Development of acoustic and diffuse mismatch models for predicting the Kapitza resistance

V I Khvesyuk1, B Liu and A A Barinov2

Bauman Moscow State Technical University, 2nd Baumanskaya Street 5, Moscow, 105005, Russia

E-mail: 1khvesyuk@bmstu.ru, 2barinove6@bmstu.ru

Abstract. This paper is devoted to the acoustic mismatch model and diffusion mismatch model of Kapitza thermal resistance. We consider that diffusion in the transition layer can be represented by variable composition and finite thickness instead of previous assumptions of a “black box” approximation. The effect of heat flow on the interface is reviewed in the acoustic mismatch model where energy is transferred between two different materials and the critical incident angles are taken into account. Finally we provide calculations of the Kapitza resistance for several interfaces (Metal-Sapphire and Metal-Silicon).

1. Introduction

In 1941 Kapitza had published an article devoted to research of thermal boundary resistance between liquid helium and copper when heat flow passes through the boundary [1]. The following results were obtained: 1) temperature jump occurs between liquid helium and copper on the contact surface; 2) heat flow is determined by the temperature difference:

\[ q = \sigma_k (T_i - T_f) \]  

where \( \sigma_k \) is Kapitza conductance; reciprocal value \( h_k = \sigma_k^{-1} \) is called Kapitza resistance. Meanwhile the temperature jump is caused by the scattering of phonons on the contact surface.

In this paper we present a general analysis of the Kapitza resistance at interfaces between two different materials, and obtain calculations of the Kapitza resistance between two solids. Special attention is paid to the problems of heat transfer through interfaces between nanostructures (especially for multilayer nanoscale structures [2, 3]). In fact, the Kapitza resistance has a little effect on the total thermal resistance in the macroscopic structures; therefore, the Kapitza resistance is generally neglected in heat transfer research for bulk materials. However, for nanostructures Kapitza resistance plays an important and sometimes a decisive role in heat transfer [4, 5].

Currently there are two theories of heat transfer through interfaces. The first one was formulated in [6], and based on the idea that the heat transport in solids is carried out by elastic waves. When waves cross the interface, the energy of elastic wave is partially transferred through the interface due to refraction. At the same time, waves are reflected at the interface which causes temperature jumps. This theory is called “Acoustic Mismatch Model” (AMM). The main limitation of AMM is the assumption that the interface is ideally smooth (for small temperatures). So this theory is only applicable to interfaces with sufficiently small roughness. In this work we will show that for nanostructures this limit does not work. If we talk about the current state of the theory, it is incomplete. For “metal-dielectric”
interfaces the theory of AMM was improved by taking into account the adhesive interaction and anharmonicity of atomic vibrations at the interface in [7]. The main task of this work is to formulate the further continuation of AMM theory.

The second theory was proposed in [8] and called the “Diffusion Mismatch Model” (DMM). The main idea of this theory is that the energy transport is carried out by quanta of elastic waves – phonons – quasi-particles without mass. Here the diffusion processes where the partially propagated energy returns with the reflected phonons are considered. This theory has not been defined in a number of aspects. In recent years DMM has been rather intensively developed by the staff of the University of Virginia and Sandia National Laboratories (SNL) [9].

2. The theory of AMM

This theory is based on the fact that there are usually two types of elastic waves propagating in solids: longitudinal acoustic waves (LA) with velocity $c_L = \sqrt{\frac{\lambda + 2\mu}{\rho}}$ and transverse acoustic waves (TA) with velocity $c_T = \sqrt{\frac{\mu}{\rho}}$. Here $\lambda$ and $\mu$ are the Lame coefficients, $\rho$ is density of the material. The general picture of reflection and refraction of a longitudinal wave is shown in figure 1.

![Figure 1. Schematic of the elastic waves on the interface: (0) the incident longitudinal or transverse wave; (1) reflected longitudinal wave; (2) reflected shear wave; (3) refracted longitudinal wave; (4) refracted transverse wave.](image)

It can be seen that while the longitudinal wave is scattered (and refracted), one longitudinal wave and one transverse wave are formed. A similar pattern occurs when the transverse wave passes. Therefore, the calculation of the Kapitza resistance is divided into the following steps.

1) Determination of the amplitude and direction of each reflected and refracted wave depending on incident angle. Meanwhile the incident waves can be longitudinal and transverse, respectively. And secondly, these solutions are made on both sides of the interface.

2) Calculation of the total energy that propagates through the interface, including the direction of flow propagation ($q_{1\rightarrow 2}$) and the opposite direction ($q_{2\rightarrow 1}$). Determination of the net heat flux through the interface: $q = q_{1\rightarrow 2} - q_{2\rightarrow 1}$.

3) Computation of the Kapitza resistance from (1), and reciprocal Kapitza conductance $h_k = \sigma_{\bar{K}}^2$.

The first step of the presented algorithm is based on the system of linear equations for four wave amplitudes: two reflected waves ($A_1$ and $A_2$) and two refracted waves ($A_3$ and $A_4$). This system of equations 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. These are the deformations and stresses caused by propagating waves. For the case where the incident wave is a longitudinal wave and there is no total internal reflection, the system of equations is given in [10].

