^2) - (q^2 + k_f^2 + Q^2 - k_i^2)^2]^{1/2}}, \quad (31)$$

where the notations $n_{e,p}$ refer to the temperatures $T_{e,p}$ of electrons and phonons in the occupation factors. There is no heat current unless they are different: $T_e \neq T_p$. These steps are similar to those of Allen²⁸ in deriving the electron-phonon energy relaxation in metals.

We now drop the factor of Q^2 since this wave vector is much smaller than the others. We define new variables $s_i^2 = k_F^2 - k_i^2$ and $s_f^2 = k_F^2 - k_f^2$. The argument of the square root in the integral for $\Phi(q)$ can be written as

$$4q^2s_i^2 - (q^2 + s_i^2 - s_f^2)^2 = [q^2 - (s_i - s_f)^2][(s_i + s_f)^2 - q^2]. \quad (32)$$

There are limits on the q integral: $s_i + s_f \geq q \geq |s_i - s_f|$. Inserting the integral over dq into the definition of Φ gives the limits

$$\begin{aligned} & \int_0^{k_F} ds_i \int_0^{k_F} ds_f \int_{|s_i - s_f|}^{s_i + s_f} dq \\ &= \int_0^{k_F} dq \left[\int_0^{k_F - q} ds_i \int_{|s_i - q|}^{s_i + q} ds_f + \int_{k_F - q}^{k_F} ds_i \int_{|s_i - q|}^{k_F} ds_f \right] \end{aligned} \quad (33)$$

$$+ \int_{k_F}^{2k_F} dq \int_{q - k_F}^{k_F} ds_i \int_{q - s_i}^{k_F} ds_f. \quad (34)$$

The order of integration has been reversed to put $\int dq$ as the last integral. It is now removed from the definition of $\Phi(q)$. The above exercise was for deriving the correct limits on the two integrals in $\Phi(q)$. The integrand is

$$\Phi(q) = \int \frac{s_i s_f}{k_i k_f} ds_i ds_f \frac{|I_{if}|^2}{\sqrt{[q^2 - (s_i - s_f)^2][(s_i + s_f)^2 - q^2]}}. \quad (35)$$

Equation (16) has a prefactor of $k_i k_f$ that cancels the same factor in the denominator in the above expression. We change integration variables to $\alpha = (s_f - s_i)/k_F$ and $\beta = (s_f + s_i)/k_F$, and define $x = q/k_F$, $y_i = k_i/k_F$, and $y_f = k_f/k_F$. The factor of I_{if} is, in these new variables,

$$I_{if} = \frac{2y_i y_f x \tilde{I}_{if}}{k_F}, \quad (36)$$

$$\tilde{I}_{if} = \frac{1}{[x^2 + (y_-)^2][x^2 + (y_+)^2]}. \quad (37)$$

Next we define the dimensionless function $\bar{\Phi}(x)$,

$$\Phi(q) = \frac{1}{k_F^2} \bar{\Phi}(x). \quad (38)$$

Collecting the above results leads to the following:

(1) For $0 \leq x \leq 1$ the limits of integration are

$$\begin{aligned} \bar{\Phi}(x) &= \frac{x^2}{8} \int_{-x}^x d\alpha \int_x^{2-|\alpha|} d\beta \frac{|\tilde{I}_{if}|^2 (\beta^2 - \alpha^2)}{\sqrt{(x^2 - \alpha^2)(\beta^2 - x^2)}} \\ &\quad \times \sqrt{[4 - (\beta - \alpha)^2][4 - (\beta + \alpha)^2]}. \end{aligned}$$

(b) For $1 \leq x \leq 2$ the integral is

$$\begin{aligned} \bar{\Phi}(x) &= \frac{x^2}{8} \int_{x-2}^{2-x} d\alpha \int_x^{2-|\alpha|} d\beta \frac{|\tilde{I}_{if}|^2 (\beta^2 - \alpha^2)}{\sqrt{(x^2 - \alpha^2)(\beta^2 - x^2)}} \\ &\quad \times \sqrt{[4 - (\beta - \alpha)^2][4 - (\beta + \alpha)^2]}. \end{aligned}$$

The function $\bar{\Phi}(x)$ is dimensionless. For the range of values $0 < x < 1$ a numerical evaluation gives the approximate expression

$$x^2 \bar{\Phi}(x) \approx 0.22 - 0.17x \quad (39)$$

VI. PHONON INTEGRALS

We collect the above results to obtain

$$J_Q = D \int_0^{W_x} W dW G(W) [n_e(W) - n_p(W)], \quad (40)$$

$$D = \frac{24}{\pi^2} \frac{\hbar n_e}{M_{AMU} A_0^2}, \quad (41)$$

$$\begin{aligned} G(W) &= \frac{1}{k_F^5} \sum_{\lambda} \int_{q < 2k_F} d^2 q \tilde{\Phi}\left(\frac{q}{k_F}\right) u^2(q) \int dq_z \delta[W \\ &\quad - \hbar \omega_{\lambda}(\mathbf{q}, q_z)] \end{aligned} \quad (42)$$

$$\begin{aligned} &\times \left| \sum_{\ell} \frac{e_{\ell}}{e} \sqrt{\frac{M_{AMU}}{M_{\ell}}} \hat{\xi}_{\lambda, \ell} \cdot (q_x, q_y, iq) \right|^2 \\ &\times \frac{\sin^2(q_z a_z)}{[\cosh(q a_z) - \cos(q_z a_z)]^2}. \end{aligned} \quad (43)$$

The prefactor of D has the units of inverse area times seconds.

