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CALCULATION OF THERMAL RECTIFICATION BY LINEAR RESPONSE THEORY

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Several investigators have found that the resistance to heat transfer at the interface between the two materials depended upon the direction of heat flow across the interface. Although many of the factors that affect the transfer of heat across the interface are reasonably well understood, the directional dependence of the thermal contact resistance has not yet been completely explained. In this paper, we evaluate the thermal contact resistance from the linear response theory by considering the scattering and transmission of phonons at the interface, it is found to be dependent on the temperature of the interface. The results of this can explain the reported behavior of thermal rectification.

1 Introduction

In 1936, Starr [1] conducted experiments with a copper-copper oxide rectifier which seemed to indicate that thermal resistance at the interface between the two materials depended upon the direction of heat flow across the interface. These results were later described in a standard text on rectifier [2]. However, in 1951, Horn [3] criticized Starr's experiments on the basis that Thomson e.m.f caused by the temperature gradient across the rectifier led to spurious results, since Starr used un-insulated thermocouples with a common lead. In 1955, Barzelay [3] found in the course of determining thermal resistance of aircraft joints that the resistance across the aluminum-stainless steel joints depended on the direction of heat flow. Since their experiments were not specifically designed to test for the presence of this effect, they proposed further experimentation in the field. Finally, Roger and his group carefully designed experimental apparatus to determine whether the asymmetric heat-conduction effect really existed [4]. Rogers found a definite directional heat transfer effect in the systems he studied.

Williams and Fletcher reviewed the various, often conflicting, investigations of thermal rectification and found that directional effects existed but that experimental data were inconsistent. This phenomenon, referred to as thermal rectification, is of significant importance in design of heat exchangers and spacecraft thermal control systems, and has potential applications in the thermal control of electronic equipment as a thermal rectifier.

In the last twenty years a growing number of works have been published on thermal contact resistance. Most of them are experimental works, but quite a few are theoretical. Although many of the factors that affect the transfer of heat across the interface are reasonably well understood, most of them are surface analysis, deformation analysis, the directional dependence of the thermal contact resistance has not yet been completely explained theoretically. It has been known that the boundary between two dissimilar materials presents a thermal resistance to the flow of phonons. In this paper, we evaluate the boundary resistance from linear response theory by considering the scattering and transmission of phonons at the interface, both the theory itself and the evaluation are exact. We found that the thermal contact resistance depends on the temperature of the interface. The directional heat transfer phenomenon at the interface of dissimilar metals in a metal-metal contact can be explained by application of these results theoretically. In section 2 we evaluate the temperature dependence of the contact thermal resistance from Kubo formula, in section 3 we analyze the thermal rectification in dissimilar metal contacts, in section 4 we discuss the results and compare with the experimental results.

2 Evaluation of the contact thermal resistance

Consider an infinite medium consisting of two solids, solid 1 and 2 in the region $z \leq 0$ and $z \geq 0$. It will be useful to calculate the average heat flux χ at time t and position z' in response to an initial temperature step ΔT imposed at position z. We define the ratio

$$K(z,z',t) = \frac{\chi(z',t)}{\Delta T(z)} \tag{1}$$

The surface conductivity K (the inverse of the surface resistance R) is obtained by setting $z = z' = 0$ and $t \to \infty$. In other words, the temperature step is imposed across the interface, and the heat flux is also measured across the interface when steady state is reached.

Acording to the linear response theory, the surface conductivity K can be calculated by

$$K(z,z',t) = \frac{2i}{\Lambda T}\int_0^t \tau d\tau \int d^2r_\perp d^2r'_\perp \times \langle J(\boldsymbol{r}',\tau)J(\boldsymbol{r},0)\rangle \tag{2}$$

where Λ is the transverse area of the sample, J is the energy current operate, and $\boldsymbol{r} = (\boldsymbol{r}_\perp, z)$, etc..

