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Computation of Interfacial Thermal Resistance by Phonon Diffuse Mismatch Model

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The thermal resistances of 1250 kinds of interface were computed at room temperature based on the phonon diffuse mismatch model. The result shows that the ratio of Debye temperature and the ratio of average sound velocity can be approximately used to characterize the difference of two materials in terms of interfacial thermal resistance. The high interfacial thermal resistances are composed of high and low Debye temperature materials. The low interfacial thermal resistances are composed of both similar Debye temperature materials, and their Debye temperatures are very high. The relation between the interfacial thermal resistance with the ratio of average sound velocity is similar to that of the ratio of Debye temperature. [doi:10.2320/matertrans.MAW200717]

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1. Introduction

The interfacial thermal resistance plays a critical role for the transport of thermal energy in large scale integrated circuit,[1)] nanocomposite,[2)] and semiconductor superlattices[3)] because the mean free path of energy carrier, for example phonon, is about 10–100 nm,[4)] thus the interface will significantly limit the transport of energy carrier in nano-structure.

When the heat flow is transported across an interface between two different materials, there is a macroscopical temperature discontinuity at the interface, which can be expressed as:

$$J = \sigma_K \Delta T \tag{1}$$

Where J is heat per unit area per unit time across the interface, σ_K is interfacial thermal conductance, ΔT is temperature drop at the interface. This had been first presented by Kapitza as early as 1941 for the interface between helium and a solid, so known as Kapitza conductance.[5)] The reciprocal of the Kapitza conductance is the interfacial thermal resistance.

Swartz and Pohl presented the phonon diffuse mismatch model (DMM) to describe this phenomenon,[6)] and assume that all the phonons are randomly and elastically scattered at the interface, the scattering probability into each material is decided by the density of phonon state in each material. The transmission probability is written as:

$$\alpha_{1,j}(\omega) = \frac{v_{2,j} g_{2,j}(\omega)}{v_{1,j} g_{1,j}(\omega) + v_{2,j} g_{2,j}(\omega)} \tag{2}$$

Where $\alpha_{i,j}(\omega)$ is phonon transmission probability of mode j in side i, ω is phonon angular frequcency, $v_{i,j}$ is phonon sound velocity of mode j in side i, $g_{i,j}(\omega)$ is density of phonon state of mode j in side i.

The interfacial thermal resistance can be given by:[6)]

$$R_{\text{int}} = \frac{1}{\sigma_K} = \frac{1}{2}\sum_{i,j}\frac{\partial}{\partial T}\int_0^{\pi/2}\int_0^{\omega_i^{\max}} \alpha_{i,j}(\theta,\omega,j) g_{i,j}(\omega) n(\omega,T)\hbar\omega v_{i,j}\cos\theta\sin\theta d\theta d\omega \tag{3}$$

Where R_{int} is interfacial thermal resistance, θ is phonon incident angle, $\omega_i^{\max}$ is maximum phonon angular frequcency in side i, $n(\omega,T)$ is Bose occupation distribution function $n(\omega,T) = \frac{1}{e^{\hbar\omega/k_B T}-1}$, $\hbar$ is Planck's constant.

It is to understand that an interface composed of two dissimilar materials has the high thermal resistance, and that of two similar materials has the low thermal resistance. In this work we use three ratios of parameter: the ratio of Debye temperature, the ratio of average sound velocity and the ratio of density to characterize the difference of two materials, and obtain the relation between the interfacial thermal resistance with three ratios of parameter by plenty of materials.

2. Methodology

We selected 50 kinds of solid material, and every two materials were combined into form interfaces, total 1250 kinds of interface, and use the phonon diffuse mismatch model to compute the interfacial thermal resistance at room temperature, and the detail solution can be found in Ref. 6).

The used parameters of materials are listed in Table 1. The Debye temperature, the sound velocity and density data mostly come from NIMS Materials Database,[7)] and symbol $*$ shows calculated value.

