Generalized model of Kapitza conductance across rough interfaces

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Abstract. This paper is devoted to the theoretical prediction of the interfacial heat transfer in nanostructured materials. The main task of this work is the analysis of interaction of elastic waves with the rough interface between two different solids. The presence of toughness leads to a significant increase in the resistance to heat transfer in nanostructures. This fundamental problem is discussed in relation to the commonly used method of wave scattering at rough surface: the Kirchhoff tangent plane method. The method assumes that at the point of the rough surface profile, the surface is regarded as locally smooth, and the reflection and transmission of the incident wave can be described by the scattering at the tangent plane of this point. Based on the elastic wave theory, we use the frequency-dependent continuity conditions to calculate the energy transmission coefficient at the interface. And then its effective value at the rough interface is estimated by using the Kirchhoff method. By substituting this effective value into the formula of Kapitza conductance, we can calculate the Kapitza conductance at the rough interface and analyze the effect of roughness on the interfacial heat transfer.

1. Introduction

The phenomenon of a temperature jump at the contact surface of two media in the heat transfer process is firstly discovered by Kapitza [1]. This indicates that part of the energy is dissipated when the heat flux passes through the surface (or interface). An important parameter characterizing heat transfer through interfaces is the Kapitza conductance $h_k$, which indicates that the heat flux transfer efficiency at the interface with Kapitza conductance plays an important role in the heat transfer between the structural elements of nano-devices. In this case, it is necessary to develop reliable methods for calculating Kapitza conductance at the interface between two solids: $q = h_k(T_1 - T_2)$, where $q$ is the heat flux, and $T_1$ and $T_2$ are the temperatures of the solid 1 and solid 2, respectively.

One of the commonly used theoretical models is the so-called acoustic mismatch model (AMM), which is based on the analysis of the elastic wave scattering at the interface [2,3]. It is generally considered that the AMM is only available for extremely low temperatures [4]. However, the recent work has shown that when taking into account the dispersion properties of elastic waves and imposing restrictions on the frequency spectrum (by analyzing the physical restrictions on the processes of wave propagation), the modified method can provide reliable predicted values of Kapitza conductance up to hundreds of Kelvin [5,6]. This is the first step in generalizing the extended theoretical model of Kapitza conductance based on the elastic wave theory.

In this work, we present the next step of generalization: the problem of determining the Kapitza conductance taking into account the roughness of the interface is formulated and solved.
This problem differs significantly from that of thermal conductivity of nano or bulk materials – the interaction of phonons with the rough surface of solids [7]. Along with scattering at a non-ideal interface between two different solids, it is necessary to study the effect of roughness on the nature of energy transfer through the interface, namely, on the energy of transmitted waves crossing the interface.

Therefore, we now formulate the features of the considered problem. First, the problem of wave scattering at the interface must be solved by using statistical methods, which are widely studies in the field of optics and acoustics [8–11]. This is necessary because the rough interfaces between two solids are difficult to accurately describe. In this case, the object of the statistical theory is the slopes of the rough surface profile: to describe the statistics of slopes, the corresponding distribution functions are used. Secondly, it is necessary to study the regularities of the scattering processes of transmitted waves, depending on the angles of inclination of the roughness. Third, on the basis of the statistical theory, the coefficients of heat transfer through the interface are determined for different polarizations of elastic waves. After that, the actual Kapitza conductance can be determined.

2. Mathematical model

The statistical description of a rough surface is based on the assumption that the deviations of the surface \( z = \zeta(x) \) relative to the mean plane \( \zeta = 0 \). And the random rough surface is Gaussian distributed. For this problem, two statistical parameters are necessary: the root-mean-square roughness \( \sigma \) and the correlation length \( L \). We consider a two-dimensional surface with generators along the axis \( y \), when \( \gamma_y = 0 \). Therefore, the derivative \( n = \zeta' \) of the normal random function obeys the distribution:

\[
  w_n(n) = \frac{1}{\sqrt{2\pi\gamma}}\exp\left(-\frac{n^2}{2\gamma}\right),
\]

where the constant \( \gamma = \sigma / L \) characterizes the variance of the first derivative of the profile \( (\zeta')^2 = \gamma^2 \) (tangents of the slope angle of the surface: \( n = \tan \varphi \)).

![Figure 1](image-url)  

**Figure 1.** The wave scattering at the rough surface.  
\( \theta_i, \theta_r, \) and \( \theta_t \) are the angles of incident, reflected and transmitted waves relative to the normal line of the tangent plane.

The next step is to establish the relationship between the angles of reflection and transmission with the angle of incidence of elastic waves on the surface, as shown in figure 1. To determine these angles, the Kirchhoff tangent plane method is used [8]. Then the coefficients of energy transfer by elastic waves of various polarizations are determined. For this, a system of elasticity equations is used; it is obtained using the boundary conditions set on the tangent planes, as at the boundaries between two solids [5, 6]. By using Kirchhoff method, we can obtain the effective transmission coefficient
\(\alpha_{\text{eff,1-2}}(\omega,\theta)\) from solid 1 to solid 2, where \(\omega\) is the frequency of the elastic wave and \(\theta\) is the angle between the incident wave and the normal to the mean plane \(\xi = 0\). By substituting the effective transmission coefficient \(\alpha_{\text{eff,1-2}}(\omega,\theta)\) into expression [5]:

\[
h_K = \frac{1}{2} \sum_{j=1}^{2} \int_{0}^{\pi/2} \int_{0}^{2\pi} f_{\text{eff},j}(\omega)\alpha_{\text{eff,1-2},j}(\theta,\omega)D_{j}(\omega) \frac{\delta f(\omega, T)}{\delta T} \cos \theta \sin \theta d\theta d\omega,
\]

we can obtain the Kapitza conductance at the rough interface.

The detailed description of computation algorithm and its application for rough aluminum/silicon interfaces are presented in article [12].

3. Results and discussion

The calculated results for rough aluminum/silicon interfaces with various root-mean-square roughness values are shown in Fig. 2.

![Figure 2](image_url)

**Figure 2.** The Kapitza resistance as a function of the temperature for various Al/Si interfaces with root-mean-square roughness \(\sigma = 0, 0.1, 0.3, 0.5, 1, 5\), and 10 nm, when the correlation length \(L = 10\) nm. The circles are the measured values of Kapitza conductance at the smooth Al/Si interface [13]. The dashed lines are the calculated results of Kapitza conductance of Al/Si interface by the AMM and diffuse mismatch model (DMM) [4].

As shown in figure 2, our model for the smooth interface [5] agrees well with the experiment [13]. As the root-mean-square roughness \(\sigma\) increases, the Kapitza conductance decreases rapidly. The AMM and DMM cannot describe the effect of roughness on the Kapitza conductance. However, the DMM can predict the Kapitza conductance of the interface with a certain roughness, which is verified by various studies before [14].
Conclusion

Based on the elastic wave theory and the Kirchhoff method, we propose a theoretical model for calculating the Kapitza conductance of the rough interface. In this model, we take into account the dispersion relations of the elastic waves and use the frequency-dependent continuity conditions of the displacement and stress at the interface. And the profile of the rough interface is described by the statistical method. The predicted values of Kapitza conductance indicate that the roughness can significantly impact the heat transfer at the interface, which plays an important role on the nanoscale. The theoretical predictions can guide the design of the nanostructured materials.

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