Calculation of thermal boundary resistance based on the analysis of elastic waves propagating at the interface

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Abstract. This work presents a method for calculating thermal boundary resistance under the assumption of the acoustic mismatch model based on the propagation of elastic waves at the interface. The main problem is to determine the energy transfer coefficient from one material to another. Its solution requires an analysis of the reflection and refraction of acoustic waves at the interface. The most important feature of the presented model is the consideration of all types of waves propagating in solids. When the solid-solid interface is smooth at low temperature, the obtained results are in good agreement with the experiment.

1. Introduction

Thermal boundary resistance is an important topic in the field of electronics cooling and cryogenic superconducting thin films and is an essential parameter in the development of electronic devices, such as thermoelectric materials, superconducting thin films, thin semiconductor films, high-power chip design, etc [1, 2]. The study of thermal boundary resistance aims not only at studying macroscopic characteristics, but also at taking into account the size effect and the phonon scattering mechanism in heat transfer processes [3].

The phenomenon of thermal boundary resistance was discovered by Kapitza in experiments with liquid helium and copper [4]. The thermal boundary conductance $\sigma_B$ is defined as the ratio of the net heat flux $q$ through the interface to the temperature difference $\Delta T$: $\sigma_B = q/\Delta T$, and thermal boundary resistance is $R_B = 1/\sigma_B$. At first theory of thermal boundary resistance between liquid helium and solid was presented by Khalatnikov [5].

The thermal boundary resistance also appears between two solid materials. This phenomenon is related to the refraction and reflection at the boundary. The theory based on phonon scattering is known as the acoustic mismatch model (AMM) [6]. For multilayer systems this problem has been examined previously in [2, 7]. For “metal-dielectric” interfaces the theory of AMM has been recently improved by taking into account the adhesive interaction and anharmonicity of atomic vibrations in [8].

This work is devoted to further development of an acoustic mismatch model for calculating thermal boundary resistance. This method is based on the propagation of elastic waves at the interface. The main problem is to determine the energy transfer coefficient from one material to another. This task requires an analysis of the reflection and refraction of acoustic waves at the interface [9]. The key features of our model are as follows. 1) All types of waves propagating in solids are taken into account,
and 2) the amplitudes of reflected and refracted waves satisfy the law of energy conservation on the interface.

2. Calculation Method
At first let us discuss the principle scheme of the reflection and refraction of elastic waves at the interface (figure 1). The incident wave can be either a longitudinal wave, P-wave, or one of two types of transverse waves, SV-wave or SH-wave.

The materials 1 and 2 have different physical properties. The characteristics of material 1, determining the elastic wave propagation at interfaces, are the Lame coefficients \(\lambda, \mu\), the substance density \(\rho\), as well as the transverse and longitudinal acoustic velocities \(c_T, c_L\), and the constants of material 2 into which refraction takes places, are designated by superscripts B, i.e., they are denoted as by \(\lambda^B, \mu^B, \rho^B, c_T^B, c_L^B\).

![Figure 1. Principle scheme of elastic wave propagating at the interface made of two different materials.](image)

Due to different sound velocities of the incident waves, the types and angles of reflected and refracted waves, amplitude ratios, and corresponding critical angles are quite different. In order to determine the energy transmission coefficient, it is necessary to consider the reflection and refraction distribution of the incident wave \(P\), as well as SV and SH waves, respectively. Moreover, since the acoustic parameters of the two materials are different, the propagation of the elastic wave at the interface needs to be analyzed in two directions.

Based on the elastic wave interface propagation analysis, the following algorithm is used to calculate the thermal boundary resistance between two solids (see figure 2).

