Thermal transport in AB superlattices

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We calculate the thermal conductivity of an AB superlattice in the cross-plane direction (perpendicular to the layers). If all of the heat is carried by phonons, the calculation has been performed often. We include the feature that one (A) or both (A and B) of the superlattice layers are electronic conductors, so they have thermal energy in the electron system as well as in the phonon system. We also assume the layers are thin, of several atomic layers, so the main thermal resistance is at the interfaces. The introduction of electron thermal energy changes the thermal conductance of the superlattice. It also changes the boundary conductance between a metal contact and the superlattice.

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I. INTRODUCTION

We calculate the heat flow and temperature profile of an AB superlattice in the cross-plane direction (perpendicular to the layers). It is composed of alternate layers $ABABAB\cdots$, where each layer is several atomic layers. We assume the thermal resistance is exclusively in the boundary resistance between adjacent layers. We further assume that layer A is a conductor and so has thermal energy in both the phonon and the electron systems. Their temperatures may not coincide, so we denote them as $(T_{A,p,n}, T_{A,e,n})$ for layer n. We work out separately the two cases for the other layer B: (i) an insulator or (ii) a conductor. If the B layer is insulating, it has only phonon energy at a temperature $T_{B,p,n+1/2}$. The ordering of layers is $(A1, B3/2, A2, B5/2, A3, \ldots, AN)$.

There have been many papers on thermal transport in superlattices, both theoretical[1–9] and experimental.[10–17] The theoretical articles have mostly been on heat carried by only phonons. The important feature of the present calculation is the inclusion of heat in the electronic system of layers that are electrical conductors. Many of the experiments are performed on superlattices which have one layer as a conductor (e.g., GaAs/AlAs).

We assume each layer is only several atomic layers thick, and the entire layer is at a single temperature. The thermal resistance is in the interface between layers. This Kapitza resistance is well studied.[18] There have been numerous experimental measurements of boundary layer thermal resistance.[19–25] There have been several theoretical calculations of the thermal boundary resistance from phonon transport.[26–29] We introduce the thermal boundary conductances G_{pp} for phonon-to-phonon heat flow, G_{ee} for electron-to-electron heat flow, and G_{ep} for electron-to-phonon heat flow. There have been several calculations of G_{ep}[30,31] between metals and nonmetals. Although we have cited much good work, the parameters G_{pp}, G_{ee}, and G_{ep} are not well understood for semiconductor superlattices such as GaAs/AlAs. Some estimates are given in Ref. 7.

We provide calculations on three different types of superlattices: (i) there is only phonon heat flow, (ii) only one type of layer has electronic energy, and (iii) both A and B have electronic energy. The first case is trivial and takes only a few lines of algebra. The majority of the article discusses the other two cases. In two cases, we find that the temperature profile is linear in distance,

$$T(x) = T_c + \frac{x}{L}(T_h - T_c), \tag{1}$$

between the cold (T_c) and hot (T_h) reservoirs, which are separated by a distance L. The main difference among the three cases is the nature of the thermal resistance between layers. We also examine the case whereby the hot and cold reservoirs are metal contacts and calculate the thermal resistance between these contacts and the semiconductor superlattice. This contact resistance is quite complicated in some cases. If both layers A and B are conductors, then Eq. (1) is modified, as discussed below.

One case involves all layers of the superlattice being insulating, and heat is carried only by phonons. The only parameter is G_{pp}. If we neglect boundary effects, the temperature is strictly linear in distance, and the thermal resistance per interface is $1/G_{pp}$:

$$T_{A,n} = T_c + \frac{n}{N}(T_h - T_c), \tag{2}$$

$$T_{B,n+1/2} = T_c + \frac{n+1/2}{N}(T_h - T_c), \tag{3}$$

$$J_Q = \frac{T_h - T_c}{\mathcal{R}_T}, \tag{4}$$

$$\mathcal{R}_T = \frac{2N}{G_{pp}}, \tag{5}$$

where N is the number of bilayers, and the number of interfaces is $\sim 2(N-1)$. The last two equations are the heat flow in watts per area and the total thermal resistance $\mathcal{R}_T$. This result is modified later to include contact effects.

II. ONLY A IS A CONDUCTOR

The most common superlattices have only alternate layers conducting, so we investigate this case first. We assume the A layers are electrically conducting and have thermal energy in the electron and also in the phonon systems. The other layers B have only phonon energy. The equations for a layer n in the interior of the superlattice has three unknowns and three equations for a general value of n. The three unknowns are the phonon temperature in the B layer ($T_{B,n+1/2}$) and the electron and phonon temperatures ($T_{A,e,n}$ and $T_{A,p,n}$, respectively) in the A layer.

