



Importance of viscoelastic and interface bonding effects in the thermal boundary conductance of solid–water interfaces



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ABSTRACT

We propose a simple analytical treatment of the thermal boundary conductance of solid/water interfaces, using a generalization of the acoustic mismatch model. The model accounts for van der Waals interactions between water and the solid, and the high frequency dynamics, which is peculiar to liquid water. Of particular interest are the viscoelastic effects that emerge at THz frequencies, and which allow transverse acoustic waves to propagate in liquid water. The parameters of the model may be found in handbooks, and as such is free from any fitting parameters. Comparison with molecular dynamics data shows that interfacial energy transfer is inelastic, and energy is transmitted up to the solid Debye frequency. Comparison with experimental data regarding metal/SAM (self-assembled monolayer)/water allows to estimate the different contributions to heat dissipation, and we found that interfacial heat transfer in this situation is limited by the SAM head/water conductance, the latter being well described by the viscoelastic model. We also discuss the dependence of the conductance on the adhesion energy between the solid and water.

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1. Introduction

Nanoscale thermal transport across solid–liquid interfaces is important in numerous applications. This covers microelectronic chips cooling to biomedical applications. In this latter example, metallic nanoparticles may be heated up following the excitation by a laser, which may result in the ultrafast local heating of the surrounding medium [1–3]. A quantity of prime importance is the thermal boundary conductance $G = q/\Delta T$ defined as the heat flux q divided by the temperature drop ΔT at the interface [4]. The thermal boundary conductance controls the heating level in the vicinity of the hot nanoparticles, and typically a relatively large value of G is desired.

On the fundamental side, our understanding of heat transport in liquids is only partial. Standard textbooks generally mention the Green–Kubo formula for the thermal conductivity [5], which is widely used in molecular dynamics simulations but which has a limited predictability for liquids. The main reason is partly ascribed to the lack of long range order in liquids, which precludes the classical description transport in terms of phonons, i.e. collective propagative excitations. For the same reasons, our understanding of

interfacial heat transport across solid/water interfaces is limited. Thermal boundary resistance at liquid/solid interfaces has been probed, both experimentally by Ge et al. [6] and from molecular dynamics (MD) [7] by Barrat and Chiaruttini, Xue et al. [8] and later by Murad and Puri [9] during the years 2000. MD work has been pursued to determine the effects of the interfacial roughness [10–12] or to show thermal rectification at solid/fluid interfaces [13]. The common conclusion of these studies is that the thermal conductance displayed by liquid/solid interfaces takes values which are not significantly lower than solid/solid interfaces. In turn, the conductance of solid/liquid interfaces is orders of magnitude larger than solid–gas interfaces [14,15]. This tends to conclude that from a vibrational point of view, liquids may not be quite different than solids. This conclusion is consistent with the recent liquid phonon theory of Bolmatov et al. [16], which takes up Frenkel's original idea [17]. According to this theory, the vibrational properties of water maybe described as those of a disordered solid with one longitudinal and two transverse waves.

Recently, the effect of the finite bonding strength between solid and liquid has been addressed. Ge et al. were the first to report experimentally that the conductance of hydrophilic interfaces is typically more than twice larger as the conductance of hydrophobic interfaces [6]. Following this pioneering work, Shenogina et al. showed using molecular dynamics simulations of self-assembled monolayers (SAM) that the thermal boundary conductance is

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proportional to the work of adhesion between the metal and water [18]. This theoretical work motivated Harikrishna et al. to measure experimentally the conductance of a series of alkane-thiol monolayers, confirming the proportionality between G and the work of adhesion [19]. Alkane-thiol monolayers have been also shown to enhance the intrinsic low conductance of gold/ethanol interface [20]. Harikrishna et al. nevertheless questioned the generality of this relation. Note to finish that the effect of the adhesion energy has been scarcely discussed within the framework of an analytical model.

In this article, we rationalize the effect of the bonding strength by using an analytical model based on a generalization of the acoustic mismatch model (AMM). Curiously, there has been no much effort to develop analytical acoustic models to predict the thermal resistance at solid/liquid interfaces, although acoustic models were initially set up for liquid Helium. Caplan et al. have recently developed an analytical framework based on the diffuse mismatch model [21]. This model considers the two extreme situations of very hydrophobic and hydrophilic interfaces, but does not describe the gradual increase of the thermal boundary conductance with the bonding strength.

In this article, we propose a viscoelastic model which is a generalization of the acoustic mismatch model [22], and which accounts for the viscoelastic properties of liquid water at high frequencies. We unveil the role of the high frequency viscoelastic properties of liquid water in the value of the thermal boundary resistance between solid and liquid water. In particular, we show that the AMM model severely underpredicts the ability of solid/fluid interfaces to transmit energy.

The article is structured as follows: In Section 2, we describe in detail the viscoelastic model. We compare the predictions of the model for bare gold/water interfaces with MD simulations data available in the literature in Section 3. In Section 4, we address the case of metal/SAM/water interfaces. We compare our predictions with available experimental data, and discuss the contributions of the different heat pathways in the experimentally relevant situations.