2.1. Block of amplitude determination
The first step of the calculation is to determine the system of equations for ratios of amplitudes: \(A_1/A_0, A_2/A_0, A_3/A_0, A_4/A_0\). This system is derived from the continuity conditions of deformation at the interface between two different materials (in two directions: along the interface and normal to the interface), and continuity of stress. For the perfect contact, the displacements and stresses are continuous along directions \(x_1\) and \(x_2\) (figure 1):

\[
\mu_j^{(0)} + \mu_j^{(1)} + \mu_j^{(2)} = \mu_j^{(3)} + \mu_j^{(4)} \tag{1}
\]

\[
\tau_{2j}^{(0)} + \tau_{2j}^{(1)} + \tau_{2j}^{(2)} = \tau_{2j}^{(3)} + \tau_{2j}^{(4)} \tag{2}
\]

where \(j = 1, 2\). The stresses are obtained by using Hook’s law:

\[
\tau_{22}^{(n)} = i k_n \left[ (\lambda + 2\mu) a_2^{(n)} p_2^{(n)} + \lambda a_1^{(n)} p_1^{(n)} \right] A_n \exp(i\eta_n) \tag{3}
\]
\[ \tau_{21}(n) = i k_n \mu \left[ \epsilon_{2}^{(n)} p_{1}^{(n)} + d_{1}^{(n)} p_{2}^{(n)} \right] A_n \exp(i\eta_n). \#(4) \]

Index \( n \) represents the type of waves – incident, reflected or refracted – as in figure 1.

Figure 2. Block diagram of developed algorithm to calculate the thermal boundary resistance between two solids.
Since the incident wave is longitudinal (P-wave), the system of equations (1)-(2) at the interface in matrix notation can be written as

\[
\begin{bmatrix}
-\sin \theta_1 & -\cos \theta_2 & \sin \theta_3 & -\cos \theta_4 \\
\cos \theta_1 & -\sin \theta_2 & \cos \theta_3 & \sin \theta_4 \\
\sin 2\theta_1 & \frac{c_l c_2}{c_T} \cos 2\theta_2 & \frac{\mu B c_l}{\mu c_T} \sin 2\theta_3 & -\frac{\mu B c_l}{\mu c_T} \cos 2\theta_4 \\
-\frac{c_l^2}{c_T} \cos 2\theta_2 & \frac{c_l}{c_T} \sin 2\theta_2 & \frac{\mu B c_l c_l^B}{\mu c_T^2} \cos 2\theta_4 & \frac{\mu B c_l}{\mu c_T} \sin 2\theta_4 \\
\end{bmatrix}
\begin{bmatrix}
A_1 \\
A_2 \\
A_3 \\
A_4 \\
\end{bmatrix}
= A_0
\begin{bmatrix}
\sin \theta_0 \\
\cos \theta_0 \\
\sin 2\theta_0 \\
\sin 2\theta_0 \\
\end{bmatrix}
\]  

(5)

By solving the system of four equations we can get the amplitude ratios, \( A_1/A_0, A_2/A_0, A_3/A_0, A_4/A_0 \) which depend on the incident angle \( \theta_0 \). Similarly, we can get the systems with transverse incident waves (SV and SH waves).

2.2. Block of transmission probability

The average energy transmissions per unit area for longitudinal (L) and transverse (T) waves may be expressed as

\[
\bar{\rho}_L = \frac{1}{2} \left( \lambda + 2\mu \right) \frac{\omega^2}{c_l} A^2 \#(6)
\]

\[
\bar{\rho}_T = \frac{1}{2} \mu \frac{\omega^2}{c_T} A^2 \#(7)
\]

Based on the obtained amplitude ratios, energy balances are considered for different incident angles, including energy transfer through the interface by reflected waves and energy carried by refracted waves. According to equation (6) and (7) and the transmission area ratio of different waves at the interface, the energy balance equation for incident longitudinal wave has the form:

\[
\left( \frac{A_1}{A_0} \right)^2 + \left( \frac{A_2}{A_0} \right)^2 \frac{\mu}{\lambda + 2\mu} c_l \cos \theta_2 + \left( \frac{A_3}{A_0} \right)^2 \frac{\lambda^B + 2\mu^B c_l \cos \theta_3}{\lambda + 2\mu} c_l \cos \theta_0 + \left( \frac{A_4}{A_0} \right)^2 \frac{\mu^B c_l \cos \theta_4}{\lambda + 2\mu} c_T \cos \theta_0 = 1 \#(8)
\]

Based on the numerical calculation for each incident angle, the sum of the energy of other waves is always equal to the incident wave energy satisfying the energy conservation condition of elastic wave propagation at the interface.