The equations that follow are continuity equations for the energy in each layer. To the left of the equal sign is the time derivative $C_j \partial T/\partial t$, where C_j is the heat capacity per area of the layer j. Since we are assuming steady state, we set to zero all time derivatives. The right-hand sides of the following equations include the heat flowing in and out of the layers from the neighboring layers. There is also a term W_A for the thermal relaxation between electrons and phonons within a layer[32]:

$$0 = G_{pp}(T_{B,p,n+1/2} + T_{B,p,n-1/2} - 2T_{A,p,n}) - W_A(T_{A,p,n} - T_{A,e,n}), \tag{6}$$

$$\begin{aligned} 0 &= G_{ep}(T_{B,p,n+1/2} + T_{B,p,n-1/2} - 2T_{A,e,n}) + W_A(T_{A,p,n} - T_{A,e,n}), \\ 0 &= G_{pp}(T_{A,p,n+1} + T_{A,p,n} - 2T_{B,p,n+1/2}) + G_{ep}(T_{A,e,n+1} + T_{A,e,n} - 2T_{B,p,n+1/2}), \end{aligned} \tag{7}$$

where G_{pp} is the thermal conductance between phonons in adjacent layers, and G_{ep} is the thermal conductance between the electron energy in A and the phonons in B. We can eliminate the factor $T_{B,p,n+1/2} + T_{B,p,n-1/2}$ from the first two equations, which yields

$$0 = (T_{A,p,n} - T_{A,e,n})(2G_{pp}G_{ep} + g_p W_A), \tag{8}$$

$$g_p = G_{pp} + G_{ep}, \tag{9}$$

which determines that $T_{A,p,n} = T_{A,e,n} \equiv T_{A,n}$. With this constraint, the equations for $T_{B,p,n}$ are

$$0 = T_{B,p,n+1/2} + T_{B,p,n-1/2} - 2T_{A,n}, \tag{10}$$

$$0 = T_{A,n+1} + T_{A,n} - 2T_{B,p,n+1/2}. \tag{11}$$

In Eq. (11), let $n \to n-1$ and then add it to the same equation:

$$\begin{aligned} T_{A,n+1} + 2T_{A,n} + T_{A,n-1} &= 2[T_{B,p,,n+1/2} + T_{B,p,n-1/2}] \\ &= 4T_{A,n}. \end{aligned} \tag{12}$$

This recursion relation has the solution that

$$T_{A,n} = T_0 + \Delta T \frac{n}{N}, \tag{13}$$

$$T_{B,n+1/2} = T_0 + \Delta T \frac{n+1/2}{N}, \tag{14}$$

where N is the number of double layers between the hot and the cold reservoirs, and $\Delta T/N$ is the change in temperature between adjacent A layers. Only solutions linear in $x = na$ are allowed in this case.

A. Three layers with A boundaries

Next we consider how heat flows into the superlattice at the boundaries. Our first calculation is for a five-layer system, from left to right:

(1) A metallic cold reservoir at temperature T_c, which is the temperature of both electrons and phonons.

(2) Semiconductor layer $A1$ with separate electron ($T_{A,e,1}$) and phonon ($T_{A,p,1}$) temperatures.

(3) Insulator layer B with phonon temperature T_B.

(4) Semiconductor layer $A2$ with separate electron ($T_{A,e,2}$) and phonon ($T_{A,p,2}$) temperatures.

(5) A metallic hot reservoir at temperature T_h, which is the temperature of both electrons and phonons.

The thermal conductances are:

(1) G_{pp} between the phonons in A and B.

(2) G_{ep} between the electrons in A and the phonons in B.

(3) The boundary conductances are assumed to be identical at the hot and cold sides.

(a) $G_{B,ee}$ between electrons in the metal and electrons in adjacent layers A.

(b) $G_{B,pp}$ between phonons in the metal and phonons in adjacent layers A.

(c) $G_{B,ep}$ between electrons in the metal and phonons in adjacent layers A.

(d) $G_{B,pe}$ between phonons in the metal and electrons in adjacent layers A.

There are five equations with five unknowns:

$$0 = g_{B,p}(T_c - T_{A,p,1}) + G_{pp}(T_B - T_{A,p,1}) - W_A(T_{A,p,1} - T_{A,e,1}), \tag{15}$$

$$0 = g_{B,e}(T_c - T_{A,e,1}) + G_{ep}(T_B - T_{A,e,1}) + W_A(T_{A,p,1} - T_{A,e,1}), \tag{16}$$

$$0 = G_{pp}(T_{A,p,2} + T_{A,p,1} - 2T_B) + G_{ep}(T_{A,e,2} + T_{A,e,1} - 2T_B), \tag{17}$$

$$0 = g_{B,p}(T_h - T_{A,p,2}) + G_{pp}(T_B - T_{A,p,2}) - W_A(T_{A,p,2} - T_{A,e,2}), \tag{18}$$

$$0 = g_{B,e}(T_h - T_{A,e,2}) + G_{ep}(T_B - T_{A,e,2}) + W_A(T_{A,p,2} - T_{A,e,2}), \tag{19}$$

$$g_{B,p} = G_{B,pp} + G_{B,ep}, \quad g_{B,e} = G_{B,ee} + G_{B,pe}. \tag{20}$$

Rearranging the first two equations gives

$$G_{pp}T_B = T_{A,p,1}(G_{pp} + g_{B,p} + W_A) - W_A T_{A,e,1} - T_c g_{B,p}, \tag{21}$$

$$G_{ep}T_B = T_{A,e,1}(G_{ep} + g_{B,e} + W_A) - W_A T_{A,p,1} - T_c g_{B,e}. \tag{22}$$

One eliminates T_B by multiplying the first by G_{ep} and the second by G_{pp}, and then subtracting. After some algebra, one finds that

$$T_{A,e,1} = T_{A,p,1} + R(T_c - T_{A,p,1}), \tag{23}$$

$$R = \frac{G_{pp}g_{B,e} - G_{ep}g_{B,p}}{G_{pp}G_{ep} + g_p W_A + G_{pp}g_{B,e}}. \tag{24}$$

Earlier it was proved that $T_{A,e,n} = T_{A,p,n}$. The proof is invalid in the boundary layer $n = 1$, where the preceding equation shows that these two temperatures are different because of the boundary conditions.