The calculated Debye temperature is given by

$$\Theta_D = \frac{\hbar\omega_D}{k_B}\quad \frac{V}{6\pi^2}\left(\frac{1}{v_L^3} + \frac{2}{v_T^3}\right)\omega_D^3 = 3N \tag{4}$$

Where Θ_D is Debye temperature, ω_D is Debye cut-off frequency, k_B is Boltzmann constant, v_L is longitudinal sound velocity, v_T is transverse sound velocity, V is volume, N is atom number.

Table 1 The used parameters of materials.

Material	Θ_D	$\bar{v}$	ρ	*Material*	Θ_D	$\bar{v}$	ρ
Diamond	1860	14.39	3.52	Mg	318	4.18	1.74
BeO	1260	8.80	3.01	NiO	317	3.35	6.72
TiB_2	1140	8.52*	4.19	Cu	315	3.30	8.96
SiC (3C)	1123	9.61	3.22	W	310	3.69	19.30
LiH	1115	8.21*	0.78	InSb	280	2.67	5.78
Al_2O_3	980	7.93	3.97	Nb_3Sn	280	3.39	8.91
MgO	941	7.36*	3.59	$SrGa_2$	272*	3.28	4.91
TiN	865*	7.26*	5.39	GaAs	264	3.73	5.32
LaB_6	773	6.17	4.67	Pt	230	2.56	21.45
LiF	645	5.44*	2.64	Ag	215	2.42	10.50
MgF_2	626*	5.28	3.17	$CeSn_3$	208*	2.49	7.84
Si	625	6.54	2.33	CdS	202*	2.58	4.80
ReO_3	560	4.95	7.39	Cd_3As_2	200	2.30	6.33
Rh	536*	4.58	12.41	$ZrSe_3$	200*	2.63*	5.74
$Ru_{0.2}Ni_{0.8}$	531*	4.21	9.70	ZnTe	198	2.95	5.72
$CaCO_3$	503*	4.57	2.72	CdTe	184*	2.32	5.85
$Fe_{0.92}O$	494	4.36	5.86	Au	170	1.99	19.32
SiO_2	470	4.76	2.66	BN	168*	1.60	2.30
Cr	460	5.06	7.19	AgBr	144	1.71	6.48
ZnS	408*	3.97*	4.09	SnTe	144*	2.28	6.47
Al	394	4.11	2.70	In	129	1.50	7.31
ZnO	387	3.96*	5.65	MnTe	122*	1.90*	6.08
Ni	375	3.85	8.90	Bi	120	1.62	9.75
CaF_2	354	4.57*	3.18	HgTe	105	1.92*	8.08
CoPt	353	3.56	15.62	Pb	88	1.43	11.35

Θ_D is Debye temperatue (K), $\bar{v}$ is average sound velocity (10^3 m/s), ρ is density (10^3 kg/m^3), Symbol $*$ shows calculated value.

The average sound velocity is given by

$$\bar{v} = \frac{v_L + 2v_T}{3} \tag{5}$$

Some sound velocities with [100] propagation direction were calculated by elastic constant[8])

$$v_L = \sqrt{\frac{C_{11}}{\rho}} v_T = \sqrt{\frac{C_{44}}{\rho}} \tag{6}$$

Where C_{11} and C_{44} is elastic constant, ρ is density.

In order to distinguish the difference of two materials clearly, the ratio of parameter is more than 1 by normalization.

3. Results and Discussion

The relation between the interfacial thermal resistances with three ratios of parameter: the ratio of Debye temperature, the ratio of average sound velocity and the ratio of density is shown in Fig. 1. It can be seen in Fig. 1(a) that the interfacial thermal resistances have approximately linear relation with the ratios of Debye temperature for various materials in the double logarithm coordinate space. When the ratios of Debye temperature become larger, the interfacial thermal resistances increase. The relation between the interfacial thermal resistance with the ratio of average sound velocity in Fig. 1(b) is similar to that of the ratio of Debye temperature. We compare the average sound velocity and the Debye temperature in Fig. 2, not including the calculated value. It can be seen that the average sound velocities have approximately linear relation with the Debye temperatures for various materials. Fig. 1(c) shows that the ratio of density doesn't determine the interfacial thermal resistance.