For one dimensional system with coordinate $\phi(z)$ and a position dependent density and modulus $M(z)$, described by the Lagrangian density

$$\mathcal{L} = \frac{1}{2}\rho(z)[\frac{\partial\phi}{\partial t}]^2 - \frac{1}{2}M(z)[\frac{\partial\phi}{\partial z}]^2 \tag{3}$$

Eventually we want $\rho(z) = \rho_1(\rho_2), M(z) = M_1(M_2)$ for $z \leq 0$ ($z \geq 0$). It is straightforward to evaluate the Hamiltonian density and the energy current

$$\mathcal{H} = \frac{\pi^2(z)}{2\rho(z)} + \frac{1}{2}M(z)[\frac{\partial\phi}{\partial z}]^2 \tag{4}$$

$$J = -\frac{M(z)}{\rho(z)}\pi(z)\frac{\partial\phi}{\partial z} \tag{5}$$

where $\pi = \rho\dot{\phi}$ is the conjugate momentum and normal ordering is everywhere understood. When (5) is inserted into (2), the correlation involves four operators at two different times, schematically

$$\begin{aligned}&\langle J(z',\tau)J(z,0)\rangle \\ &\quad\sim \langle \pi(z',\tau)\phi(z',\tau)\pi(z,0)\phi(z,0)\rangle \\ &\quad\sim \langle \pi(z',\tau)\pi(z,0)\rangle\langle\phi(z',\tau)\phi(z,0)\rangle \\ &\quad+\langle \pi(z',\tau)\phi(z,0)\rangle\langle\phi(z',\tau)\pi(z,0)\rangle\end{aligned} \tag{6}$$

by Wick's theorem. The other contraction does not contribute, since each J is normal ordered and there is no connected four point function since the Hamiltonian is quadratic. All results can thus be expressed in terms of the correlation function $F(z,z',t) = \langle\phi(z,t)\phi(z',0)\rangle$ and some algebra leads to

$$K = -\frac{2iM(z)M(z')}{T}\int_0^\infty tdt \left[\frac{\partial^2 F}{\partial t^2}\frac{\partial^2 F}{\partial z\partial z'} + \frac{\partial^2 F}{\partial t\partial z'}\frac{\partial^2 F}{\partial t\partial z}\right] \tag{7}$$

Since we wish to calculate χ when steady state is achieved, the time integral has been extended to infinity and for one dimension, Λ has been set to 1.

The freedom to choose z and z' allows us to average over these positions e.g., by $(1/L)\int_0^L dz$. For convenience, we shall restrict $z \leq 0$ and $z \geq 0$, so $M(z) = M_2, M(z') = M_1$ are constants in the average. Since z, z', t are now all under the integral sign, we may freely integrate by parts; a little arithmetic then shows that the second term in (7) makes the same contribution as the first.

secondly we introduce the Fourier transform

$$F(z,z',t) = \int\frac{d\omega}{2\pi}\tilde{F}(z,z',\omega)e^{-i\omega t} \tag{8}$$

which is related to the retarded Green's function

$$G(z,z',t) = -i\Theta(t)\langle[\phi(z,t)\phi(z',0)]\rangle \quad (9)$$

by [5]

$$\tilde{F}(z,z',\omega) = \frac{-2}{1-e^{-\beta\omega}} Im\tilde{G}(z,z',\omega) \quad (10)$$

Inserting these into (7) then gives

$$K = -\frac{8M_1M_2}{T^2}\int_0^\infty \frac{d\omega}{2\pi}\frac{\omega^2 e^{-\beta\omega}}{(1-e^{-\beta\omega})^2}H(\omega) \quad (11)$$

where

$$H(\omega) = Im\frac{\partial}{\partial z}\tilde{G}(z,z',\omega) Im\frac{\partial}{\partial z'}\tilde{G}(z,z',\omega) \quad (12)$$

and the right hand side is understood to be averaged over z, z'. Note that in (12), the two factors of $\tilde{G}$ are forced to the frequency by the infinite time integral in (7).

The Green's function can be evaluated from the defining equation, written in the frequency domain as

$$[-\rho(z)\omega^2 - \frac{\partial}{\partial z}M(z)\frac{\partial}{\partial z}]\tilde{G}(z,z',\omega) = -\delta(z-z') \quad (13)$$