Another equation is derived from from Eqs. (21) and (22) by adding them:

$$g_p T_B = g_p T_{A,p,1} + (T_{A,p,1} - T_c)(H - RG_{ep}), \tag{25}$$

$$g_{B,T} = g_{B,p} + g_{B,e}, \quad H = g_{B,T} - Rg_{B,e}. \tag{26}$$

We can derive a similar set of equations for the layers near the hot side; simply change T_c to T_h and the layer index for A to 2:

$$T_{A,e,2} = T_{A,p,2} + R(T_h - T_{A,p,2}), \tag{27}$$

$$g_p T_B = g_p T_{A,p,2} + (T_{A,p,2} - T_h)(H - RG_{ep}). \tag{28}$$

Combining these equations, along with Eq. (17), gives a solution for all of the temperatures:

$$T_{A,p,1} = T_c + \delta T, \tag{29}$$

$$T_{A,p,2} = T_h - \delta T, \tag{30}$$

$$\delta T = \frac{g_p(T_h - T_c)}{2(g_p + H - RG_{ep})}, \tag{31}$$

$$T_B = \tfrac{1}{2}(T_h + T_c). \tag{32}$$

The constant heat flow through the device is

$$J_Q = g_{B,p}(T_{A,p,1} - T_c) + g_{B,e}(T_{a,e,1} - T_c) \tag{33}$$

$$= H(T_{A,p,1} - T_c) \tag{34}$$

$$= \mathcal{G}(T_h - T_c), \tag{35}$$

$$\mathcal{G} = \frac{g_p H}{2(g_p + H - RG_{ep})}. \tag{36}$$

The total thermal resistance is

$$\mathcal{R}_T = \frac{1}{\mathcal{G}} = \frac{2}{g_p} + \frac{2}{H}\left(1 - \frac{RG_{ep}}{g_p}\right). \tag{37}$$

The first term is from the two interfaces between the A and B layers, each of which has a thermal resistance of $1/g_p$. The last term is the thermal resistance from the two metallic boundaries. If the superlattice has N layers of A, the total thermal resistance of the superlattice is

$$\mathcal{R}_T = \frac{2(N-1)}{g_p} + \mathcal{R}_L + \mathcal{R}_R. \tag{38}$$

The last two terms are from the boundaries:

$$\mathcal{R}_{L,R} = \frac{1}{H}\left(1 - \frac{RG_{ep}}{g_p}\right) \tag{39}$$

$$= \frac{1}{g_p} \frac{g_p(G_{pp}G_{ep} + g_p W_A) + G_{pp}^2 g_{B,e} + G_{ep}^2 g_{B,p}}{g_{B,T}(G_{pp}G_{ep} + g_p W_A) + g_{B,e} g_{B,p} g_p}. \tag{40}$$

This formula is one of the major results of this calculation. It provides the thermal boundary resistance between a metal contact and an AB superlattice.

B. B boundaries

The preceding formula gives the thermal boundary resistance when the layer A, which is conducting, is adjacent to the metal boundary contact. Here we derive the other case where the boundary layer is B, which has no electrical conduction and no heat content from electrons.

Again we consider a five-layer system, from left to right: (i) metal contact at temperature T_c, layer $B1$, layer A, layer $B2$, and metal contact at temperature T_h. Because layer A is surrounded by two B layers, $T_{A,p} = T_{A,e}$. The three unknown temperatures are T_{B1}, T_A, and T_{B2}. The three equations are

$$0 = g_{B,L,p}(T_c - T_{B1}) + g_p(T_A - T_{B1}), \tag{41}$$

$$0 = g_p(T_{B1} + T_{B2} - 2T_A), \tag{42}$$

$$0 = g_{B,R,p}(T_h - T_{B2}) + g_p(T_A - T_{B2}). \tag{43}$$

The solution is

$$T_{B1} = T_c + \frac{g_p g_{B,R,p}(T_h - T_c)}{D_B}, \tag{44}$$

$$T_A = T_c + \frac{g_{B,R,p}(g_p + g_{B,L,p})(T_h - T_c)}{D_B}, \tag{45}$$

$$T_{B2} = T_c + \frac{g_{B,R,p}(2g_{B,L,p} + g_p)}{D_B}(T_h - T_c), \tag{46}$$

$$D_B = 2g_{B,L,p}g_{B,R,p} + g_p(g_{B,L,p} + g_{B,R,p}). \tag{47}$$

The heat current is

$$J_Q = \frac{T_h - T_c}{\mathcal{R}_T}, \tag{48}$$

$$\mathcal{R}_T = \frac{2}{g_p} + \frac{1}{g_{B,L,p}} + \frac{1}{g_{B,R,p}}. \tag{49}$$

The first term is from the two AB interfaces. The last two are the thermal resistance between the B boundary layers and the two metal contacts. For a typical superlattice with N_i boundaries between A and B, the total thermal resistance is

$$\mathcal{R}_T = \frac{N_i}{g_p} + \frac{1}{g_{B,L,p}} + \frac{1}{g_{B,R,p}}. \tag{50}$$

The most general formula for the thermal resistance of the AB superlattice is

$$\mathcal{R}_T = \frac{N_i}{g_p} + \mathcal{R}_{B,L} + \mathcal{R}_{B,R}, \tag{51}$$

where the first term is from the N_i-AB interfaces in the superlattice, and the last two terms are from the left and right metallic contacts. If the boundary layer of the superlattice is B, the thermal contact resistance is $\mathcal{R}_{B,j} = 1/g_{B,j,p}$. If the boundary layer of the superlattice is a conducting layer A, the thermal contact resistance is given in Eq. (40).