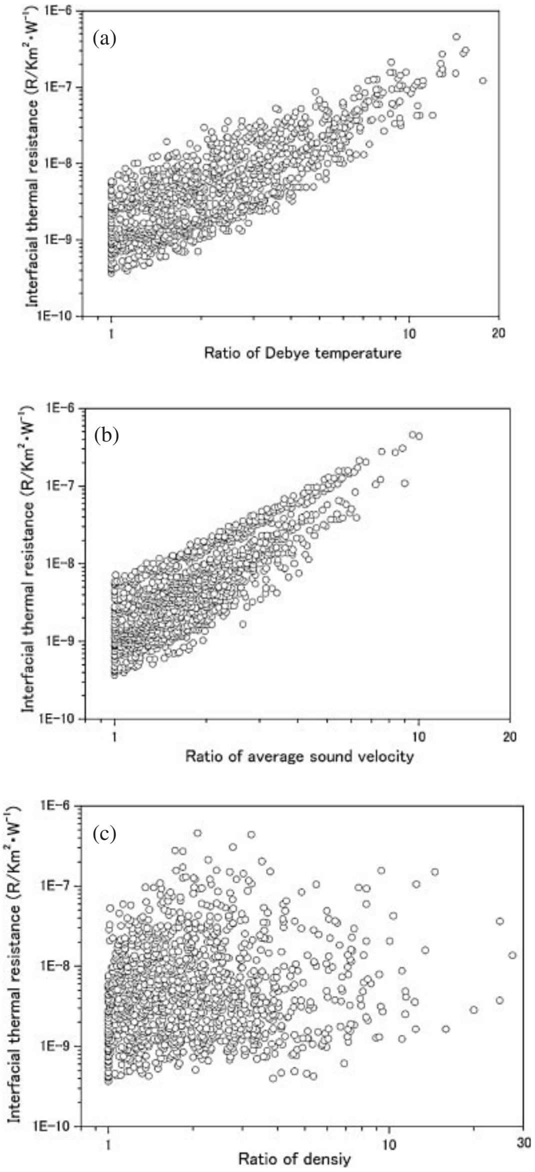

Fig. 1 Interfacial thermal resistance vs. ratios of parameter.

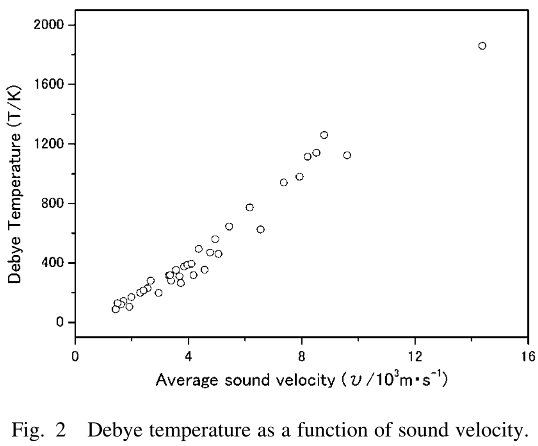

Fig. 2 Debye temperature as a function of sound velocity.