2. Model

The model we use is inspired by a generalization of the acoustic mismatch (AMM) model [24,23,22]. We retain here AMM since we are interested in comparing the predictions of our model with the thermal conductance at atomically sharp interfaces. Generally speaking, when the incident phonons have wavelengths larger than the interfacial roughness rms, diffuse scattering is unlikely and specular scattering suffices to describe the thermal boundary conductance, as discussed by several authors [25–27]. MD simulations also demonstrate that the AMM model describes satisfactorily heat transfer at interfaces having a roughness rms smaller than 2.5 nanometers [29,28].

In its original version, the AMM model depends only on the bulk properties of the two media in contact. Recently, it has been generalized to account for the finite bonding strength between two media [22]. In this generalized version, the phonon transmission coefficient is given by:

$$t = \frac{4Z_1 Z_2 \cos \theta_1 \cos \theta_2}{(Z_1 \cos \theta_1 + Z_2 \cos \theta_2)^2 + \frac{\omega^2}{K_{12}^2} (Z_1 Z_2 \cos \theta_1 \cos \theta_2)^2} \quad (1)$$

where Z_1 and Z_2 are the acoustic impedances of the two media defined by $Z_i = \rho_{m,i} v_i$, $\rho_{m,i}$ being the mass density and v_i the sound velocity in medium i ; θ_1 and θ_2 are the incident and refraction angles related by the equivalent of Snell Descartes's laws: $\sin \theta_1 / v_1 = \sin \theta_2 / v_2$, see Fig. 1.

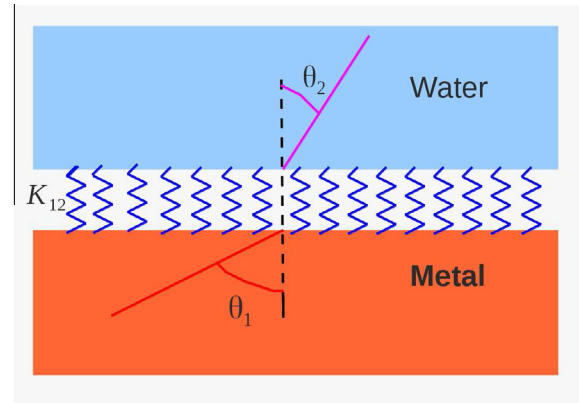


Fig. 1. Schematic illustration of the energy transmission across solid/water interfaces.

In particular, when medium 2 has the largest sound velocity, phonons propagating towards medium 2 are confined in a cone making a critical angle $\theta_c = \sin^{-1}(v_1/v_2)$, and phonons having an incident angle larger than θ_c are completely reflected by the interface. Finally, the transmission coefficient Eq. (1) depends on the interaction strength between the two media through the spring constant (per unit area) K_{12} . If the interaction between the two media is supposed to be of van der Waals type, and characterized by the Lennard–Jones potential

$$V_{12}(r) = 4\epsilon_{12} \left(\left(\frac{\sigma_{12}}{r} \right)^{12} - \left(\frac{\sigma_{12}}{r} \right)^6 \right) \quad (2)$$

the spring constant per unit area is given by:

$$K_{12} = n_s \left(\frac{d^2 V_{12}}{dr^2} \right)_{r=r_0} = \frac{72}{2^{1/3}} \frac{n_s \epsilon_{12}}{\sigma_{12}^2} \quad (3)$$

where $r_0 = 2^{1/6} \sigma_{12}$ is the equilibrium distance between two neighbouring atoms defined by $(dV_{12}/dr)_{r_0} = 0$ and n_s is the number of surface atoms per unit area [22].

We generalize Eq. (1) through two aspects: we differentiate phonons with different polarisations-*i.e.* longitudinal and transverse, and we introduce a cut-off frequency $\omega_x(T) = 1/\tau_x(T)$ which is the inverse of the water viscoelastic relaxation time $\tau_x(T)$. Next, we follow Frenkel's original idea according to which liquids may support shear waves at high frequencies $\omega > 1/\tau$ where τ is the atom jumping time between two equilibrium positions [17]. Indeed as expressed in the liquid phonon theory of Bolmatov et al. there are two kinds of motion in liquids: phonon motions at high frequencies $\omega > \omega_F$, where $\omega_F = 1/\tau$ is Frenkel frequency, and diffusional motions due to an atom jumping between two equilibrium positions [16]. Therefore, at high frequencies there is no difference between a liquid and a disordered solid from a vibrational point of view and phonon modes may propagate which may be decomposed as one longitudinal wave and two transverse waves. For lower frequencies $\omega < \omega_F$ only one longitudinal wave may propagate in the liquid. These hypotheses have been verified using inelastic X ray scattering [31,30]. The transition frequency ω_F is found to be well approximated by the inverse of the liquid viscoelastic relaxation time $\omega_F \simeq \omega_x(T) = 1/\tau_x(T)$ where $\tau_x(T) = \eta(T)/G_\infty(T)$ is the ratio between the temperature dependent shear viscosity $\eta(T)$ and the infinite frequency shear modulus $G_\infty(T)$. Following these considerations, we describe the vibrations in liquid in the following way: for frequency $\omega > \omega_x(T)$, liquid water behaves as a three-dimensional solid and as such may support both longitudinal and transverse acoustic waves; on the other

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