In the high-temperature limit, where $k_B T > W_x$, the occupation factors can be expanded,

$$[n_e(W) - n_p(W)] \approx \frac{k_B}{W} (T_e - T_p), \quad (44)$$

$$J_Q = \sigma (T_e - T_p), \quad \sigma = \sigma_0 \mathcal{I}, \quad (45)$$

$$\mathcal{I} = \int_0^{W_x} dW G(W), \quad (46)$$

$$\sigma_0 = k_B D = \sigma_{00} \frac{a_0 \Omega_0}{A_0^2}, \quad (47)$$

$$\sigma_{00} = \frac{24 k_B}{\pi^2} \frac{\hbar n_e}{M_{AMU} a_0}, \quad (48)$$

where a_0 is the Bohr radius. Using the electron density n_e of aluminum, the constant σ_{00} has the numerical value of $\sigma_{00} = 7.28$ GW/m² K, which is larger than the experimental data shown in Table I. However, \mathcal{I} is less than 1 because of several factors including the ion mass. The integral in Eq. (46) is

TABLE I. Room-temperature values of Kapitza conductance in units of MW/m² K. Data from Stoner and Maris (Ref. 7). Metals on top, and insulators on left.

	Al	Au	Pb
BaF ₂	100	40	62
Al ₂ O ₃	105	45	55
Diamond	46	40	31

dimensionless and does not contain the energy of the phonons,

$$\begin{aligned} \mathcal{I} = & \frac{1}{k_F^5} \sum_{\lambda} \int_{q < 2k_F} d^2 q \tilde{\Phi} \left(\frac{q}{k_F} \right) u(q)^2 \int dq_z \\ & \times \left| \sum_{\ell} \frac{e_{\ell}}{e} \sqrt{\frac{M_{AMU}}{M_{\ell}}} \hat{\xi}_{\lambda, \ell} \cdot (q_x, q_y, iq) \right|^2 \\ & \times \frac{\sin^2(q_z a_z)}{[\cosh(q a_z) - \cos(q_z a_z)]^2}. \end{aligned} \quad (49)$$

It is merely an integral over wave vectors in the Brillouin zone (BZ).

The only phonon part of the integral in Eq. (49) consists of displacement eigenvectors $\hat{\xi}_{\lambda, \ell, \mu}$ which depend upon the phonon mode λ (e.g., TA and LO), atom in the unit cell (ℓ), and vector component $\mu = (x, y, z)$. For a crystal with N_a atoms per unit cell, there are $3N_a$ values of λ . The polarization vectors obey the orthogonality relation

$$\sum_{\lambda=1}^{3N_a} \hat{\xi}_{\lambda, \ell, \mu} \hat{\xi}_{\lambda, \ell', \nu} = \delta_{\ell \ell'} \delta_{\mu \nu}. \quad (50)$$

In the formula for \mathcal{I} , the summation over λ eliminates all cross terms in the square of the matrix element,

$$\sum_{\lambda} \left| \sum_{\ell} \frac{e_{\ell}}{e} \sqrt{\frac{M_{AMU}}{M_{\ell}}} \hat{\xi}_{\lambda, \ell} \cdot (q_x, q_y, iq) \right|^2 \quad (51)$$

$$= \sum_{\lambda \ell} \left(\frac{e_{\ell}}{e} \right)^2 \frac{M_{AMU}}{M_{\ell}} [\xi_{\lambda, \ell, x}^2 q_x^2 + \xi_{\lambda, \ell, y}^2 q_y^2 + q^2 \xi_{\lambda, \ell, z}^2] \quad (52)$$

$$= \sum_{\ell} \left(\frac{e_{\ell}}{e} \right)^2 \frac{M_{AMU}}{M_{\ell}} [q_x^2 + q_y^2 + q^2] \quad (53)$$

TABLE II. Factors entering the Kapitza conductance at room temperature. Final column contains theoretical results in units of MW/m² K.