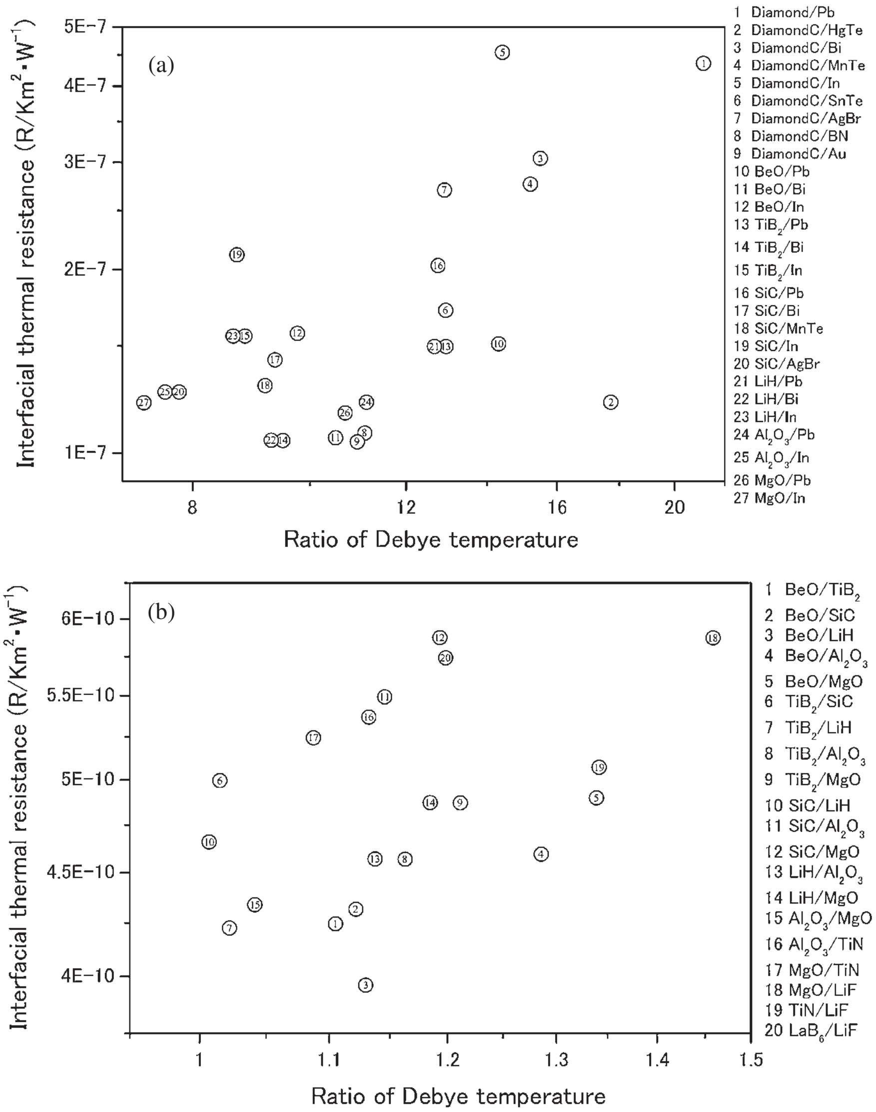

Fig. 3 (a) Interfacial thermal resistance $>1 \times 10^{-7}$ Km^2/W (b) interfacial thermal resistance $<6 \times 10^{-10}$ Km^2/W.

We only consider the ratio of Debye temperature in the following because the ratio of average sound velocity and the ratio of Debye temperature are similar.

We enlarge the high and low interfacial thermal resistances in Fig. 1(a) to Fig. 3(a) and Fig. 3(b) in order to observe the relation between the interfacial thermal resistance with the ratio of Debye temperature in detail. The ratios of Debye temperature are higher than 7 in Fig. 3(a), and the high interfacial thermal resistances are composed of one kind of high Debye temperature material (>900 K) and another kind of low Debye temperature material (<200 K). For the low interfacial thermal resistances (Fig. 3(b)), the ratios of Debye temperature are lower than 1.5, and the low interfacial thermal resistances are composed of two kinds of similar Debye temperature material, and the Debye temperatures of two materials are very high, which can be seen in Table 1.

Dividing the value of interfacial thermal resistance into four regions 10^{-7}, 10^{-8}, 10^{-9}, 10^{-10} Km^2/W, we can obtain the map of interfacial thermal resistance in Fig. 4. The materials are sorted ascendingly by the Debye temperature. The upper and lower map is symmetrical along the diagonal, and the four colors are used to show the interfacial thermal resistance region. The green region shows the high interfacial thermal resistance, and the blue region shows the low interfacial thermal resistance. The magenta and yellow show the middle interfacial thermal resistance. We can obtain the range of interfacial thermal resistance from the map.

We compare the phonon diffuse mismatch model and the experiment data in Fig. 5. The experiment data come from Ref. 9) and 10). We can see that the difference between DMM and experiment data is mostly below a factor of 3, which shows that the theoretical model can be used to determine the interfacial thermal resistance.

