A generalized model of the Kapitza resistance

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Abstract. This work devoted to a new generalized model of Kapitza conductance. At present, the problem of the development of the theory of contact resistances between solids is particularly relevant due to growth of nanotechnology, where it plays an important and sometimes main role in the heat transport. Presented model takes into all specified properties of acoustic waves. First of all, it is refraction and reflection of acoustic waves that caused simultaneously both longitudinal and transverse waves. Secondly, it is considered the phenomenon of total internal reflection, which makes a significant contribution to the Kapitza resistance. These facts totally change the formulation of the problem, especially, the boundary conditions on the contact surface (interface). Results shows a good agreement with the experimental data, better than in previous works.

1. Introduction
The existence of a thermal boundary resistance between a solid (copper) and superfluid helium was the first time discovered by Kapitza in the presence of a heat flow [1]. This phenomenon is called Kapitza resistance. Heat transfer between two dissimilar substances is characterized by a temperature jump $T_1 - T_2$ caused on the interface by a heat flow $q$. It is described by thermal conductance Kapitza coefficient $\sigma_K$ defined by relation

$$q = \sigma_K (T_1 - T_2).$$

Often during the consideration of macroscopic thermal physics the Kapitza resistance is neglected. But at studying heat transfer within nanoscale structures (for example multilayers or superlattices) contribution of Kapitza resistance in general thermal resistance becomes significant [2]. Therefore the development of a reliable method of calculation of the Kapitza resistance is very important problem at present. In this letter the method of calculation of thermal boundary resistance is presented in the framework of acoustic mismatch model (AMM) [3, 4]. Initial idea of AMM is emergence of the resistance as a result of scattering of acoustic waves on the interface of two dissimilar materials. Unfortunately basic positions of [4] do not match to modern theory of reflection and transmission of acoustic waves on the interface of two dissimilar elastic solids [5]. In this work we formulated a generalized model based on the theory from the Achenbach book [5].

2. Basics of the generalized model
In this paper the propagation of plane harmonic waves in an infinite medium consisting of two joined elastic half-space of different material properties is considered. In such a composite
medium, systems of plane waves can superposed to represent an incident, reflection and refraction waves at the interface separating the two media. The unit propagation vectors of the system of incident $p^{(0)}$, reflected $p^{(1)}$ and $p^{(2)}$, refracted $p^{(3)}$ and $p^{(4)}$ waves are shown in figure 1 (following page). The material properties of medium carrying the incident and reflected waves are the Lame elastic constants $\lambda$, $\mu$ and the mass density $\rho$. The material constants of the second medium (where refraction waves propagate) are $\lambda^B$, $\mu^B$, $\rho^B$. The incident waves can be both longitudinal and transverse waves. Below is assumed that (0), (1), (3) are longitudinal (transverse) waves, (2) and (4) are transverse (longitudinal) waves.

Heat flow across interface is defined as

$$ q = q_{1\rightarrow2} - q_{2\rightarrow1}. $$

$q_{1\rightarrow2}$ – heat flow from half-space where incident wave is propagated to half-space where refracted waves are propagate, $q_{2\rightarrow1}$ – backward heat flow.

By assuming that phonons are equilibrium at either side, the heat flow from medium $i$ to medium $j$ can be expressed as

$$ q_{i\rightarrow j} = \int \int c_i\hbar f(T_i, \omega)\Pi_{i\rightarrow j}(\theta_0) D(\omega) \cos \theta_0 \sin \theta_0 d\theta_0 d\psi d\omega. $$

$\Pi_{i\rightarrow j}(\theta_0)$ – coefficient of energy transmission, $\theta_{cr}$ – critical angle, $\theta_0$ – see figure 1. The main problem is determination of $\Pi_{i\rightarrow j}(\theta_0)$. The solution of this problem is obtained on the basis of theory of wave propagation across interface of two dissimilar materials [2]. It includes two steps. First step is to receive the dependences of ratios of wave amplitudes $A_1/A_0$, $A_2/A_0$, $A_3/A_0$ and $A_4/A_0$ which are the function of $\theta_0$ – the angle between incident wave and the normal to the interface. Second step is computation of distribution of energy between different waves.

