Lattice-dynamical calculation of the Kapitza resistance between fcc lattices

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The temperature dependence of the Kapitza resistance (thermal boundary resistance) at the interface between two dissimilar solids is calculated for a model system consisting of two semi-infinite, harmonic fcc lattices in register. The spectral density of phonon flux transmitted across the interface is obtained from a numerical calculation of the phonon transmission coefficient and group velocity and is used to calculate the Kapitza resistance. Results for the spectral density of the transmitted phonon flux, the spectral dependence of the phonon transmission coefficient, and the temperature dependence of the thermal boundary resistance are presented. Calculation of the thermal boundary resistance for real systems using the results of this calculation is discussed.

I. INTRODUCTION

New techniques have recently made possible measurements[1,2] of the temperature dependence of the Kapitza resistance at temperatures up to room temperature. It has long been understood[3] that the Kapitza resistance between two dissimilar materials is due to the reflection of phonons at the interface. In the past, most investigations of the Kapitza resistance were concerned with the interface between a solid and liquid helium or with the interface between two solids at low temperatures. Since thermal phonons at low temperatures are long-wavelength acoustic phonons, nearly all theoretical work in the field[4–10] has employed a continuum mechanical model to calculate the reflection of these phonons at the interface. This model, the acoustic-mismatch model, gives the transmission coefficient at the interface for long-wavelength acoustic phonons in terms of the acoustic properties of the two materials on either side of the interface. Unfortunately, the acoustic-mismatch model does not account for phonon dispersion, the cutoff in the phonon density of states for high frequencies, or weak bonding at the interface. To account for these effects it is necessary to use a lattice model to describe phonon propagation in the two lattices and transmission across the interface between them. Lattice model calculations have been performed for one-dimensional[11,12] and two-dimensional[13] lattices of masses and springs but it is difficult to infer propagation behavior in three-dimensional solids from these results.

In this paper we present a calculation of phonon transmission and the Kapitza conductance at the interface between two semi-infinite fcc lattices which have different masses and spring constants. The interatomic forces are taken to be nearest-neighbor central forces. A description of the model is given in Sec. II and equations of motion are derived in a convenient form. Expressions for the transmission coefficient and Kapitza conductance are developed in Sec. III, followed by a brief outline of the numerical algorithm used to evaluate these quantities. In Sec. IV we present the numerical results for the transmission coefficient as a function of frequency and the Kapitza conductance as a function of temperature.

II. MODEL

The model we consider is two fcc lattices (lattice A and lattice B) divided by an interface between two adjacent (001) planes of atoms. The relative position of adjacent atoms on opposite sides of the interface preserves the fcc structure. In lattice A, atoms of mass M are connected to their 12 nearest neighbors by springs of stiffness K, and in lattice B, atoms of mass M' are connected to their 12 nearest neighbors by springs of stiffness K'. Nearest-neighbor atoms on opposite sides of the interface are connected by springs of stiffness K''. Atoms lying in a plane perpendicular to the interface are shown in Fig. 1. The spacing between nearest neighbors is $a\sqrt{2}$.

A. Equations of motion

We define $\mathbf{u}_{lmn}$ to be the displacement from equilibrium of the atom with equilibrium position $\mathbf{r}_{lmn}=(la,ma,na)$ in the lattice. The definition of the lattice constant a is indicated in Fig. 1, and l,m,n are integers whose sum is even. The equation of motion for the atom lmn (assumed to be an atom away from the interface in lattice A) is

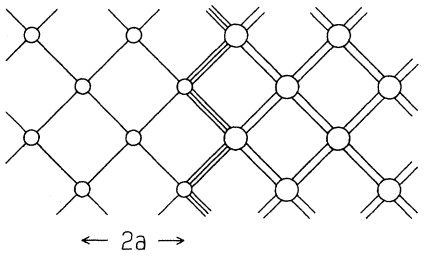

FIG. 1. Atoms lying in a plane perpendicular to the interface. Small atoms of mass M are connected to each other by springs of stiffness K (single lines). Large atoms of mass M' are connected by springs of stiffness K' (double lines). Atoms on opposite sides of the interface are connected by springs of stiffness K'' (triple lines).

$$M\ddot{u}^x_{lmn}=K/2(u^x_{l+1,m+1,n}+u^x_{l+1,m,n+1}+u^x_{l+1,m-1,n}+u^x_{l+1,m,n-1}+u^x_{l-1,m+1,n}$$
$$+u^x_{l-1,m,n+1}+u^x_{l-1,m-1,n}+u^x_{l-1,m,n-1}-8u^x_{lmn}$$
$$+u^y_{l+1,m+1,n}-u^y_{l+1,m-1,n}+u^y_{l-1,m-1,n}-u^y_{l-1,m+1,n}+u^z_{l+1,m,n+1}-u^z_{l+1,m,n-1}$$
$$+u^z_{l-1,m,n-1}-u^z_{l-1,n,m+1}) . \tag{1}$$