4. Conclusions

We have obtained the relation between the interfacial thermal resistance with the ratio of Debye temperature and the ratio of average sound velocity by plenty of materials, and two ratios can be approximately used to characterize the material difference in terms of interfacial thermal resistance. The high interfacial thermal resistances are composed of high and low Debye temperature materials. The low interfacial thermal resistances are composed of both similar Debye

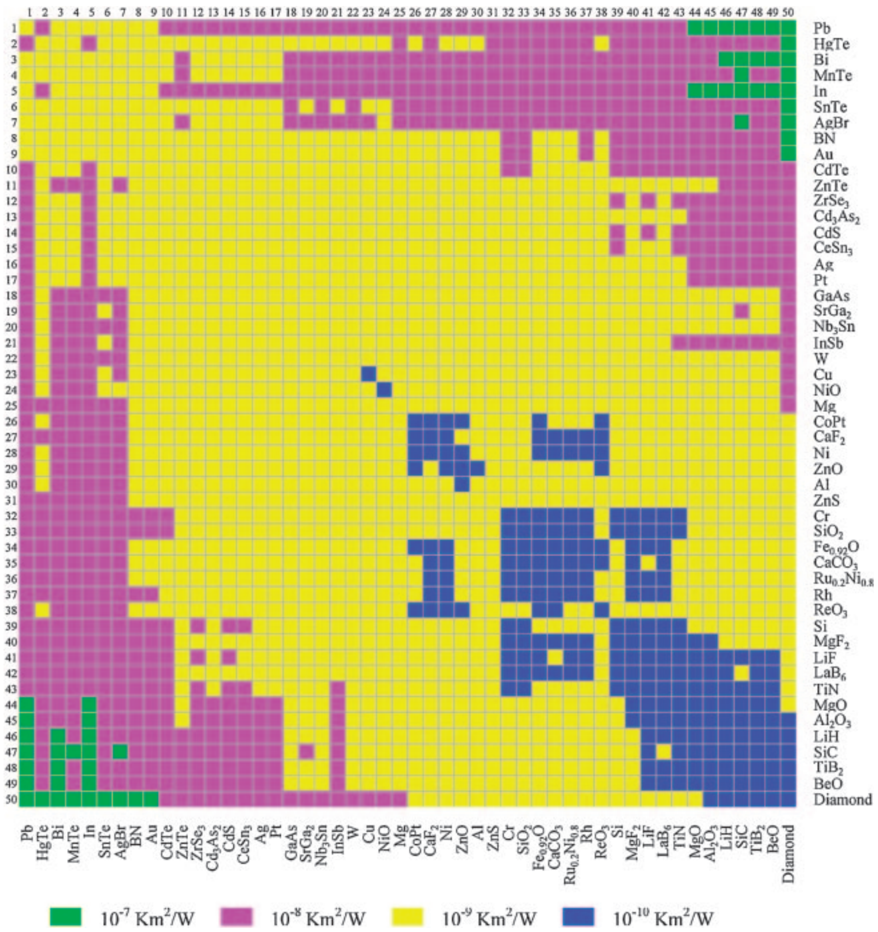

Fig. 4 Map of interfacial thermal resistance.

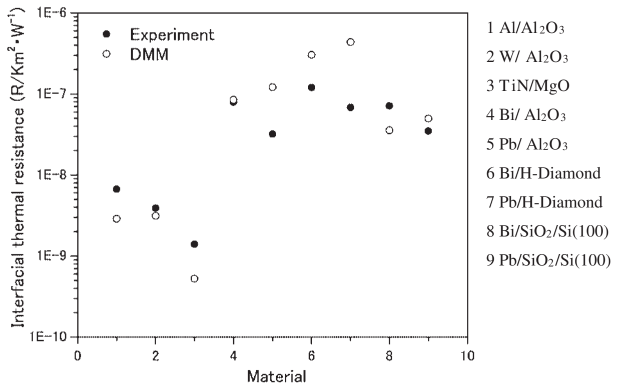

Fig. 5 Interfacial thermal resistance of several materials of experiment at room temperature.

temperature materials, and their Debye temperatures are very high. The relation between the interfacial thermal resistance with the ratio of average sound velocity is similar to that of the ratio of Debye temperature.

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