The set of equations for wave amplitudes that are derived from the condition of continuity of deformations and stresses at the interface:
\[ A_0 \sin \theta_0 + A_1 \sin \theta_1 + A_2 \cos \theta_2 - A_3 \cos \theta_3 + A_4 \cos \theta_4 = 0, \]  
\[ A_0 \cos \theta_0 - A_1 \cos \theta_1 + A_2 \sin \theta_2 - A_3 \sin \theta_3 - A_4 \sin \theta_4 = 0, \]  
\[ A_0 \sin(2\theta_0) - A_1 \sin(2\theta_1) - A_2 \frac{c_L}{c_T} \cos \theta_2 - A_3 \frac{\mu_B}{\mu} \frac{c_L}{c_L} \sin(2\theta_3) + A_4 \frac{\mu_B}{\mu} \frac{c_L}{c_T} \cos(2\theta_4) = 0, \]  
\[ A_0 \left( \frac{\lambda}{\mu} + 2 \cos^2 \theta_0 \right) + A_1 \left( \frac{\lambda}{\mu} + 2 \cos^2 \theta_1 \right) - A_2 \frac{c_L}{c_T} \sin(2\theta_2) - A_3 \frac{\mu_B}{\mu} \frac{c_L}{c_L} \left( \frac{\lambda}{\mu} + 2 \frac{\mu_B}{\mu} \cos^2 \theta_3 \right) - A_4 \frac{\mu_B}{\mu} \frac{c_L}{c_T} \sin(2\theta_4) = 0. \] 

In equations (3)–(6) is assumed that incident wave is longitudinal wave, \( \theta_0, \theta_1, \theta_2, \theta_3 \) and \( \theta_4 \) are shown in figure 1; \( c_L, c_L^T \) – velocities of the longitudinal waves in materials 1 and 2; \( c_T, c_T^L \) are velocities of the transverse waves in materials 1 and 2. The energy conservation equation is written as

\[ \left( \frac{A_1}{A_0} \right)^2 + \left( \frac{A_2}{A_0} \right)^2 \frac{c_T}{c_L} \cos \theta_2 + \left( \frac{A_3}{A_0} \right)^2 \frac{c_B}{c_L} \cos \theta_3 + \left( \frac{A_4}{A_0} \right)^2 \frac{c_T}{c_T} \cos \theta_4 = 1. \]  

The first member on the left side is the part of full energy that leaves interface with reflected longitudinal wave. Second member is the relative energy of reflected transverse wave, third member is the relative energy of refracted longitudinal wave, and fourth member is the relative energy of refracted transverse wave. Therefore the transmission energy from one side to second side is

\[ \Pi_{i \rightarrow j}(\theta_0) = \left( \frac{A_3}{A_0} \right)^2 \frac{c_B}{c_L} \cos \theta_3 + \left( \frac{A_4}{A_0} \right)^2 \frac{c_T}{c_T} \cos \theta_4, \]  
\[ \text{where} \quad \cos \theta_3 = \sqrt{1 - \left( \frac{c_L^T}{c_L} \right)^2 \sin^2 \theta_0}, \quad \cos \theta_4 = \sqrt{1 - \left( \frac{c_L^T}{c_L} \right)^2 \sin^2 \theta_0}. \]

Using equations 2 and 4 the value \( q_{1 \rightarrow 2} \) can be determined.

### 3. Method of determination of Kapitza conductivity

In this section the method of computation of Kapitza conductance based on the set of equations (1)–(8) is presented.

Step 1. First of all, it needs to set of material properties. Then equations (3)–(6) are solved for both conditions: when incident wave is longitudinal wave and when incident wave is transverse wave.

Step 2. Secondly, the procedure of the determination of Kapitza conductivity is performed. The values \( q_{1 \rightarrow 2}^1 \) and \( q_{2 \rightarrow 1}^1 \) are determined in case when incident wave is longitudinal wave. The values \( q_{1 \rightarrow 2}^2 \) and \( q_{2 \rightarrow 1}^2 \) are determined in case when incident wave is transverse wave.

Step 3. Using these results we determine the heat flow across interface transmitted both longitudinal \( (q^l) \) and transverse \( (q^t) \) waves:

\[ q^l = \frac{1}{3} (q_{1 \rightarrow 2}^1 - q_{2 \rightarrow 1}^1), \]  
\[ q^t = \frac{2}{3} (q_{1 \rightarrow 2}^1 - q_{2 \rightarrow 1}^1). \] 

Factors in equations (9) and (10) take into account that in an infinite medium contains one longitudinal and two transverse waves.
Step 4. Determine the Kapitza conductivities $\sigma_K^l$ and $\sigma_K^t$ from equations 9 and 10. Final result is

$$ \sigma_K = \sigma_K^l + \sigma_K^t. \quad (11) $$

As an example of calculation of Kapitza conductivity the thermal contact between copper and superfluid helium is considered. As a result the following formula was obtained:

$$ \sigma_K = \frac{\pi^2 k_B^4}{30 \hbar^3 c_1^2} T^3. \quad (12) $$

On figure 2 the estimations show that calculation by this formula agrees well with experimental data [6]. For example for $T = 1.5$ K, $\sigma_K = 1.555$ kW/m$^2$K.

4. Conclusion
In this work the generalized method of determination of Kapitza conductivity is presented. It based on the theory of acoustic waves propagation across interface of two dissimilar solids [5]. All possible reflected and refracted waves are taken into account. Preliminary calculations show that if incident wave is longitudinal wave, then refracted and reflected transverse waves bring relatively small contribution in energy transmission across interface between two solids. The set of equation presented here requires detailed study.

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