The equations for $\ddot{u}^y_{lmn}$ and $\ddot{u}^z_{lmn}$ are obtained by cyclic permutation of the subscripts and the superscript in Eq. (1). Solutions to these equations are of the form

$$u^\alpha_{lmn}=e_\alpha \exp i(\mathbf{k}\cdot\mathbf{r}_{lmn}-\omega t) , \tag{2}$$

where e_α is the α component of the polarization vector $\mathbf{e}$ of the wave and $\mathbf{k}$ is the wave vector. Substitution of Eq. (2) into Eq. (1) yields

$$\underline{D}\mathbf{e}=\omega^2\mathbf{e} . \tag{3}$$

where the elements of the dynamical matrix $\underline{D}$ are

$$D_{11}=\frac{K}{2M}\{8-\exp[i(k_x+k_y)a]-\exp[-i(k_x+k_y)a]-\exp[i(k_x-k_y)a]-\exp[-i(k_x-k_y)a]$$
$$-\exp[i(k_x+k_z)a]-\exp[-i(k_x+k_z)a]-\exp[i(k_x-k_z)a]-\exp[-i(k_x-k_z)a]\} ,$$
$$D_{12}=\frac{K}{2M}\{-\exp[i(k_x+k_y)a]-\exp[-i(k_x+k_y)a]+\exp[i(k_x-k_y)a]+\exp[-i(k_x-k_y)a]\} . \tag{4}$$

The other elements are given by permutation. The condition that Eq. (3) have a solution is that the determinant of the coefficients vanish

$$|\underline{D}-\omega^2\underline{I}|=0 . \tag{5}$$

This equation, the secular determinant, is a third-degree polynomial in ω^2 which, for a given value of the wave vector $\mathbf{k}$ can be solved algebraically for the three roots in ω^2. On the other hand, given a value of ω^2 and any two components of the wave-vector $\mathbf{k}$, Eq. (5) in its present form must be solved numerically for the third component of the wave vector. Solving the equation for the secular determinant in this situation is a necessary part of the calculations which will follow. Since numerical solution of Eq. (5) is difficult in a significant fraction of cases and requires a large amount of computation time, we transform Eq. (5) to a form which can be solved algebraically.

The desired transformation is more or less obvious if we expand the determinant in Eq. (5) using the explicit form of the elements $\underline{D}_{ij}$ found in Eq. (4). First we note that this expression is unchanged when any or all components of the wave vector $\mathbf{k}$ are replaced by their negative value. Next, multiplying this expression for the determinant by $\exp[3ia(k_x+k_y+k_z)]$ produces a function which can be regarded as a sixth-degree polynomial in $\exp(ik_za)$. Hence we may write Eq. (5) in the form

$$\prod_{l=1}^{6}[\exp(ik_za)-\exp(ik_{zl}a)]=0 , \tag{6}$$

where each of the k_{zl} for $l=1,\ldots,6$ is one of the roots of the determinant for a particular set of values of ω^2, k_x, and k_y. For each root k_{zl} there must be a corresponding root $k_{zl'}=-k_{zl}$. This allows us to write Eq. (6) in the form

$$\prod_{l=1}^{3}[\cos(k_za)-\cos(k_{zl}a)]=0 . \tag{7}$$

Thus we have converted a sixth-degree polynomial into a third-degree polynomial, each of whose roots yields two roots of the original sixth-degree polynomial.

To carry out this transformation we define

$$X=2\cos(k_xa), \quad Y=2\cos(k_ya), \quad Z=2\cos(k_za) , \tag{8}$$

and

$$\Omega=(2M\omega^2/K)-8 . \tag{9}$$

After some algebra, Eq. (5) can then be written in the form

$$[4(X+Y)]Z^3+[(8+3XY)\Omega+8XY+32-8(X^2+Y^2)+4X^2Y^2]Z^2$$
$$+[2(X+Y)\Omega^2+3XY(X+Y)\Omega+8XY(X+Y)+4(X^3+Y^3)-32(X+Y)]Z$$
$$+[\Omega^3+2XY\Omega^2+8(X^2+Y^2-6)\Omega+4(X^2+Y^2)XY-32XY+32(X^2+Y^2)-8X^2Y^2-128]=0 . \tag{10}$$

For given k_x, k_y, and ω, Eq. (10) can be solved to give three roots for Z, and, therefore, the six solutions for the $\{k_{zl}\}$. In the calculations we also need to find the phonon frequencies for given k_x, k_y, and k_z. To do this we rearrange Eq. (10) as a cubic polynomial in Ω,

$$\Omega^3+C_2\Omega^2+C_1\Omega+C_0=0 . \tag{11}$$

The coefficients C_0, C_1, and C_2 are

$$
\begin{aligned}
C_0 &= 4(XYZ)^2+4(X^2+Y^2)(XY-Z^2) \\
&\quad +4(Y^2+Z^2)(YZ-X^2) \\
&\quad +4(Z^2+X^2)(ZX-Y^2)+32(X^2+Y^2+Z^2) \\
&\quad -32(XY+YZ+ZX)+8(X+Y+Z)XYZ-128 , \\
C_1 &= 3(X+Y+Z)XYZ+8(X^2+Y^2+Z^2)-48 , \qquad (12) \\
C_2 &= 2(XY+YZ+ZX) .
\end{aligned}
$$

The roots of Eq. (11) for Ω can then be used to obtain the phonon frequencies from Eq. (9). We may also derive a simple expression for the group velocity in terms of these transformed variables. The z component of the group velocity is

$$
v_z = \frac{\partial\omega}{\partial Z}\frac{dZ}{dk_z} = -\frac{Ka}{2M\omega}\frac{\partial\Omega}{\partial Z}\sin(k_z a) \qquad (13)
$$

and implicit differentiation of Eq. (11) yields

$$
v_z = \frac{Ka}{2M\omega}\left[\left\{\Omega^2\frac{\partial C_2}{\partial Z}+\Omega\frac{\partial C_1}{\partial Z}+\frac{\partial C_0}{\partial Z}\right\}\Big/(3\Omega^2+2C_2\Omega+C_1)\right]\sin(k_z a) . \qquad (14)
$$

Analogous expressions for the x and y component of the group velocity are obtained in the same way.