We have derived systems of equations for incident transverse wave in the absence of total internal reflections and for both types of incident waves in the presence of total internal reflections. A similar
theory was considered in [11] for electromagnetic waves, but for elastic waves the situation is more complicated due to the presence of two different types of waves. Therefore, the system of equations in the case of incident longitudinal wave at the interface has the following form:

\[
A_i \sin \theta_i + A_i \sin \theta_i + A_i \cos \theta_i - A_i \sin \theta_i + A_i \cos \theta_i = 0
\]  

(2)

\[
A_i \cos \theta_i - A_i \cos \theta_i + A_i \sin \theta_i - A_i \cos \theta_i - A_i \sin \theta_i = 0
\]  

(3)

\[
A_i \sin (2\theta_i) - A_i \sin (2\theta_i) - \frac{c_l}{c_l} \cos (2\theta_i) - \frac{\mu}{\mu} c_l \frac{c_l}{c_l} \sin (2\theta_i) + A_i \frac{\mu}{\mu} \frac{c_l}{c_l} \cos (2\theta_i) = 0
\]  

(4)

\[
A_i \frac{\lambda + 2 \mu \cos^2 \theta_i}{\mu} + A_i \frac{\lambda + 2 \mu \cos^2 \theta_i}{\mu} - A_i \frac{c_l}{c_l} \sin (2\theta_i) - A_i \frac{c_l}{c_l} \frac{\lambda + 2 \mu \cos^2 \theta_i}{\mu}
\]  

(5)

The amplitudes \( A_i \) are obtained by solving the system of linear equations (2)-(5), where the values of \( A_i \) and \( \theta_i \) are fixed (other angles \( \theta_j \), \( j=1,...,4 \), depend on \( \theta_0 \) from Slack law).

Next using \( A_i \) we solve the energy conservation equation

\[
\left( \frac{A_i}{A_i} \right)^2 + \left( \frac{A_i}{A_0} \right)^2 \frac{c_l}{c_l} \cos \theta_i + \left( \frac{A_i}{A_0} \right)^2 \frac{\lambda + 2 \mu \cos^2 \theta_i}{\mu} + \left( \frac{A_i}{A_0} \right)^2 \frac{\lambda + 2 \mu \cos^2 \theta_i}{\mu} \frac{c_l}{c_l} \cos \theta_i \frac{\lambda + 2 \mu \cos^2 \theta_i}{\mu} = 1,
\]  

(6)

where each term represents the energy ratio of the corresponding wave to the wave incident on the interface. In this expression, the 3-rd and the 4-th terms in the left side represent the part of energy carried by the wave through the interface.

The ratio of energy transferred by refracted waves on the interface made of lead (Pb) and sapphire is shown in figure 2 (where \( E_i / E_o = A_i / A_0 \)). The process can be divided into three parts.

1) When the incident angle is from zero to the first critical angle, energy is transmitted to the second material by the longitudinal and transverse refracted waves.

2) While the angle is between the first critical value and the second critical angle, the energy is carried only by the transverse refracted wave.

3) After the second critical angle, there are only two reflected waves and no energy transferred through the interface.
Finally, it is necessary to add one important remark about the applicability of the theory of AMM to the analysis of the Kapitza resistances for nanostructures. The usual view that the theory is only suitable within low temperatures is incorrect for nanoscale. This is due to two circumstances. First, the roughness of nanostructures is significantly less than that of macroscopic samples; they are about tenths of a nanometer. Second, the frequency of elastic waves is limited by the maximum value (from dispersion relations). A detailed analysis shows that these two circumstances ensure a sufficiently large values of the ratio of the elastic wavelengths to the average roughness up to temperatures of the order of 1000 K.

3. The theory of DMM

The theory of diffusion mismatch model (DMM) was proposed in article [8]. The main idea is that the phonons are incident on the interface, some of them are forward scattered and some are backscattered. However the physical mechanism of this process is not discussed. It is assumed that

1) Before the interaction with the interface the characteristics of phonon are energy $\omega$, wave vector $k$ and polarization $j$.

2) After the interaction they are wave vector $k'$ and polarization $j'$; meanwhile they may be changed but the absolute value of the wave vector is preserved.

3) Only elastic interactions are considered, which means that energy is conserved. Actually, these conditions correspond to the assumption that the phonon “forgets” its original state after passing through the interface. Here an important note should be made. If there are only phonon-phonon interactions in the process, the phonon energy $\hbar \omega$ is not conserved. This is possible only for interaction of phonons with impurities or lattice imperfection (vacancies, etc.). However the possibility of changing the mode with such interactions is not considered as it assumed in the DMM (and no one has mentioned these previously).

