A new look at Kapitza conductance calculation (thermal boundary resistance)

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Abstract. The Kapitza resistance of the sapphire-lead interface was calculated using the propagation analysis of the elastic wave at the interface; results are in a good agreement with the experimental data. We present a detailed analysis of the elastic wave propagation at the interface between two different materials. The energy distribution of the waves transmitted through the interface as a function of the incident angle is obtained to calculate the Kapitza resistance. For the first time, the Kapitza resistance was determined during the heat flux from both sides: from the sapphire side and from the lead side.

1. Introduction

In 1941, Kapitza reported the discovery of a temperature jump at the interface between liquid helium and copper when the heat flow passes [1]. This phenomenon is associated with the presence of heat transfer resistance, which appears at the interface between two objects of different materials. It is called the Kapitza resistance. In 1952, Khalatnikov presented the acoustic mismatch model (AMM) for calculating the phenomena that occur on the contact surfaces between two materials when the heat flow through [2]. The essence of this model is that when an elastic wave passes through the interface of two contact objects, it transfers energy from one of them accompanied by reflection and refraction. The reflection of waves leads to heat resistance and occurs the temperature jump. In the same year, an independently similar model was proposed in [3] devoted to the study of energy transfer by seismic waves across the rock-water boundary. In work [3] the problem of determining the thermal resistance is not proposed, but the problem of determining the amplitude of the reflected wave and the refracted wave is completely solved. This work is usually not referred to, but it contains a more accurate version of the theory. Further, the AMM model was developed in order to determine the Kapitza resistance between two solids [4].

It is well-known that in the study of heat transfer between different solids, the AMM model is used for process analysis at low temperatures under assumption that the wavelength is greater than the roughness. This guarantees the specular reflection of the elastic wave at the interface, which is assumed in this work. When this approximation is violated, the diffusion mismatch model (DMM), proposed in [4], is used to calculate Kapitza resistance. In the framework of both models, the connection between the temperature jump at the interface $T_i - T_s$ and the heat flux $q$ passing through is given by:
where \( \sigma_x \) – Kapitza conductance. The reciprocal \( h_x = \sigma_x^{-1} \) is called Kapitza resistance.

Thus, the problem of heat transfer through contact surfaces between two objects is transformed into determining the indicated variables and their dependencies on temperature and the properties of the corresponding materials. In this case, two semi-infinite solids that are in contact with each other are generally considered. The properties of materials, on which the intensity of heat transfer by acoustic waves depends, are the Lame coefficients, \( \lambda, \mu \), density of the substance, \( \rho \), as well as transverse and longitudinal velocities \( c_T, c_L \), which are determined using these values.

Often during the consideration of macroscopic thermal physics the Kapitza resistance is neglected [5]. However, in nanoscale structures (for example multilayers or superlattices [6, 7]) contribution of Kapitza resistance in general thermal resistance becomes significant [8, 9]. Therefore, the development of a reliable method of calculation of the Kapitza resistance becomes very important. The purpose of this paper is to give a detailed calculation method for determining Kapitza resistance based on AMM model (corresponding to two oppositely directed heat fluxes, both from the first material to the second and in the opposite direction).

2. Calculation Method

Figure 1 shows the modes that must be considered when calculating the heat transfer through the interface: \( p^{(0)} \) – wave incident on interface (amplitude \( A_0 \)). It can be either a longitudinal wave (P-wave) or a transverse wave (SV- or SH-wave). Further, \( p^{(1)} \) – the reflected wave of the same type as the incident wave (amplitude \( A_1 \)), \( p^{(2)} \) – the reflected wave of a different type from the incident wave (amplitude \( A_2 \)), \( p^{(3)} \) – refracted wave of the same type as the incident wave (amplitude \( A_3 \)), \( p^{(4)} \) – refracted wave different from the type of incident wave (amplitude \( A_4 \)).

The following is the sequence of Kapitza resistance calculations.