B. Boundary conditions

To calculate the phonon transmission coefficients we have to apply boundary conditions at the interface between the two lattices. We consider an incident phonon of wave-vector $\mathbf{k}^{(0)}$, frequency ω, polarization $\mathbf{e}^{(0)}$, and amplitude A_0. The reflected phonons have wave-vectors $\mathbf{k}^{(1)}$, $\mathbf{k}^{(2)}$, $\mathbf{k}^{(3)}$, and the transmitted phonons have wave-vectors $\mathbf{k}^{(4)}$, $\mathbf{k}^{(5)}$, $\mathbf{k}^{(6)}$. The displacements of atoms in lattice A are then given by

$$
u^{\alpha}_{lmn} = \sum_{p=0}^{3} A_p e^{(p)}_{\alpha}\exp i(\mathbf{k}^{(p)}\cdot\mathbf{r}_{lmn}-\omega t) . \qquad (15)
$$

In lattice B the displacement of the atom (l,m,n) in direction α is

$$
w^{\alpha}_{lmn} = \sum_{p=4}^{6} A_p e^{(p)}_{\alpha}\exp i(\mathbf{k}^{(p)}\cdot\mathbf{r}_{lmn}-\omega t) . \qquad (16)
$$

The boundary conditions are obtained by considering the equations of motion of the atoms in lattices A and B immediately adjacent to the interface. Because of the translational invariance parallel to the interface, it is sufficient to consider the motion of just one atom on each side of the boundary. For convenience, we choose the origin of coordinates to be at the position of an atom in lattice A which is next to the interface. The equation of motion for the x component of the displacement of this atom is similar to Eq. (1), except for the replacement of some springs of strength K by K'',

$$
\begin{aligned}
M\ddot{u}^{x}_{000} &= (K/2)(u^{x}_{1,1,0}+u^{x}_{-1,1,0}+u^{x}_{1,0,-1}+u^{x}_{1,-1,0}+u^{x}_{-1,-1,0}+u^{x}_{-1,0,-1} \\
&\quad +u^{y}_{1,1,0}-u^{y}_{1,-1,0}+u^{y}_{-1,-1,0}-u^{y}_{-1,1,0}-u^{z}_{1,0,-1}+u^{z}_{-1,0,-1}-6u^{x}_{000}) \\
&\quad +(K''/2)(u^{x}_{-1,0,1}+u^{x}_{1,0,1}-u^{z}_{-1,0,1}+u^{z}_{1,0,1}-2u^{x}_{000}) . \qquad (17)
\end{aligned}
$$

The equation for the other two components of $\mathbf{u}_{000}$, and the equations of motion for an atom next to the interface in lattice B follow in a similar way.

Substitution of Eqs. (15) and (16) into Eq. (17) yields one of the six boundary conditions for the amplitudes A_p; the other five are obtained from the equations for u^{y}_{000}, u^{z}_{000}, and for the atom in lattice B. The six equations are expressed in matrix form as

$$
\sum_{q=1}^{6} M_{pq}A_q = M_{p0}A_0 . \qquad (18)
$$

The coefficients M_{pq} are given in the Appendix.

III. CALCULATIONS

The analysis of heat flow across the interface in our model system and the connection with real systems requires information about the density of states and the Debye temperature. The density of phonon states $D(\omega)$ per unit volume is given by

$$
D(\omega) = \frac{1}{V}\sum_{\mathbf{k},j}\delta(\omega-\omega(\mathbf{k},j)) , \qquad (19)
$$

where V is the volume, and the sum is over all wave-vectors $\mathbf{k}$ in the first Brillouin zone and over all polarizations j. The histogram in Fig. 2 is an approximation of

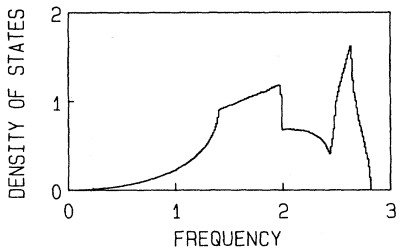

FIG. 2. Density of states per volume a^3 for a fcc lattice with masses $M=1$, spring constants $K=1$.

$D(\omega)$ obtained by summing over one million random uniformly distributed wave vectors in the first Brillouin zone. The density of states histogram in Fig. 2 is for spring constant $K=1$ and mass $M=1$. For a different spring constant K' and mass M' the density of states extends over a frequency range $\sqrt{K'/M'}$ times as large and accordingly has $\sqrt{K'/M'}$ times fewer states in a unit frequency range. The lattice model with nearest-neighbor central forces that we have used gives a phonon density of states qualitatively similar to the density of states determined experimentally for several fcc metals, e.g., aluminum[14] and copper.[15]

We now relate the phonon spectrum of the model to the Debye phonon spectrum. This will provide means by which we can associate the properties of real solids with the lattices used in this model. Each branch of the phonon spectrum is replaced by the same linear dispersion relation $\omega=kc$, with a maximum value of the magnitude of the wave vector $k=k_D$ for each branch. Equating the volume $4(\pi/a)^3$ of the first Brillouin zone for our model crystal to the equivalent reciprocal space volume $4\pi k_D^3/3$ in the Debye model we obtain $\omega_D=(3\pi^2)^{1/3}ac_D$. The velocity c_D is given by

$$c_D=(\langle c_1^{-3}+c_2^{-3}+c_3^{-3}\rangle/3)^{1/3}, \tag{20}$$

where c_1,c_2,c_3 are the sound velocities of the three polarizations and $\langle\ \rangle$ denotes an angular average. We obtain $c_D=0.9584(Ka^2/M)^{1/2}$, and therefore a Debye frequency $\omega_D=2.965\sqrt{K/M}$, and a Debye temperature $\Theta_D=2.965(\hbar/k_B)\sqrt{K/M}$.