According to this assumptions, the probability of passing through the interface depends only on frequency (or energy), that is $\alpha = \alpha(\omega)$. So from the diffusion mismatch model [8] it follows

$$\alpha_i(\omega) = 1 - \alpha_{\perp i}(\omega)$$

Figure 2. The energy distribution of the waves transmitted (a) from Pb to sapphire and (b) from Sapphire to Pb. 1 – longitudinal reflected wave, 2 – transverse reflected wave, 3 – longitudinal refracted wave, 4 – transverse refracted wave; 12.5° – the first critical angle $\theta_{cr1}$, 22° – the second critical angle $\theta_{cr2}$. 
(Index 3−i follows from the fact that when i = 1 we get 3−i = 2, and when i = 2 we have 3−i = 1). This means that the probability of phonons transferred from material 1 to material 2 is exactly equal to the probability of the reflection of phonons from material 2 back to this material. The convenience of this assumption is that it completes the theory and allows us to get some result. But there is no physical justification for this hypothesis. The authors say nothing about the type of interaction that can provide this type of condition. Within this theory, the transition layer is practically not considered, although its existence is tacitly assumed. This is a kind of a “black box” with the phonon interaction processes which are not considered.

The fundamental question, without solving which it is impossible to build a reasonable model – what is the transition layer from one body to another? For example, we can assume a perfect border, smooth and infinitely thin, but the problem of the transition of a phonon from one material to another will arise. The fact is that in each material there are unique connections between the frequencies and the wave vectors of phonons – dispersion relations. This problem can be solved using the following method. When a phonon reaches a boundary in another material, we suppose that this phonon interacts with the phonons from another material. Using this approach, energy transport is apparently possible. This assumption due to a slightly different situation was made in the work [12].

Another way is the presence of a transition layer between two materials. We assume that in the transition layer the composition changes from one hundred percent content of the first material to one hundred percent content of the second material (figure 3). In this case, diffusion transport of phonons is possible. But the new question appears: how does this happen?

Finally let us consider how the diffusion in the transition layer can be represented. Not in the approximation of a “black box”, but in a real transition layer of variable composition and finite thickness. One of the important features of the transition layer is the disorder of atoms (or amorphous structure), that is the absence of a crystal lattice typical to solids. Under these conditions, it is impossible to talk about the presence of dispersion relations, the determination of phonon lifetimes, and so on. The assumption that some phonons are in an amorphous structure is proposed. For example, in the absence of dispersion relations, it can be assumed that phonons in the transition layer can have any relationship between the frequency and the wave vector. Hence for any phonons an “access” to the transition layer is possible. Since the reflection is possible only at the boundaries of the transition layer, so the absence of dispersion relations does not give an answer to the question of determining the phonon velocity. Therefore the solution to the problem of existence of longitudinal and transverse phonons is also unclear.

![Figure 3](image)

**Figure 3.** Illustration of the transition layer (green circles) between two bodies (blue and red circles). Lines represent the changes in the composition.

**Conclusion**

In this work we introduce a detailed analysis of two models for calculating the thermal boundary resistance: acoustic mismatch model and diffusion mismatch model.

For acoustic mismatch model we carry out the numerical calculations of the Kapitza resistance from both sides of material 1 and material 2 for several solid-solid interfaces. For the first time, the Kapitza resistance was determined during the heat flux from both sides: from the semiconductor side and from
the metal side. Calculation parameters $\rho, c_L, c_T$ are taken from [8], and results are presented in Table 1. It seems that the values of Kapitza resistances from different directions ($1 \to 2$ and $2 \to 1$) are different. This is due to the fact that dispersions of materials have a different frequency intersections.

Table 1. Calculated resistance Kapitza for several interfaces, multiplied by $T^3$ with units $K^3W^{-1}cm^2$.

|            | Sapphire | Silicon |
|------------|----------|---------|
|            | $1 \to 2$ | $2 \to 1$ | $1 \to 2$ | $2 \to 1$ |
| Aluminum   | 20.99    | 24.06   | 11.61    | 14.30    |
| Copper     | 17.70    | 20.58   | 13.83    | 17.67    |
| Indium     | 21.04    | 23.19   | 12.07    | 13.94    |
| Lead       | 18.29    | 21.04   | 12.13    | 14.59    |
| Tungsten   | 21.72    | 27.96   | 21.49    | 30.70    |
| Chromium   | 16.59    | 20.27   | 13.81    | 15.92    |
| Magnesium  | 25.45    | 29.52   | 12.25    | 15.04    |
| Nickel     | 17.85    | 20.86   | 13.55    | 18.42    |
| Platinum   | 19.79    | 25.54   | 19.03    | 27.38    |
| Rhodium    | 19.02    | 22.97   | 17.59    | 22.66    |
| Silver     | 17.57    | 20.50   | 13.40    | 16.95    |

For diffuse mismatch model, we proposed the following model. In the transition layer, phonons can have any combination of frequency and wave vector. This allows phonons to freely penetrate into this layer from both sides and diffuse inside the transition layer. It is also possible to assume the absence of the concept of transverse and longitudinal phonon. Then this model will correspond to the basic provisions of the model [8]. It can be assumed that all phonons have a certain average velocity. Within this model, it is possible to use the Monte Carlo method to analyze phonon diffusion in the transition layer. The question remains: how does the phonon transport from the transition layer to another material occur?

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