Next step is to determine the phonon transmission probability, that is, the ratio of energy transferred to another material when acoustic wave is incident on the interface between two materials: from material 1 to material 2 \( \Pi_{1\to2} \), and in the opposite direction \( \Pi_{2\to1} \). These values are equal to the ratios of the energy transmitted through the interface to the energy incident on it and depend on the amplitudes \( A_3/A_0 \) and \( A_4/A_0 \):

\[
\Pi_{1\to2}(\theta_0) = \begin{cases} 
\left( \frac{A_3}{A_0} \right)^2 \rho^B \frac{c_l^B \cos \theta_3}{\rho \ c_j \cos \theta_0} + \left( \frac{A_4}{A_0} \right)^2 \rho^B \frac{c_T^B \cos \theta_4}{\rho \ c_j \cos \theta_0}, & 0 \leq \theta_0 < \theta_{cr1} \\
\left( \frac{A_4}{A_0} \right)^2 \rho^B \frac{c_T^B \cos \theta_4}{\rho \ c_j \cos \theta_0}, & \theta_{cr1} \leq \theta_0 < \theta_{cr2} \\
0 , & \theta_{cr2} \leq \theta_0 \leq \frac{\pi}{2} 
\end{cases}
\]  

(9)

\[
\Pi_{2\to1}(\theta_0) = \begin{cases} 
\left( \frac{A_3}{A_0} \right)^2 \rho^B \frac{c_l^B \cos \theta_3}{\rho \ c_j \cos \theta_0} + \left( \frac{A_4}{A_0} \right)^2 \rho^B \frac{c_T^B \cos \theta_4}{\rho \ c_j \cos \theta_0}, & 0 \leq \theta_0 < \theta_{cr1} \\
\left( \frac{A_4}{A_0} \right)^2 \rho^B \frac{c_T^B \cos \theta_4}{\rho \ c_j \cos \theta_0}, & \theta_{cr1} \leq \theta_0 < \theta_{cr2} \\
0 , & \theta_{cr2} \leq \theta_0 \leq \frac{\pi}{2} 
\end{cases}
\]  

(10)

Where using the Snell’s law: \( \cos \theta_3 = [1 - (c_l^B/c_l)^2 \sin^2 \theta_0]^{1/2}, \cos \theta_4 = [1 - (c_T^B/c_l)^2 \sin^2 \theta_0]^{1/2} \).
2.3. Block of heat flux and Kapitza resistance

As an example, let us consider the heat flux transferred through the interface when a longitudinal wave is incident from material 1. Then the heat flux is written as:

\[
q^p_{1\rightarrow 2} = \frac{1}{4\pi} \int_0^{\pi/2} \int_0^{\omega_{\text{max}}} \hbar \omega f(\omega, T_1) D(\omega) \Pi_{1\rightarrow 2}(\theta_0) \cos \theta_0 \sin \theta_0 d\theta_0 d\phi d\omega \quad (#11)
\]

where \(f(\omega, T_1)\) is the Bose-Einstein phonon distribution function in the first medium, and \(D(\omega) = \omega^2 (2\pi^2 c_L^2)^{-1}\) is the phonon density of states.