The Kapitza conductance $\sigma(T)$ at temperature T is the ratio of the heat flow across the interface per unit area per unit time to the temperature difference across the interface. We may calculate this quantity by first considering the heat flow across the interface per unit time $\dot{Q}(T,T')$ when the temperatures of the two lattices are T and T'. This is given by

$$\dot{Q}(T,T')=\frac{S_0}{V}\left[\sum_{\mathbf{k},j}{}^{+}\hbar\omega(\mathbf{k},j)n(\omega(\mathbf{k},j),T)v_z(\mathbf{k},j)t(\mathbf{k},j)+\sum_{\mathbf{k}',j'}{}^{-}\hbar\omega(\mathbf{k}',j')n(\omega(\mathbf{k}',j'),T')v_z(\mathbf{k}',j')t(\mathbf{k}',j')\right]. \tag{21}$$

The first sum $\sum^+$ is over phonons incident on the interface from lattice A and the second sum $\sum^-$ is over phonons which are incident on the interface from lattice B, i.e., in each lattice only phonons with group velocity directed towards the interface are to be included in the sum. S_0 is the area of the interface. Each term in the sums is the product of the energy $\hbar\omega$ of the incident phonon, the transmission coefficient t, the component of the velocity normal to the interface v_z, and the Bose-Einstein number density n.

If both lattices are at the same temperature there can be no net flow of heat across the interface. Therefore, the two sums in Eq. (21) must be equal for $T=T'$, and this must be true for all temperatures $T=T'$. We conclude that there can be no net flow of heat due to phonons of a given frequency ω, and hence,

$$F(\omega)=\frac{1}{V}\sum_{\mathbf{k},j}{}^{+}v_z(\mathbf{k},j)t(\mathbf{k},j)\delta(\omega-\omega(\mathbf{k},j))$$
$$=-\frac{1}{V}\sum_{\mathbf{k}',j'}{}^{-}v_z(\mathbf{k}',j')t(\mathbf{k}',j')\delta(\omega-\omega(\mathbf{k}',j'))\,. \tag{22}$$

These sums are over wave-vectors $\mathbf{k}$ and polarizations j which correspond to a wave traveling toward the interface. We call $F(\omega)$ the transmission spectral density.

It is useful to define an average value of the z component of the velocity $\langle v_z(\omega)\rangle$ for phonons of frequency ω.

$$\langle v_z(\omega)\rangle=\frac{2}{VD(\omega)}\sum_{\mathbf{k},j}{}^{+}v_z(\mathbf{k},j)\delta(\omega-\omega(\mathbf{k},j))\,. \tag{23}$$

The factor of 2 is included because the sum $\sum^+$ includes only half of the wave vectors in the Brillouin zone. Similarly we define $\langle t(\omega)\rangle$, the average transmission coefficient for incident phonons of frequency ω,

$$\langle t(\omega)\rangle=\frac{1}{VD(\omega)\langle v_z(\omega)\rangle}\times\sum_{\mathbf{k},j}{}^{+}v_z(\mathbf{k},j)t(\mathbf{k},j)\delta(\omega-\omega(\mathbf{k},j))\,, \tag{24}$$

where the sum is over wave vectors $\mathbf{k}$ and polarizations j which correspond to a wave traveling toward the interface.

Using the definition of $F(\omega)$, Eq. (21) can be written in the form

$$\dot{Q}(T,T')=S_0\int_0^\infty[n(\omega,T)-n(\omega,T')]\hbar\omega F(\omega)d\omega \tag{25}$$

and, hence, the Kapitza conductance is

$$\sigma(T)=\frac{\dot{Q}(T,T+\Delta T)}{S_0\Delta T}$$
$$=\int_0^\infty\frac{\partial n(\omega,T)}{\partial T}\hbar\omega F(\omega)d\omega\,. \tag{26}$$

The Kapitza conductance $\sigma(T)$ can be written in a more illuminating form using the definitions of $\langle v_z(\omega)\rangle$ and $\langle t(\omega)\rangle$. We find

$$\sigma(T)=\tfrac{1}{2}\int_0^\infty C(\omega,T)\langle v_z(\omega)\rangle\langle t(\omega)\rangle d\omega\,, \tag{27}$$

where $C(\omega,T)=D(\omega)\hbar\omega\,\partial n(\omega,T)/\partial T$ is the specific heat per unit volume of the phonons of frequency ω.

A brief outline of the calculation of $F(\omega)$, which is used in Eq. (26) to calculate $\sigma(T)$, is as follows. We approximate the sum for $F(\omega)$ using a large number of random, uniformly distributed wave vectors in the first Brillouin zone. For each wave vector $\mathbf{k}$ and each polarization j in the sum, we use the secular determinant [Eq. (11)] to determine the frequency $\omega(\mathbf{k},j)$ for the incident wave and hence for the reflected and transmitted waves. The six wave vectors (three each for the reflected and

transmitted waves) needed to calculate the transmission coefficient $t(\mathbf{k},j)$ are determined by solving the secular determinant [Eq. (10)] subject to two requirements. First, the component of each wave vector parallel to the interface (k_x and k_y) must be equal to the component of the incident-wave wave vector parallel to the interface. This requirement allows six reflected-wave wave vectors and six transmitted-wave wave vectors. Using Eq. (14) to calculate the velocity for these waves, the six allowed wave vectors in each case are reduced to three by choosing those wave vectors which correspond to waves propagating away from the interface or which are exponentially small far from the interface. Having determined the allowed wave vectors for the reflected and transmitted waves, the polarization vector is calculated for each wave using Eq. (3) and then the boundary conditions are applied to determine the relative amplitude of each wave. From the amplitude and velocity of each wave we obtain the energy flux and thus the transmission coefficient t, which is the ratio of the transmitted energy flux to the incident energy flux. For each wave vector, the calculation is checked for accuracy by summing the total amount of flux leaving the surface in the form of reflected and transmitted waves and comparing it to the total amount of flux incident on the surface in the form of the incident wave.