III. BOTH LAYERS CONDUCTING

Now consider the case of an AB superlattice in which both layers have conduction electrons. Now there are four variables: $T_{A,p,n}$, $T_{A,e,n}$, $T_{B,p,n+1/2}$, and $T_{B,e,n+1/2}$ for the electron (e) and phonon (p) temperatures in layers A and B. There are four boundary conductances: G_{pp} between phonons in both layers, G_{ee} between electrons in both layers, G_{ep} between electrons in A and phonons in B, and G'_{ep} between electrons in B and phonons in A. An important parameter is the total conductance,

$$g_T = G_{pp} + G_{ee} + G_{ep} + G'_{ep}. \tag{52}$$

The thermal resistance between layers is $1/g_T$. The steady-state equations are

$$\begin{aligned} 0 &= G_{pp}(T_{B,p,n+1/2} + T_{B,p,n-1/2} - 2T_{A,p,n}) \\ &\quad + G'_{ep}(T_{B,e,n+1/2} + T_{B,e,n-1/2} - 2T_{A,p,n}) \\ &\quad - W_A(T_{A,p,n} - T_{A,e,n}), \end{aligned} \tag{53}$$

$$0 = G_{ee}(T_{B,e,n+1/2} + T_{B,e,n-1/2} - 2T_{A,e,n}) + G_{ep}(T_{B,p,n+1/2} + T_{B,p,n-1/2} - 2T_{A,e,n}) + W_A(T_{A,p,n} - T_{A,e,n}), \tag{54}$$

$$0 = G_{pp}(T_{A,p,n+1} + T_{A,p,n} - 2T_{B,p,n+1/2}) + G_{ep}(T_{A,e,n+1} + T_{A,e,n} - 2T_{B,p,n+1/2}) - W_B(T_{B,p,n} - T_{B,e,n}), \tag{55}$$

$$0 = G_{ee}(T_{A,e,n+1} + T_{A,e,n} - 2T_{B,e,n+1/2}) + G'_{ep}(T_{A,p,n+1} + T_{A,p,n} - 2T_{B,e,n+1/2}) + W_B(T_{B,p,n} - T_{B,e,n}). \tag{56}$$

The first two equations have a solution:

$$T_{B,p,n+1/2} + T_{B,p,n-1/2} = M^A_{pp}T_{A,p,n} - M^A_{pe}T_{A,e,n}, \tag{57}$$
$$T_{B,e,n+1/2} + T_{B,e,n-1/2} = M^A_{ee}T_{A,e,n} - M^A_{ep}T_{A,p,n}, \tag{58}$$
$$M^A_{ee} = \frac{1}{D}[2G_{pp}g_e + g_p W_A] = 2 + M^A_{ep}, \tag{59}$$
$$M^A_{pp} = \frac{1}{D}[2G_{ee}g'_p + g'_e W_A] = 2 + M^A_{pe}, \tag{60}$$
$$M^A_{ep} = \frac{1}{D}[2G_{ep}g'_p + g_p W_A], \tag{61}$$
$$M^A_{pe} = \frac{1}{D}[2G'_{ep}g_e + g'_e W_A], \tag{62}$$
$$g'_p = G_{pp} + G'_{ep}, \quad g'_e = G_{ee} + G'_{ep}, \tag{63}$$
$$D = G_{ee}G_{pp} - G_{ep}G'_{ep}. \tag{64}$$

A similar solution is found for the second pair of equations:

$$T_{A,p,n+1} + T_{A,p,n} = M^B_{pp}T_{B,p,n+1/2} - M^B_{pe}T_{B,e,n+1/2}, \tag{65}$$
$$T_{A,e,n+1} + T_{A,e,n} = M^B_{ee}T_{B,e,n+1/2} - M^B_{ep}T_{B,p,n+1/2}, \tag{66}$$
$$M^B_{ee} = \frac{1}{D}[2G_{pp}g'_e + g'_p W_B] = 2 + M^B_{ep}, \tag{67}$$
$$M^B_{pp} = \frac{1}{D}[2G_{ee}g_p + g_e W_B] = 2 + M^B_{pe}, \tag{68}$$
$$M^B_{ep} = \frac{1}{D}[2G'_{ep}g_p + g'_p W_B], \tag{69}$$
$$M^B_{pe} = \frac{1}{D}[2G_{ep}g'_e + g_e W_B]. \tag{70}$$

These equations can be written in vector notation as

$$\mathcal{T}_{A,n} = \begin{pmatrix} T_{A,p,n} \\ T_{A,e,n} \end{pmatrix}, \tag{71}$$
$$\mathcal{T}_{B,n+1/2} = \begin{pmatrix} T_{B,p,n+1/2} \\ T_{B,e,n+1/2} \end{pmatrix}, \tag{72}$$
$$\mathcal{T}_{B,n+1/2} + \mathcal{T}_{B,n-1/2} = \mathcal{M}_A\mathcal{T}_{A,n}, \tag{73}$$
$$\mathcal{T}_{A,n+1} + \mathcal{T}_{A,n} = \mathcal{M}_B\mathcal{T}_{B,n+1/2}. \tag{74}$$