1) The amplitude ratios of the reflected and refracted waves to the incident wave \( (A_0/A_1), (A_0/A_2), (A_0/A_3), (A_0/A_4) \) are depended on the angle of the wave incident on the interface. These values are determined in the case where the incident wave is a longitudinal wave and a transverse wave, respectively. In addition, such calculations are carried out both from the side of the material with higher temperature and from the side of the material with low temperature. System of equations for determining these quantities is obtained from the boundary conditions on the interface surface. The boundary conditions are obtained from the requirement of continuity of deformations and stresses at the interface between two materials during the transition from material 1 to material 2 [10].

When the incident wave is a longitudinal wave, the system of equations used to determine the relative amplitudes of the various waves at the interface is depended on the angle of incidence:

\[
A_3 \sin \theta_3 + A_4 \sin \theta_4 + A_3 \cos \theta_3 - A_4 \sin \theta_4 + A_4 \cos \theta_4 = 0
\]  \hspace{1cm} (2)

\[
A_3 \cos \theta_3 - A_4 \cos \theta_4 + A_2 \sin \theta_2 - A_3 \cos \theta_3 - A_4 \sin \theta_4 = 0
\]  \hspace{1cm} (3)
Based on the obtained results, we determine energy balances on both sides, including energy transfer through the interface by elastic waves and energy reflection at the interface of the two materials. For the longitudinal incident wave from one side of two materials, the energy balance equation has the form:

\[ \frac{A_3 \sin (2 \theta_s)}{\mu} - A_1 \frac{c_\lambda \cos (2 \theta_s)}{\mu} - A_2 \frac{c_\mu \mu \cos (2 \theta_s)}{\mu} + A_4 \frac{c_\mu \mu \sin (2 \theta_s)}{\mu} = 0 \]  

(4)

\[ A_6 \frac{\lambda + 2 \mu \cos^2 \theta_s}{\mu} + A_1 \frac{c_\lambda \cos \theta_s}{\mu} - A_2 \frac{c_\mu \mu \cos \theta_s}{\mu} - A_3 \frac{c_\lambda \lambda \mu \sin \theta_s}{\mu} - A_4 \frac{\lambda + 2 \mu \cos^2 \theta_s}{\mu} = 0 \]  

(5)

2) Based on the obtained results, we determine energy balances on both sides, including energy transfer through the interface by elastic waves and energy reflection at the interface of the two materials. For the longitudinal incident wave from one side of two materials, the energy balance equation has the form:

\[ \left( \frac{A_3}{A_0} \right)^2 + \left( \frac{A_4}{A_0} \right)^2 \frac{c_\lambda \cos \theta_s}{\mu} + \left( \frac{A_1}{A_0} \right)^2 \frac{c_\mu \mu \cos \theta_s}{\mu} + \left( \frac{A_2}{A_0} \right)^2 \frac{c_\mu \mu \cos \theta_s}{\mu} = 1 \]  

(6)

where each term is the energy of the corresponding waves (reflected and refracted waves), referred to the energy of the wave incident on the interface. That is, they are the relative fractions of the corresponding waves in the total energy balance.

3) Next we obtain the fraction of energy transferred through the interface from side 1 to side 2 – \( \Pi_{1 \rightarrow 2} \) and in the opposite direction – \( \Pi_{2 \rightarrow 1} \), that is important for determining the Kapitza resistance (conductance). \( \Pi_{1 \rightarrow 2} \) and \( \Pi_{2 \rightarrow 1} \) are equal to the ratios of the energies transmitted through the interface to the energy incident on it and depend on the amplitudes \( \left( A_j / A_k \right) \) and \( \left( A_j / A_k \right) \). When there is no full internal reflection at the interface, the corresponding expression is:

\[ \Pi_{1 \rightarrow 2}(\theta_s) = \left( \frac{A_3}{A_0} \right)^2 \frac{c_\lambda \cos \theta_s}{\mu} + \left( \frac{A_4}{A_0} \right)^2 \frac{c_\mu \mu \cos \theta_s}{\mu} \]  

(7)