Histograms of the function $F(\omega)$ are produced by dividing the interval between zero and the maximum frequency supported in the lattice into 100 equal size bins. As we sum over wave vectors, the results for $v_z(\mathbf{k},j)t(\mathbf{k},j)$ in each case are accumulated in the appropriate bins.

IV. RESULTS AND DISCUSSION

A. Transmission spectral density

We have calculated the transmission spectral density $F(\omega)$ [Eq. (22)] for a broad range of combinations of springs and masses in the two lattices.[16] Histograms of these results, which were obtained by approximating the sum for $F(\omega)$ using at least 10 000 random, uniformly distributed wave vectors in the first Brillouin zone, are shown in Figs. 3–5. In these calculations the lattice parameter a is equal to 1. For each of these histograms, lattice A has springs K and masses M equal to 1. The spring constant K' in lattice B ranges from 0.5 to 16.0 as indicated in the figures, while the masses M' in lattice B are 0.5, 1.0, and 2.0 in Figs. 3, 4, and 5, respectively. The interface spring constant K'' is $(K+K')/2$ in all cases.

We have verified by direct calculation that detailed balance holds, i.e., that the alternative expressions for $F(\omega)$ in Eqs. (22) (involving sums over $\mathbf{k},j$ and $\mathbf{k}',j'$) give the same results. Equation (22) lead to a further symmetry property of $F(\omega)$. Since F has dimensions length^{-2} we must be able to write it in the form

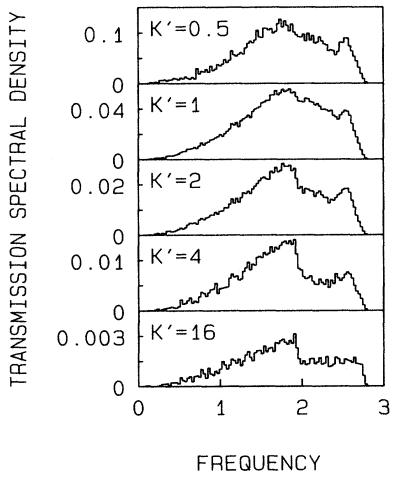

FIG. 3. Transmission spectral density $F(\omega)$ [Eq. (22)] across the interface between a lattice with $K=1, M=1$ and several lattices with $M'=0.5$. The interface springs K'' are in each case equal to $(K+K')/2$, and the lattice parameter $a=1$.

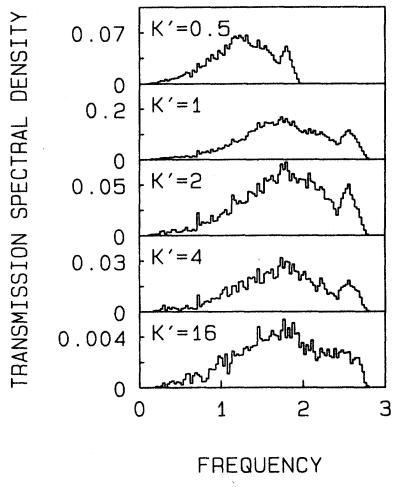

FIG. 4. Transmission spectral density as in Fig. 3 but with $M'=1$.

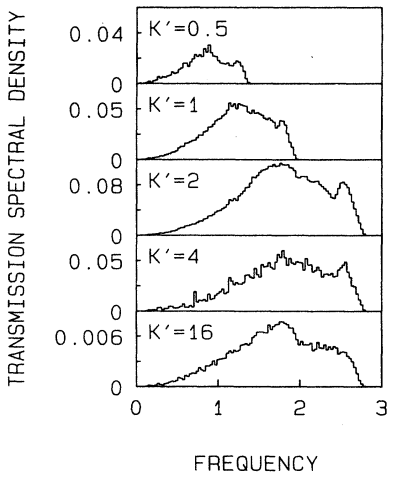

FIG. 5. Transmission spectral density as in Fig. 3 but with $M'=2$.

$$F(\omega)=f\left[\frac{M'}{M},\frac{K'}{K},\frac{\omega}{\omega_D}\right]\Big/a^2 \tag{28}$$

involving the dimensionless function f of three dimensionless variables. Thus, from Eq. (22) we have the symmetry condition

$$f\left[\frac{M'}{M},\frac{K'}{K},\frac{\omega}{\omega_D}\right]=f\left[\frac{M}{M'},\frac{K}{K'},\frac{\omega}{\omega_D'}\right]. \tag{29}$$