In Eq. (74), if one changes n to $n-1$ and then adds the result to Eq. (74), one gets

$$\mathcal{T}_{A,n+1} + 2\mathcal{T}_{A,n} + \mathcal{T}_{A,n-1} = \mathcal{M}_B[\mathcal{T}_{B,n+1/2} + \mathcal{T}_{B,n-1/2}] \tag{75}$$
$$= \mathcal{M}_B\mathcal{M}_A\mathcal{T}_{An}. \tag{76}$$

We get a simple recursion relation for $\mathcal{T}_{A,n}$. The 2×2 matrix $\mathcal{M}_B\mathcal{M}_A$ has one eigenvalue that is $\lambda = 4$. It gives the solution that

$$T_{A,j,n} = T(n) = T_0 + nC, \tag{77}$$
$$T_{B,j,n+1/2} = T(n+1/2) = T_0 + (n+1/2)C, \tag{78}$$

where $T_0 \sim T_c$ and $C \sim \Delta T/N_i$ are derived in the Appendix.

The other eigenvalue of the 2×2 matrix is $\lambda = \lambda_A\lambda_B$, where

$$\lambda_A = (2 + M^A_{ep} + M^A_{pe}) = \frac{1}{D}\left[2g_e g'_p + g_T W_A\right], \tag{79}$$
$$\lambda_B = \left(2 + M^B_{ep} + M^B_{pe}\right) = \frac{1}{D}[2g'_e g_p + g_T W_B]. \tag{80}$$

One can show that $\lambda \geqslant 4$ and

$$T_{A,p,n} - T_{A,e,n} = Fe^{-n\phi} + Ge^{-\phi(N+1-n)}, \tag{81}$$
$$\lambda = 2[1 + \cosh(\phi)] = \lambda_A\lambda_B. \tag{82}$$

Below we show $G = -F$ and therefore define

$$\mathcal{F}(n) = e^{-n\phi} - e^{-\phi(N+1-n)}. \tag{83}$$

The preceding two eigenvalues can be derived directly. For example, define $t_{j,n} = T_{j,p,n} - T_{j,e,n}$. Subtracting the two sets of equations, Eqs. (57) and (58) and Eqs. (65) and (66), gives

$$t_{B,n+1/2} + t_{B,n-1/2} = \lambda_A t_{A,n}, \tag{84}$$
$$t_{A,n+1} + t_{A,n} = \lambda_B t_{B,n+1/2}. \tag{85}$$

In Eq. (85), let $n \to n-1$ and add this new equation to the old one:

$$t_{A,n+1} + 2t_{A,n} + t_{A,n-1} = \lambda_B(t_{B,n} + t_{B,n-1}) = \lambda_A\lambda_B t_{A,n}. \tag{86}$$

This equation has the solution $t_{A,n} = F\mathcal{F}(n)$, where ϕ is defined in Eq. (82).

The other eigenvalue is found by taking the following weighted averages:

$$s_{A,n} = g'_p T_{A,p,n} + g_e T_{A,e,n}, \tag{87}$$
$$s_{B,n+1/2} = g_p T_{B,p,n+1/2} + g'_e T_{B,e,n+1/2}. \tag{88}$$

We take these weighted averages of Eqs. (57) and (58), and Eqs. (65) and (66), and find, after some algebra,

$$s_{A,n} + s_{A,n+1} = 2s_{B,n+1/2}, \tag{89}$$
$$s_{B,n+1/2} + s_{B,n-1/2} = 2s_{A,n}. \tag{90}$$

These equations have the eigenvalue $\lambda = 4$ and the linear solution

$$s_{A,n} = g_T T(n), \tag{91}$$
$$s_{B,n} = g_T T(n+1/2). \tag{92}$$

Next we prove that these are the only two solutions. We make an ansatz that the temperatures have the following dependence on layer index:

$$T_{A,(e,p),n} = t_{A,(e,p)}\sinh(n\phi), \tag{93}$$
$$T_{B,(e,p),n} = t_{B,(e,p)}\sinh[(n+1/2)\phi]. \tag{94}$$

Then every term in Eqs. (57) and (58) has a common factor of $\sinh(n\phi)$ that can be factored out. Similarly, every term in

Eqs. (65) and (66) has a factor of $\sinh[(n+1/2)\phi]$. Denote the eigenvalue as $\Lambda = 2\cosh(\phi/2)$. The remaining equations can be written in matrix form:

$$0 = \begin{bmatrix} M_{pp}^A & -M_{pe}^A & -\Lambda & 0 \\ -M_{ep}^A & M_{ee}^A & 0 & -\Lambda \\ -\Lambda & 0 & M_{pp}^B & -M_{pe}^B \\ 0 & -\Lambda & -M_{ep}^B & M_{ee}^B \end{bmatrix} \begin{bmatrix} t_{A,p} \\ t_{A,e} \\ t_{B,p} \\ t_{B,e} \end{bmatrix}. \quad (95)$$

The solution is obtained by setting the determinant of the matrix to zero. The equation for the eigenvalue is

$$0 = (\Lambda^2 - 4)(\Lambda^2 - \lambda_A\lambda_B), \quad (96)$$

$$\Lambda^2 = [2\cosh(\phi/2)]^2 = 2[1+\cosh(\phi)] = \lambda, \quad (97)$$

so that the two equations are the ones we had earlier:

(1) The first solution is

$$2[1+\cosh(\phi)] = 4, \quad \phi = 0. \quad (98)$$

This case has the solution $T_{j,n} = T(n) = T_0 + Cn$ and is the linear solution.