The equation of heat fluxes transferred through the interface is written as:

\[
q^p = q^p_{1\rightarrow 2} - q^p_{2\rightarrow 1}, \quad p = P, SV, SH \quad (#12)
\]

The thermal boundary resistance can now be obtained as \(R^p_B = (T_1 - T_2)/q^p\), and by assuming that the temperature difference is small [6], we can approximate \(R^p_B\) by

\[
R^p_B = \frac{30 \hbar^3 c_p^2}{\pi^2 k_B^4 \Gamma_{1\rightarrow 2}^p} \quad (#13)
\]

where \(\Gamma_{1\rightarrow 2}^p = 2 \int_0^{\pi/2} \Pi_{1\rightarrow 2}(\theta_0) \cos \theta_0 \sin \theta_0 d\theta_0\). And then the total thermal boundary resistance is obtained:

\[
R_B = \left( \frac{1}{R^P_B} + \frac{1}{R^SV_B} + \frac{1}{R^{SH}_B} \right)^{-1} \quad (#14)
\]

Theoretical calculations were carried out on the basis of the equations presented above for the interface between sapphire and lead. Material parameters \(\rho, c_T, c_L\) are taken from [10]. The calculation results of the interface between sapphire and lead are presented in Figure 3.

\[\text{Figure 3. The thermal boundary conductance } \sigma_B \text{ between sapphire and lead as a function of temperature.}\]

The feature of classical acoustic mismatch model [6, 13, 14] is that the transfer is taken into account only by longitudinal waves (not by the transverse one). A number of other factors also remain unconsidered (for example, the critical angles of incident waves, etc.). However, in our model, the thermal boundary resistance of the P wave, SV wave, and SH wave are calculated separately, taking into account the critical angle. For the first time, the thermal boundary resistance was obtained during
the heat flux from material 1 and from material, separately. In this case, our theoretical calculation results are in good agreement with the experimental results.

3. Conclusion

A complete theoretical calculation of the thermal boundary resistance using the framework of the acoustic mismatch model (AMM) has been performed. Both reflection and refraction of the elastic waves are considered separately in different incident waves (one longitudinal P-wave and two types of transverse SV-wave and SH-wave) and different heat flux directions (from material 1 to material 2 and backwards, $2 \rightarrow 1$). The relationships between the energy propagation coefficient and the incident angle have been obtained (9, 10).

We have found that the calculation under the framework of the acoustic mismatch model needs to satisfy the following condition: the wavelength of the elastic wave is greater than the average roughness of the interface. Highly accurate results have been achieved based on elastic wave propagation at the interface. Specifically, at low temperature, when the solid-solid interface is smooth, the obtained results are in a good agreement with the experimental data (see figure 3).

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References

[1] Khvesyuk V I 2016 Tech. Phys. Let. 42 (10) 985
[2] Khvesyuk V I and Barinov A A 2017 J. Phys. Conf. Ser. 891 012352
[3] Khvesyuk V I and Scryabin A S 2017 High Temp. 55 (3) 434
[4] Kapitza P L 1941 J. Phys. USSR 4 181
[5] Khalatnikov I M 1952 Zh. Eksp. Teor. Fiz. 22 687
[6] Little W A 1959 Can. J. Phys. 37 334
[7] Khvesyuk V I and Chirkov A Yu 2017 J. Phys. Conf. Ser. 891 012330
[8] Slepenv A G 2017 Physics of the Solid State 59 (7) 1468
[9] Swartz E and Pohl R 1989 Rev. Mod. Phys. 61 605
[10] Zhang Z M 2007 Nano/Microscale Heat Transfer (N.Y.: Mc Grow Hill) p 479
[11] Achenbach J D 1973 Wave Propagation in Elastic Solids (N.Y.: Elsevier Pub. Co.) p 165
[12] Nitsche F and Schumann B 1980 J. Low. Temp. Phys. 39 119
[13] Peterson R E and Anderson A C 1973 J. Low Temp. Phys. 11 639
[14] Cheeke J D N, Ettinger H and Herbal B 1976 Can. J. Phys. 54 1749