The transmission spectral density between two lattices with the same masses and spring constants is included in Fig. 4 (histogram with $K'=1$). Of course, for all frequencies this $F(\omega)$ is larger than the $F(\omega)$ between any pair of lattices in which either or both the masses or springs are different. For a given ratio M'/M of the masses the maximum transmission across the interface occurs when the ratio of the spring constants is approximately

$$\frac{K'}{K}=\frac{M'}{M}. \tag{30}$$

For this ratio of spring constants the maximum phonon frequency and the phonon density of states in the two lattices is the same, and so this condition is not surprising. The significance of the density of states is confirmed by looking at further details in Figs. 3–5. Consider, for example, the results for $K'=1,M'=0.5$ (Fig. 3), $K'=2,M'=1$ (Fig. 4), and $K'=4,M'=2$ (Fig. 5). In each of these three cases lattice B has the same phonon density of states, and the transmission spectral densities are very similar both in magnitude and frequency-dependence. The set $K'=0.5,M'=0.5$ (Fig. 3), $K'=1,M'=1$ (Fig. 4), and $K'=2,M'=2$ (Fig. 5) also have the same density of states. The frequency dependence of $F(\omega)$ is very similar for these three sets of parameters, but the magnitude of $F(\omega)$ is much larger for the case $K'=1,M'=1$ since then the lattices are perfectly matched. Note that the pair $K'=0.5,M'=0.5$ and $K'=2,M'=2$ should have exactly the same $F(\omega)$ [see Eqs. (28) and (29)], and this is indeed the case to within the statistical accuracy of the calculation.

The phonon density of states $D(\omega)$ contains van Hove singularities at critical frequencies ω_c (Fig. 2). These arise from phonons whose group velocity is zero. $F(\omega)$ shows weaker singularities. Clearly, this is because relative to $D(\omega)$ it contains in the summation over $\mathbf{k}$ the component $v_z(\mathbf{k},j)$ of the group velocity normal to the surface which vanishes for those phonons that give rise to the singularities.

B. Phonon transmission coefficient

Using Eq. (24), we have calculated $\langle t(\omega)\rangle$ for phonons going from a lattice with $K=1$ and $M=1$ into other lattices. Results for $M'=0.5$, 1, and 2 are shown in Figs. 6, 7, and 8, respectively. The springs K' are as indicated in the figures and the interface springs K'' are $(K+K')/2$. From these figures we see that for most combinations of springs and masses in the two lattices the transmission coefficient is approximately independent of frequency. (The large fluctuations in the transmission coefficient that occur at low frequencies are not significant, and arise because of the relatively small number of low-frequency phonons which leads to poor statistical averaging at these frequencies.) This approximate constancy of $\langle t(\omega)\rangle$ is particularly remarkable when one considers that the incident flux is predominantly from transverse phonons at low frequencies, and entirely from longitudinal phonons at the highest frequencies.

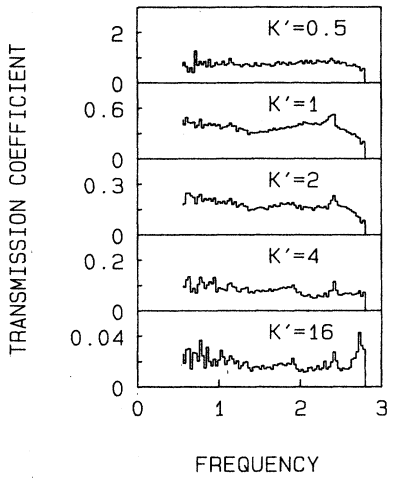

FIG. 6. Average phonon transmission coefficient $\langle t(\omega)\rangle$ as a function of frequency for phonons incident on an interface between a lattice with $K=1,M=1$ and several lattices with $M'=0.5$. The interface springs K'' are in each case equal to $(K+K')/2$.

The transmission coefficient has a large frequency dependence when the maximum frequency in lattice B is less than that in lattice A, i.e., when $K'/M'<K/M$. In these cases $\langle t(\omega)\rangle$ is zero above the cutoff frequency $\omega_{\max}=\sqrt{8K'/M'}$, and below this frequency is a rapidly decreasing functions of ω.

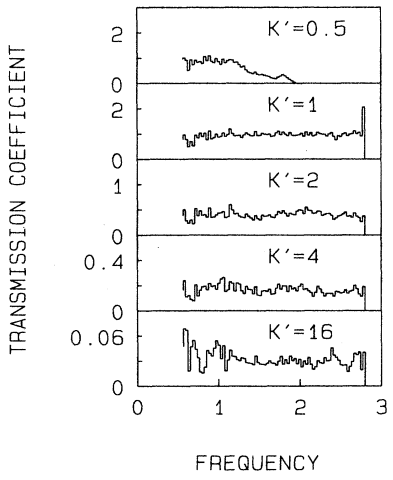

FIG. 7. Average phonon transmission coefficient $\langle t(\omega)\rangle$ as in Fig. 6 but with $M'=1$.

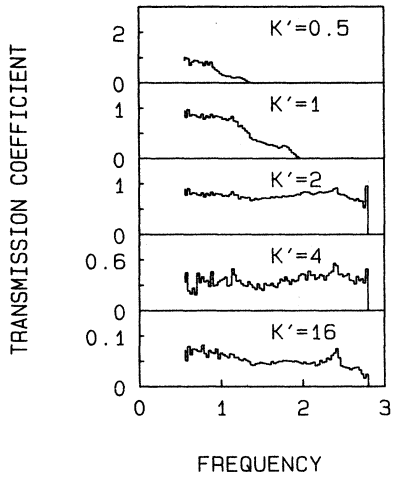

FIG. 8. Average phonon transmission coefficient $\langle t(\omega)\rangle$ as in Fig. 6 but with $M'=2$.