(2) The second solution is

$$2[1+\cosh(\phi)] = \lambda_A\lambda_B. \quad (99)$$

This case is the exponentially decaying solution $T_{j,n} = A\mathcal{F}(n)$ since $\lambda_A\lambda_B > 4$.

(3) Equation (96) seems to permit negative eigenvalues $\lambda = -2$, $\lambda = -\sqrt{\lambda_A\lambda_B}$. One can show that there are no new solutions for either of these negative eigenvalues.

The two solutions can be used to find all four temperatures in the superlattice. Define

$$\delta T_A = F_A\mathcal{F}(n), \quad (100)$$

$$\delta T_B = F_B\mathcal{F}(n+1/2), \quad (101)$$

where the last two Eqs. (100) and (101) are relaxations, where the phonon and electron temperatures equilibrate over distance starting from the $n=1$ edges. A similar relaxation happens at the other edge ($n=N$). The solutions are

$$T_{A,p,n} = T(n) + \frac{g_e}{g_T}\delta T_A, \quad (102)$$

$$T_{A,e,n} = T(n) - \frac{g_p'}{g_T}\delta T_A, \quad (103)$$

$$T_{B,p,n+1/2} = T(n+1/2) + \frac{g_e'}{g_T}\delta T_B, \quad (104)$$

$$T_{B,e,n+1/2} = T(n+1/2) - \frac{g_p}{g_T}\delta T_B. \quad (105)$$

Then $s_{A,n} = g_T\bar{T}(n)$ and $s_{B,n} = g_T\bar{T}(n+1/2)$, which satisfy Eqs. (89) and (90). Also, $t_{A,n} = \delta T_A$ and $t_{B,n} = \delta T_B$, and Eqs. (84) and (85) are satisfied, provided

$$\sqrt{\lambda_A}F_A = \sqrt{\lambda_B}F_B \equiv F. \quad (106)$$

The boundary resistances for this case are more complicated due to the spatial relaxation terms $\mathcal{F}(n)$. The thermal resistance in the bulk of the superlattice is $\mathcal{R} = N_i/g_T$ for N_i interfaces. The boundary resistance from a metal contact is derived in the Appendix.

IV. DISCUSSION

We calculated the thermal conductivity of an alternate superlattice ($ABAB\cdots$) in the cross-plane direction. The thermal conductivity of the device is given by the ratio of the temperature difference divided by the total thermal resistance:

$$J_Q = \frac{T_h - T_c}{\mathcal{R}_T}, \quad (107)$$

$$\mathcal{R}_T = N_i\mathcal{R}_I + \mathcal{R}_{LB} + \mathcal{R}_{RB}, \quad (108)$$

where $\mathcal{R}_I$ is the thermal resistance of a single interface and N_i is the number of $A-B$ interfaces; $\mathcal{R}_{LB}, \mathcal{R}_{RB}$ are the thermal resistances at the interfaces between the heat reservoirs at the left and right boundaries. For a single interface:

(1) For heat flow only by phonons, $\mathcal{R}_I = 1/G_{pp}$.

(2) For A a conductor and B an insulator, then $\mathcal{R}_I = 1/g_p = (G_{pp} + G_{ep})^{-1}$.

(3) For both A and B conductors, then $\mathcal{R}_I = 1/g_T = (G_{pp} + G_{ee} + G_{ep} + G_{ep}')^{-1}$.

A similar list is given for the boundary conductances:

(1) For heat flow only by phonons, $\mathcal{R}_{jB} = 1/g_{B,p}$.

(2) If A is a conductor and B is an insulator, and A is at the boundary, the result is Eq. (40).

(3) If A is a conductor and B is an insulator, and B is at the boundary, the result is $\mathcal{R}_{jB} = 1/g_{B,p}$.

(4) If both A and B are conductors, the result is Eq. (A51) if A is the bounding layer.

We hope these expressions are useful for interpreting experimental measurements. The present theoretical need is to derive expressions for the conductances G_j for semiconductors, which are the layers in most superlattices.

A popular method of measuring the thermal conductivity of thin films and superlattices is called the 3-ω method.[33] Our analysis shows that boundary resistance at the contacts does not change the measurement, in complete agreement with Cahill's analysis[33] for bulk samples.

APPENDIX

Here we derive in detail the surface resistance for an AB superlattice for the cases that both layers (A and B) are conducting. We begin by summarizing some formulas derived earlier:

$$T_{A,p,n} = T(n) + \frac{g_eF}{g_T\sqrt{\lambda_A}}\mathcal{F}(n), \quad (A1)$$

$$T_{A,e,n} = T(n) - \frac{g_p'F}{g_T\sqrt{\lambda_A}}\mathcal{F}(n), \quad (A2)$$

$$T_{B,p,n+1/2} = T(n+1/2) + \frac{g_e'F}{g_T\sqrt{\lambda_B}}\mathcal{F}(n+1/2), \quad (A3)$$

$$T_{B,p,n+1/2} = T(n+1/2) + \frac{g_pF}{g_T\sqrt{\lambda_B}}\mathcal{F}(n+1/2), \quad (A4)$$

$$\mathcal{F}(n) = e^{-n\phi} - e^{-\phi(N+1-n)}. \quad (A5)$$

Assume that N is an odd integer, which makes the middle layer A. Then the middle layer is $N_m = (N+1)/2$. By symmetry, the temperatures of this layer must be

$$T_{A,p,N_m} = T_{A,e,N_m} = T(N_m) = \frac{(T_c + T_h)}{2} \equiv \bar{T}, \tag{A6}$$

$$T_0 + CN_m = \bar{T}. \tag{A7}$$

Note that $\mathcal{F}(N_m) = 0$. This solution requires $G = -F$. The theory has three unknowns: T_0, C, and F. Equation (A7) is the first of three equations.