Crystal	a_l (Å)	e^*	$\varepsilon_l(\infty)$	x_0	$\tilde{\Lambda}$	σ
LiF	4.02	0.87	1.93	0.879	0.0072	100
NaF	4.62	0.93	1.75	0.765	0.0051	40
NaCl	5.64	0.74	2.35	0.626	0.0029	10

$$= 2q^2 \sum_{\ell} \left(\frac{e_{\ell}}{e} \right)^2 \frac{M_{AMU}}{M_{\ell}}. \quad (54)$$

For a binary crystal, where the anion and cation have equal and opposite Szigetzi charges³⁰ $e^* = e_{\ell}/e$, the result is given by the reduced mass μ of the two ions,

$$\begin{aligned} \mathcal{I} = & 2(e^*)^2 \frac{M_{AMU}}{\mu k_F^5} \int_{q < 2k_F} q^2 u(q)^2 d^2 q \tilde{\Phi} \left(\frac{q}{k_F} \right) \\ & \times \int dq_z \frac{\sin^2(q_z a_z)}{[\cosh(q a_z) - \cos(q_z a_z)]^2} = I_0 \tilde{\Lambda}, \end{aligned} \quad (55)$$

$$I_0 = 4\pi (e^*)^2 \frac{M_{AMU}}{\mu}, \quad (56)$$

$$\tilde{\Lambda} = \int_0^{x_0} x^3 u(x)^2 dx \tilde{\Phi}(x) \int_0^{z_0} dz \frac{\sin^2(zc)}{[\cosh(xc) - \cos(zc)]^2}, \quad (57)$$

$$c = k_F a_z, \quad z_0 = \sqrt{x_0^2 - x^2}. \quad (58)$$

The Fermi-surface restriction is that $x = q/k_F < 2$. The above integral is evaluated for aluminum, which has a very large value of k_F . Then the effective restriction on the integral over phonon wave vectors is that they should be confined to the Brillouin zone of the insulator since all these wave vectors in the BZ obey the constraint $q < 2k_F$. Since we do not know the orientation of the insulator, we do not know the projection of the BZ on the interface. So we made an approximate calculation by assuming that the BZ was a sphere, and the above integral is confined to a hemisphere. The sphere with the same volume as the BZ in rocksalt (fcc) lattices has a radius q_0 ,

$$x_0 = \frac{q_0}{k_F} = \frac{2\pi}{k_F a_l} \left(\frac{3}{\pi} \right)^{1/3}, \quad (59)$$

where a_l is the lattice constant. Table II shows results for three crystals with the sodium chloride structure. This case has the prefactor of

$$\frac{\Omega_0}{A_0^2} = \frac{1}{a_l}. \quad (60)$$

The theoretical prediction for σ varies from 100 to 10 MW/m² K. These results are similar to the experimental values in Table I. The values for σ become smaller as one goes down the column. This is partly due to: (1) the increase

in ion mass, (2) the smaller value of e^* , (3) the increase in lattice constant, and (4) the increase in the insulator dielectric constant $\varepsilon_i = \varepsilon(\infty)$. Note the strong dependence of $\tilde{\Lambda}(x_0)$. The insulators in Table I all have one ion mass that is light (C,O,F), which probably contributes to the large values found experimentally. The present theory gives a value of the Kapitza conductance in general agreement with the available experimental data.

VII. DISCUSSION

We present a theory of heat flow between the conduction electrons in a metal and the phonons in an insulator. We propose that these two systems interact through the surface charges caused by the image potential that the ions in the insulator make on the surface of the metal. When the ions vibrate, the surface charges oscillate, which provides direct coupling to the electrons in the metal. This interaction takes place only in the surface region, where the tails of the conduction electrons have a small region of overlap with the tail of the image potential.

We derived an analytic theory for this interaction. We also make an approximate evaluation of this Kapitza resistance for three alkali halide crystals. They were chosen because all parameters are known, and our theory has no adjustable parameters. The predicted thermal conductances are the same magnitude as found experimentally for more complex insulators. The theory predicts that the values of boundary conductance are independent of temperature above the Debye temperature of the insulator. This prediction agrees with the experiments.⁷

A better calculation of our theory requires knowledge of which crystal face of the metal is bonded to which crystal

face of the insulator. That information is presently lacking. Also, the surface charges can be treated better, with a non-zero width, which gives a slightly improved image potential in the surface region. Two-dimensional crystal surfaces have two-dimensional reciprocal-lattice vectors \mathbf{G}_j . An electron scattering from the surface can have its wave vector changed by one of these reciprocal-lattice vectors. Such processes are well known in photoemission and in low-energy electron diffraction. They can contribute to heat flow through the boundary since a phonon of parallel wave vector \mathbf{q} can scatter the parallel wave vector of the electron by $\mathbf{q} + \mathbf{G}$. These processes are not included here since we do not know which crystal faces are involved nor the matrix element for such scattering. For incommensurate surfaces, there are two sets of such reciprocal-lattice vectors: one for the metal and one for the insulator.

Most people tell us that diamond is not an ionic crystal, and should not be described by our theory. We agree that it is not an ionic crystal, but aver that it should be described by our theory. The standard bond polarizability model of group-IV elements, such as diamond and silicon, puts the bonding charges between the ions. When the ions vibrate, the bonding electrons stay midway between the ions. These electrons are polarizable. This model has positive ions and negative electrons, which are all that are needed for the present theory. Recently we applied this model³¹ to derive the infrared properties of graphite, another carbon compound. The fact that the experimental values for diamond are the same magnitude as those for the ionic materials suggests they have a common theory. Solid argon is an example of a crystal that is not described by the present theory. We hope to derive a theory for it, based on Eq. (2), in the near future.

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