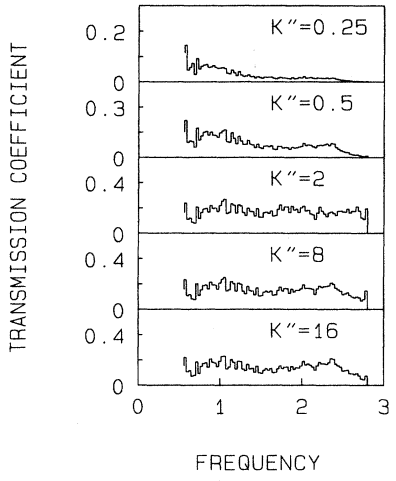

FIG. 10. Average phonon transmission coefficient $\langle t(\omega)\rangle$ as in Fig. 9. The interface springs are as indicated.

C. Effect of varying the interface spring constant

The results presented so far have all been obtained using an interface spring constant K'' equal to the average value of the spring constant in either lattice. Calculating the transmission spectral density for other values of K'', we find no appreciable difference in the results provided that K'' lies in the range between K and K'. This is demonstrated in Fig. 9 where we show $\langle t(\omega)\rangle$ for the values $K=1$, $M=1$, $K'=4$, $M'=1$, with K'' taking five values between K and K'.

If K'' is outside this range there can be a significant reduction in the transmission spectral density and the phonon transmission coefficient. If the interface spring is much stronger than the springs in either lattice we find that the transmission is reduced only slightly, with the greatest reduction at high frequencies. An example of this is shown in Fig. 10 ($K=1$, $M=1$, $K'=4$, $M'=1$) for $K''=16$. One can understand the reason for the fairly small reduction for large K'' by considering the limiting case of $K''\rightarrow\infty$. Then, at least for phonons at normal incidence to the interface, it is straightforward to see that the effect of the change in the interface springs results, in effect, in a plane of atoms at the interface each with mass equal to the sum of the masses in the two lattices. This plane of atoms is connected to atoms in lattices A and B by springs of strength K and K', respectively. The reduction in flux due to this plane of heavier atoms is not large.

For K'' less than the smaller of K and K' the transmission is also reduced, and clearly as $K''\rightarrow 0$ the transmis-

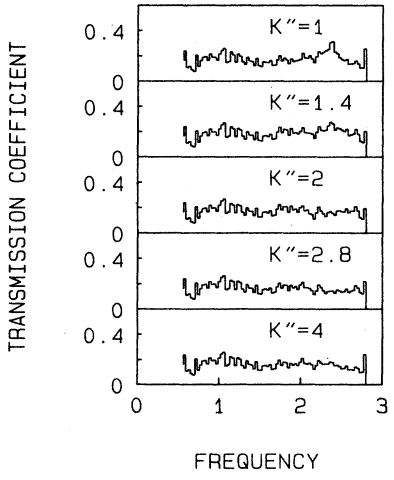

FIG. 9. Average phonon transmission coefficient $\langle t(\omega)\rangle$ as a function of frequency for phonons incident on an interface between a lattice with $K=1, M=1$ and a lattice with $K'=4$, $M'=1$. The interface springs are as indicated.

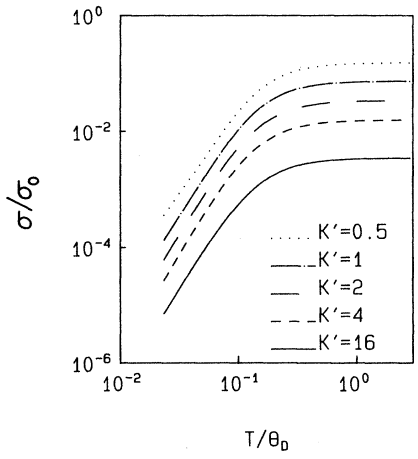

FIG. 11. Kapitza conductance σ divided by σ_0 as a function of T/Θ_D at an interface between a lattice with $K=1$, $M=1$ and several lattices with $M'=0.5$.

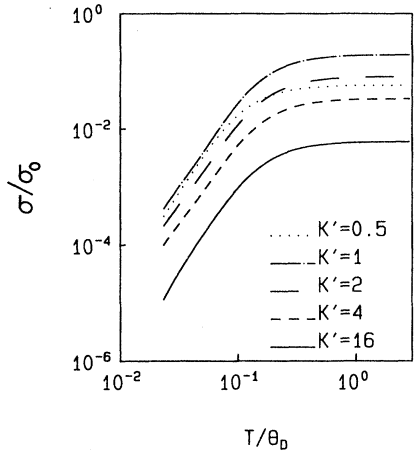

FIG. 12. Kapitza conductance σ divided by σ_0 as a function of T/Θ_D at an interface between a lattice with $K=1, M=1$ and several lattices with $M'=1$.

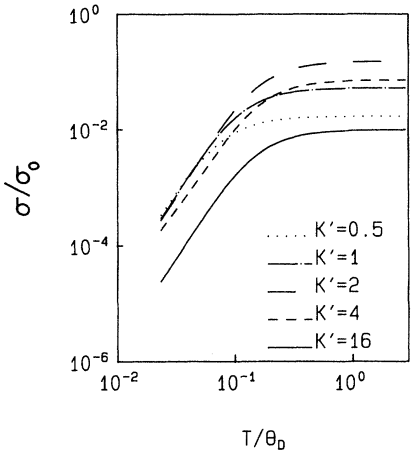

FIG. 13. Kapitza conductance σ divided by σ_0 as a function of T/Θ_D at an interface between a lattice with $K=1, M=1$ and several lattices with $M'=2$.

sion must tend to zero, presumably as K''^2. As can be seen from Fig. 10 the reduction in $\langle t(\omega)\rangle$ is largest at high frequencies.