Two equations from the second layer, and from the second-to-last layer, are

$$0 = G_{pp}T_{A,p,1} + G_{ep}T_{A,e,1} - g_pT(1) + F\mathcal{L}_c, \tag{A8}$$

$$0 = G'_{ep}T_{A,p,1} + G_{ee}T_{A,e,1} - g'_eT(1) - F\mathcal{L}_c, \tag{A9}$$

$$\mathcal{L}_c = \frac{D\mathcal{F}(2)}{g_T\sqrt{\lambda_A}} - \frac{\mathcal{F}(3/2)}{\sqrt{\lambda_B}}\left[W_B + \frac{2g'_eg_p}{g_T}\right], \tag{A10}$$

$$\mathcal{L}_c = \frac{D}{g_T\sqrt{\lambda_A}}\left[\mathcal{F}(2) - \sqrt{\lambda_A\lambda_B}\mathcal{F}(3/2)\right] = -\frac{D}{g_T\sqrt{\lambda_A}}\mathcal{F}(1), \tag{A11}$$

$$0 = G_{pp}T_{A,p,N} + G_{ep}T_{A,e,N} - g_pT(N) + F\mathcal{L}_h, \tag{A12}$$

$$0 = G'_{ep}T_{A,p,N} + G_{ee}T_{A,e,N} - g'_eT(N) - F\mathcal{L}_h, \tag{A13}$$

$$\mathcal{L}_h = \frac{D\mathcal{F}(N-1)}{g_T\sqrt{\lambda_A}} - \frac{\mathcal{F}(N-1/2)}{g_T\sqrt{\lambda_B}}[g_TW_B + 2g'_eg_p] = -\mathcal{L}_c. \tag{A14}$$

Adding Eqs. (A8) and (A9), and also Eqs. (A12) and (A13), we get

$$0 = g'_pT_{A,p,1} + g_eT_{A,e,1} - g_TT(1), \tag{A15}$$

$$0 = g'_pT_{A,p,N} + g_eT_{A,e,N} - g_TT(N). \tag{A16}$$

We next use the definitions

$$D_p = g_{B,p} + g'_p + W_A = \tilde{g}'_p + W_A, \tag{A17}$$

$$D_e = g_{B,e} + g_e + W_A = \tilde{g}_e + W_A, \tag{A18}$$

$$\mathcal{D} = D_pD_e - W_A^2 = \tilde{g}'_p\tilde{g}_e + W_A(g_T + g_{B,T}), \tag{A19}$$

$$D = G_{pp}G_{ee} - G_{ep}G'_{ep}, \tag{A20}$$

to express the following functions:

$$\mathcal{D}T_{A,p,1} = \tilde{g}_e\left[T_cg_{B,p} + g'_pT(3/2) + \frac{FD}{g_T\sqrt{\lambda_B}}\mathcal{F}(3/2)\right] + W_A[T_cg_{B,T} + g_TT(3/2)],$$

$$\mathcal{D}T_{A,e,1} = \tilde{g}'_p\left[T_cg_{B,e} + g_eT(3/2) - \frac{FD}{g_T\sqrt{\lambda_B}}\mathcal{F}(3/2)\right] + W_A[T_cg_{B,T} + g_TT(3/2)],$$

$$\mathcal{D}T_{A,p,N} = \tilde{g}_e\left[T_hg_{B,p} + g'_pT(N-1/2) + \frac{FD}{g_T\sqrt{\lambda_B}}\mathcal{F} \times (N-1/2)\right] + W_A[T_hg_{B,T} + g_TT(N-1/2)], \tag{A21}$$

$$\mathcal{D}T_{A,e,N} = \tilde{g}'_p\left[T_hg_{B,e} + g'_pT(N-1/2) + \frac{FD}{g_T\sqrt{\lambda_B}}\mathcal{F} \times (N-1/2)\right] + W_A[T_hg_{B,T} + g_TT(N-1/2)]. \tag{A22}$$

Multiplying Eq. (A15) by $\mathcal{D}$ and using the top two equations, we get

$$\mathcal{D}g_TT(1) = \alpha_1T_c + \alpha_2T(3/2) + \alpha_3F, \tag{A23}$$

$$\alpha_1 = g'_p\tilde{g}_eg_{B,p} + g_e\tilde{g}'_pg_{B,e} + g_Tg_{B,T}W_A, \tag{A24}$$

$$\alpha_2 = \tilde{g}_e(g'_p)^2 + \tilde{g}'_p(g_e)^2 + g_T^2W_A, \tag{A25}$$

$$\alpha_3 = \frac{D\mathcal{F}(3/2)}{g_T\sqrt{\lambda_B}}(g'_p\tilde{g}_e - g_e\tilde{g}'_p). \tag{A26}$$