In terms of energy transfer by elastic waves the total internal reflection has an important feature compared to the refraction of an electromagnetic wave. It lies in the fact that there are two critical angles. One is when the refracted longitudinal wave is reflected, the second is when the refracted transverse wave is reflected.

\[ \Pi_{1 \rightarrow 2}(\theta_s) = \left( \frac{A_3}{A_0} \right)^2 \frac{c_\lambda \cos \theta_s}{\mu} + \left( \frac{A_4}{A_0} \right)^2 \frac{c_\mu \mu \cos \theta_s}{\mu}, \quad 0 \leq \theta_0 \leq \theta_{crit} \]  

(8)

where \( \theta_{crit} \) – the first critical angle, \( \theta_{crit} \) – the second critical angle.

Figure 2 shows the dependence of energy transmitted by the elastic wave on the angle of incidence at the sapphire-lead interface. Since the velocity of longitudinal wave is greater than the velocity of transverse wave, the angle between longitudinal wave and the interface normal is always greater than the angle of transverse wave.

3) The equation of heat fluxes transferred through the interface by incident longitudinal wave is written as:

\[ q^i = q_{1 \rightarrow 2} - q_{2 \rightarrow 1} \]  

(9)

and by incident transverse wave:

\[ q^i = q_{1 \rightarrow 2} - q_{2 \rightarrow 1} \]  

(10)

We assume that the velocity of acoustic waves in medium 1 is less than the velocity in medium 2, that is, there is no total internal reflection. As an example, let us consider the heat flux transferred through the interface when a longitudinal wave is incident on it:
\[ q_{1 \to 2} = \frac{1}{4\pi} \int \int \int \hat{h}(\omega) \cdot f_s(\omega, T_i) \cdot \Pi_{1 \to 2}(\theta, \phi) \cdot \cos \theta \cdot \sin \theta \cdot d\theta \cdot d\phi \cdot d\omega \]  \quad (11)

where \( f_s(\omega, T_i) \) - Bose-Einstein phonon distribution function in the first medium, \( D(\omega) = \omega^2 / (2\pi^2 c_s^3) \) - phonon density of states. Separately, the integral is calculated

\[ \Gamma_{1 \to 2}(\theta, \phi) = \frac{1}{4\pi} \int \int \Pi_{1 \to 2}(\theta, \phi) \cdot \cos \phi \cdot d\theta \cdot d\phi = \frac{1}{2} \int \int \Pi_{1 \to 2}(\theta) \cdot \cos \phi \cdot \sin \phi \cdot d\theta \cdot d\phi \]  \quad (12)

and we have

\[ q_{1 \to 2} = \Gamma_{1 \to 2}(\theta, \phi) \int_{0}^{\pi} \frac{\hat{h}(\omega) \cdot d\omega}{2\pi^2 c_s^3} \left[ \exp \left( \frac{\hat{h}(\omega)}{k_s T_i} \right) - 1 \right] = \frac{\Gamma_{1 \to 2}(\theta, \phi) k_s^4 T_i^4}{2\pi^2 c_s^3 h^3} \int_{0}^{\pi} x^3 \cdot e^x - 1 \]  \quad (13)

\[ \frac{E_1}{E_0} \begin{array}{c|c|c|c} \theta_0 \text{(deg)} & 0 & 20 & 40 & 60 & 80 & 100 \\ \hline 3+4 & 1 & 0.8 & 0.6 & 0.4 & 0.2 & 0 \\ 3 & 1 & 0.8 & 0.6 & 0.4 & 0.2 & 0 \\ 4 & 1 & 0.8 & 0.6 & 0.4 & 0.2 & 0 \\ \end{array} \]

\[ \frac{E_1}{E_0} \begin{array}{c|c|c|c} \theta_0 \text{(deg)} & 0 & 20 & 40 & 60 & 80 & 100 \\ \hline 3+4 & 1 & 0.8 & 0.6 & 0.4 & 0.2 & 0 \\ 3 & 1 & 0.8 & 0.6 & 0.4 & 0.2 & 0 \\ 4 & 1 & 0.8 & 0.6 & 0.4 & 0.2 & 0 \\ \end{array} \]

**Figure 2.** The energy distribution of the waves transmitted through the sapphire-lead interface (a) and from sapphire to lead (b): 3 – longitudinal wave, 4 – transverse wave. 12.5° – the first critical angle \( \theta_{cr1} \), 22° – the second critical angle \( \theta_{cr2} \).