D. Kapitza resistance

The Kapitza conductance $\sigma(T)$ is obtained from the transmission spectral density by numerical integration of Eq. (26). Results of these calculations are shown in Figs. 11–13. In all of these calculations the interface spring constant has the value $K''=(K+K')/2$. We have plotted the Kapitza conductance divided by σ_0, defined by

$$\sigma_0=\frac{k_B}{a^2}\left[\frac{K}{M}\right]^{1/2}=\frac{0.337k_B^2\Theta_D}{\hbar a^2}\ , \tag{31}$$

as a function of T/Θ_D.

The conductivity is in all cases proportional to T^3 at low temperatures and independent of T for $T>\Theta_D$. (We believe that some small deviations from T^3 dependence that can be seen in Figs. 11–13 are an artifact arising from poor statistical averaging at low frequencies.) The temperature dependence of σ is thus similar to that of the specific heat. A more detailed comparison shows that as T is raised $\sigma(T)$ increases less rapidly than does $C(T)$. This is due to the increase in the number of high-frequency phonons which have low group velocity and transmission coefficient. The effect is most marked when $\Theta_D'<\Theta_D$, since then the phonon transmission coefficient is zero above a certain frequency. As an example of this effect, see the results for $K'/K=0.5, M'/M=2.0$ in Fig. 13.

To apply these model calculations to estimate the conductance between two real solids one can use the relation

$$\frac{K'}{K}=\frac{M'}{M}\left[\frac{\Theta_D'}{\Theta_D}\right]^2\ . \tag{32}$$

The conductance can then be estimated from Figs. 11–13, provided that the ratio of the masses is no more than 2:1. Notice that the conductance must have the symmetry

$$\sigma(K,M,K',M',T)=\sigma(K',M',K,M,T)\ , \tag{33}$$

i.e., must be the same when the two lattices are interchanged. Thus, one can always choose the lattices so that K'/K is larger than 1, i.e., in the range included in Figs. 11–13.

We have recently completed a series of measurements of the temperature dependence of the Kapitza resistance for several different interfaces. In a subsequent paper we plan to compare these and other[1,2] data with the calculations described in this paper.

ACKNOWLEDGMENTS

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APPENDIX

The coefficients M_{pq} for the incident wave ($q=0$) and the three reflected waves ($q=1,2,3$) are

$$M_{1q}=[(1-K''/K')-\exp(-ik_z^{(q)}a)\cos(k_xa)]K'e_x^{(q)}+[i\exp(-ik_z^{(q)}a)\sin(k_xa)]K'e_z^{(q)}\ ,$$

$$M_{2q}=[(1-K''/K')-\exp(-ik_z^{(q)}a)\cos(k_ya)]K'e_y^{(q)}+[i\exp(-ik_z^{(q)}a)\sin(k_ya)]K'e_z^{(q)}\ ,$$

$$M_{3q}=[i\exp(-ik_z^{(q)}a)\sin(k_xa)]K'e_x^{(q)}+[i\exp(-ik_z^{(q)}a)\sin(k_ya)]K'e_y^{(q)}$$
$$+\{2(1-K''/K')-\exp(-ik_z^{(q)}a)[\cos(k_xa)+\cos(k_ya)]\}K'e_z^{(q)}\ ,$$
$$M_{4q}=[\cos(k_xa)]K''e_x^{(q)}a+[i\sin(k_xa)]K''e_z^{(q)}\ ,$$
$$M_{5q}=[\cos(k_ya)]K''e_y^{(q)}a+[i\sin(k_ya)]K''e_z^{(q)}\ ,$$
$$M_{6q}=[i\sin(k_xa)]K''e_x^{(q)}a+[i\sin(k_ya)]K''e_y^{(q)}+[(\cos(k_xa)+\cos(k_ya)]K''e_z^{(q)}\ .$$

The coefficients M_{pq} for the three transmitted waves ($q=4,5,6$) are

$$M_{1q}=[\cos(k_xa)]K''e_x^{(q)}a-[i\sin(k_xa)]K''e_z^{(q)}\ ,$$
$$M_{2q}=[\cos(k_ya)]K''e_y^{(q)}a-[i\sin(k_ya)]K''e_z^{(q)}\ ,$$
$$M_{3q}=-[i\sin(k_xa)]K''e_x^{(q)}a-[i\sin(k_ya)]K''e_y^{(q)}+[\cos(k_xa)+\cos(k_ya)]K''e_z^{(q)}\ ,$$
$$M_{4q}=[(1-K''/K)-\exp(ik_z^{(q)}a)\cos(k_xa)]Ke_x^{(q)}-[i\exp(ik_z^{(q)}a)\sin(k_xa)]Ke_z^{(q)}\ ,$$
$$M_{5q}=[(1-K''/K)-\exp(ik_z^{(q)}a)\cos(k_ya)]Ke_y^{(q)}-[i\exp(ik_z^{(q)}a)\sin(k_ya)]Ke_z^{(q)}\ ,$$
$$M_{6q}=-[i\exp(ik_z^{(q)}a)\sin(k_xa)]Ke_x^{(q)}-[i\exp(ik_z^{(q)}a)\sin(k_ya)]Ke_y^{(q)}$$
$$+\{2(1-K''/K')-\exp(ik_z^{(q)}a)[\cos(k_xa)+\cos(k_ya)]\}Ke_z^{(q)}\ .$$

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