Note that

$$g_T\mathcal{D} = \alpha_1 + \alpha_2. \tag{A27}$$

The similar expression for the hot end is

$$\mathcal{D}g_TT(N) = \alpha_1T_h + \alpha_2T(N-1/2) - \alpha_3F, \tag{A28}$$

since $\mathcal{F}(N-1/2) = -\mathcal{F}(3/2)$. We add the two expressions (A23) and (A28) and use the feature that $T(1) + T(N) = 2T(N_m)$, $T(3/2) + T(N-1/2) = 2T(N_m)$ to get

$$2g_T\mathcal{D}T(N_m) = 2\alpha_1\bar{T} + 2\alpha_2T(N_m). \tag{A29}$$

This equation proves that $T(N_m) = \bar{T}$, as asserted earlier. Next we subtract these two expressions to get ($\Delta T = T_h - T_c$)

$$g_T\mathcal{D}[T(N) - T(1)] = (T_h - T_c)\alpha_1 + [T(N-1/2) - T \times(3/2)]\alpha_2 - 2\alpha_3F,$$

$$C(N-1)(\alpha_1 + \alpha_2) = \Delta T\alpha_1 + C(N-2)\alpha_2 - 2\alpha_3F. \tag{A30}$$

Rearranging gives

$$\alpha_1\Delta T = C[\alpha_1(N-1) + \alpha_2] + 2\alpha_3F. \tag{A31}$$

This is our second of the three equations for the coefficients. Clearly, $C \sim \Delta T/N$. For the third equation, we use Eq. (A8):

$$0 = \mathcal{D}[G_{pp}T_{A,p,1} + G_{ep}T_{A,e,1}] - \mathcal{D}[g_pT(1) - F\mathcal{L}_c], \tag{A32}$$

$$0 = [\mathcal{D}L_c + \beta_3]F - g_p\mathcal{D}T(1) + \beta_1T_c + \beta_2T(3/2), \tag{A33}$$

$$\beta_1 = G_{pp}\tilde{g}_eg_{B,p} + G_{ep}\tilde{g}'_pg_{B,e} + g_pg_{B,T}W_A, \tag{A34}$$

$$\beta_2 = G_{pp}\tilde{g}_eg'_p + G_{ep}\tilde{g}'_pg_e + g_pg_TW_A, \tag{A35}$$

$$\beta_3 = \frac{D\mathcal{F}(3/2)}{g_T\sqrt{\lambda_B}}[D + G_{pp}g_{B,e} - G_{ep}g_{B,p}]. \tag{A36}$$

The results can be expressed as a matrix

$$\begin{bmatrix} 1 & N_m & 0 \\ 0 & M_{22} & M_{23} \\ M_{31} & M_{32} & M_{33} \end{bmatrix}\begin{bmatrix} T_0 \\ C \\ F \end{bmatrix} = \begin{bmatrix} \bar{T} \\ \alpha_1\Delta T \\ \beta_1T_c \end{bmatrix}, \tag{A37}$$

where

$$M_{22} = \alpha_1(N-1) + \alpha_2 = 2N_m\alpha_1 + (\alpha_2 - 2\alpha_1), \quad \text{(A38)}$$

$$M_{23} = 2\alpha_3 \quad M_{31} = g_p\mathcal{D} - \beta_2 = \beta_1, \quad \text{(A39)}$$

$$M_{32} = g_p\mathcal{D} - \tfrac{3}{2}\beta_2 = \beta_1 - \tfrac{1}{2}\beta_2, \quad \text{(A40)}$$

$$M_{33} = -\beta_3 - \mathcal{D}L_c. \quad \text{(A41)}$$

The determinant of the 3×3 matrix is

$$\mathcal{M} = M_{22}M_{33} - M_{23}M_{32} + N_m\beta_1 M_{23} \quad \text{(A42)}$$

$$= N_m[2\alpha_1 M_{33} + \beta_1 M_{23}] + [(\alpha_2 - 2\alpha_1)M_{33} - M_{23}M_{32}] \quad \text{(A43)}$$

and the coefficients are

$$T_0 = T_c + \frac{\Delta T}{2\mathcal{M}}[(\alpha_2 - 2\alpha_1)M_{33} - M_{23}M_{32}], \quad \text{(A44)}$$

$$C = \frac{\Delta T}{2\mathcal{M}}[2\alpha_1 M_{33} + \beta_1 M_{23}] \approx \frac{\Delta T}{N}[1 + O(1/N)], \quad \text{(A45)}$$

$$F = \frac{\Delta T}{2\mathcal{M}}[\alpha_1\beta_2 - \alpha_2\beta_1]. \quad \text{(A46)}$$

The heat current from layer A to layer B is

$$J_Q = G_{pp}[T_{B,p,n+1/2} - T_{A,p,n}] + G_{ee}[T_{B,e,n+1/2} - T_{A,e,n}] + G_{ep}[T_{B,p,n+1/2} - T_{A,e,n}] + G_{ep'}[T_{B,e,n+1/2} - T_{A,p,n}] \quad \text{(A47)}$$

$$= g_T[T(n+1/2) - T(n)] = \frac{g_T C}{2} \quad \text{(A48)}$$

$$= \frac{\Delta T}{\mathcal{R}_T}, \quad \text{(A49)}$$

$$\mathcal{R}_T = \frac{N_i}{g_T} + \mathcal{R}_L + \mathcal{R}_R, \quad \text{(A50)}$$

$$\mathcal{R}_{L,R} = \frac{1}{g_T}\frac{2\alpha_2 M_{33} + \beta_2 M_{23}}{2\alpha_1 M_{33} + \beta_1 M_{23}}, \quad \text{(A51)}$$

where the number of interfaces between layers is $N_i = 2(N-1)$. We tried writing out this result using the definitions of the terms, but the result is quite long.

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