The function G has the interpretation of being a wave produced by a harmonic point source at z' (< 0) and observed at the point z (> 0). The solution to (13) is just plane waves in each region with a gradient discontinuity at $z = z'$. The wave vectors for the plane waves are $g_i = \omega/v_i$ in the two region $i = 1,2$, and $v_i = \sqrt{M_i/\rho_i}$. The retarded nature selects outgoing waves at infinity. The amplitudes of the plane waves are obtained by matching $\tilde{G}$ across the three regions ($z < z', z' < z < 0, 0 < z$) and the result is best expressed in terms of the impedance $Z_i = \rho_i v_i$ and the amplitude reflection coefficient $r = (Z_1 - Z_2)/(Z_1 + Z_2)$. Then it is easily shown that

$$H = -\frac{1}{8}\frac{1-r^2}{M_1M_2} \quad (14)$$

The factor $1 - r^2$ is just the energy transmission coefficient $\mathcal{T}$. We then obtain

$$K = \frac{1}{T^2}\int_0^\infty \frac{d\omega}{2\pi}\frac{\omega^2 e^{-\beta\omega}}{(1-e^{-\beta\omega})^2}\mathcal{T} \quad (15)$$

which gives

$$K = \frac{\pi}{6}\mathcal{T}T \quad (16)$$

linear in the temperature T for such a one dimensional system.

3 Evaluation of the thermal rectification

The directional heat transfer phenomenon at the interface of different metals in a metal-metal contact can be explained theoretically by application of the result of the previous section.

Let us consider the two different metals in a metal-metal contact system consisting a metal 1 of thickness l_1 and of metal 2 of thickness l_2, both have the same cross section. let $l_1 = l_2$, k_i denote the thermal conductivity of the metal $i (i = 1,2)$ and T_i ($i = 1,2$) denote the temperature of the end of the two metals respectively. The heat flow rate q can be expressed mathematically as follows [6]:

$$q = K\Delta T \quad (17)$$

where K is the surface thermal conductivity at the interface evaluated in section 2 and ΔT is the variation of the temperatures of the two ends of metals.

Suppose $T_1 > T_2$, heat will flow from metal 1 to metal 2, the heat flow rate will be

$$q_{12} = \frac{\pi}{6}\mathcal{T}T_{12}\Delta T \quad (18)$$

Now, suppose we reverse the interface temperatures, heat will now flow metal 2 to metal 1.

$$q_{21} = \frac{\pi}{6}\mathcal{T}T_{21}\Delta T \quad (19)$$

We can calculate T_{12} and T_{21} by application of Fourier's law of heat conduction.

$$T_{12} = \frac{k_1T_1 + k_2T_2}{k_1 + k_2} \quad (20)$$

$$T_{21} = \frac{k_1T_2 + k_2T_1}{k_1 + k_2} \quad (21)$$

Therefore, the ratio of these quantities is given by the expression,

$$\frac{q_{12}}{q_{21}} = \frac{k_1T_1 + k_2T_2}{k_1T_2 + k_2T_1} \tag{22}$$

From equation (22), if two metals are different ($k_1 \neq k_2$), we will have

$$q_{12} \neq q_{21} \tag{23}$$

Therefore, we can prove clearly that the directional heat-transfer phenomenon exist at the interface of dissimilar metals in a metal-metal contact system.

4 Discussion

This paper has given a qualitative explanation of asymmetric heat flow at the interface between dissimilar metals. In Table 1, we give some exact quantitative calculations of this effect, and we find that thermal rectification effect at the interface of Fe-Ag contact is biggest in these contact systems. On the other hand, the Calculation result of the ratio of hear flow rate at Al-Fe contact interface compares favorably with L. S. Fletcher's value [7] of approximately 0.76.

Table 1: Calculation result of the ratio of heat flow rate at the dissimilar metal-metal contact interface

Metal 1	Metal 2	q_{12}/q_{21}
Al	Ag	0.934425
Al	Au	0.954392
Al	Si	1.092150
Fe	Ag	0.793798
Fe	Au	0.817426
Fe	Si	0.911356
Fe	Al	0.844628

Using Eq. (23) thermal rectification can be shown to exist for the contact between two different metals through which heat is flowing. It is possible to explain this phenomenon as a consequence of the temperature dependence of boundary resistance, it bases on the microscopic properties of the contacting material. An important aspect of this conclusion is that thermal rectification is a strong function of both the material properties. Because the total heat flux through the interface is carried by electrons and phonons, in this paper we only analyze the contact resistance on phonon conduction. For further study, we should take into account 1) electron conduction 2) physical properties of any interstitial materials.

In summary, it is apparent that thermal rectification is a function of both the material properties. For dissimilar materials, the thermal contact conductivity is higher when the interface has higher temperature.

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