Similarly, the expression for \( q_{1 \to 1} \) is obtained. The final expression for \( q' \) is:

\[ q' = \frac{k_s^4}{2\pi^2 h^3} \left[ \frac{\Gamma_{1 \to 2}(\theta, \phi) T_i^4}{c_s^3} \int_{0}^{\pi} x^3 \cdot e^x - 1 \right] \]

\[ \frac{\Gamma_{1 \to 2}(\theta, \phi) k_s^4 T_i^4}{2\pi^2 c_s^3 h^3} \int_{0}^{\pi} x^3 \cdot e^x - 1 \]  \quad (14)

It should be noted that for \( T_i = T_2 \) equation (15) should be satisfied:

\[ \frac{\Gamma_{1 \to 2}(\theta, \phi) k_s^4 T_i^4}{2\pi^2 c_s^3 h^3} \int_{0}^{\pi} x^3 \cdot e^x - 1 \]

\[ \frac{\Gamma_{1 \to 2}(\theta, \phi) k_s^4 T_i^4}{2\pi^2 c_s^3 h^3} \int_{0}^{\pi} x^3 \cdot e^x - 1 \]  \quad (15)

Similar expressions are obtained for heat flux transferred by a transverse wave from medium 1 to 2. As a result, we obtain the total heat flux crossing the interface:

\[ q_z = q' + q'' \]  \quad (16)
4) Finally, using equation (1) Kapitza resistance was determined. For example, we consider sapphire-lead interface and use parameters $\rho, \varepsilon_1, \varepsilon_2$ from [4]. The calculation results are presented in figure 3 and compared with the experimental data [11]. As it is seen, results are in a good agreement with the experimental data for low roughness since we consider a specular reflection on the interface.

![Figure 3](image_url)

**Figure 3.** The thermal boundary resistance $r_s$ for sapphire-lead interface, multiplied by $T^2$, as a function of temperature $T$. Pb-Sapphire – theoretical value of Kapitza resistance when the heat flow is from lead to sapphire, Sapphire-Pb – from sapphire to lead, $r_s$ – surface roughness of the contact surface between sapphire and lead [11].

3. Conclusion

Numerical calculations were carried out on the basis of the equations (2)-(5) presented above for the sapphire-lead interface. The order of steps to calculate Kapitza resistance is as follows: first, specify the type of incident wave (longitudinal or transverse) and angle of incidence on the interface $\theta_0$, then determine the dependencies of the amplitudes of all reflected and refracted waves on $\theta_0$. After that, determine the coefficients of energy transfer (8) through the interface and obtain expressions for heat fluxes (14), (16). Finally, the equation for Kapitza resistance is obtained (1).

For the first time in this work the following consideration were taken into account.

1) The Kapitza resistance was determined during the heat flux from both sides: from the sapphire side and from the lead side. In this case, the differences are within ten percent.

2) The distribution of the amplitude of each wave is considered completely when the critical angle occurs. For example, when a longitudinal wave is incident, there are two critical angles: when the incident angle increases, the refracted longitudinal wave first reaches $90^\circ$, and then refracted transverse wave reaches $90^\circ$. In this case, in the region between these two critical angles, the amplitudes of the waves become complex. A similar situation occurs when the critical angle is reached by an electromagnetic wave [12]. For electromagnetic waves, one critical angle takes place, and the existence of the complex amplitude of the reflected wave is associated with the fact that when the angle of incidence exceeds the critical angle, the wave partially penetrates into the second material, and then reflects [12].

4. References

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