# Exercise 5.1

*Thermal boundary resistance.* Estimate the thermal boundary resistance between two materials with the following properties on the basis of the diffuse interface scattering model: material 1: $v_1 = 3900\,\mathrm{ms^{-1}}$, $C_1 = 1.67 \times 10^6\,\mathrm{Jm^{-3}K^{-1}}$; material 2: $v_2 = 6400\,\mathrm{ms^{-1}}$, $C_2 = 1.66 \times 10^6\,\mathrm{Jm^{-3}K^{-1}}$. For a heat flux of $10^8\,\mathrm{Wm^{-2}}$, estimate the temperature drop occurring at the interface.

## Solution

In diffuse interface scattering model (also known as diffuse mismatch model), phonons lose the information of their orgin after scattered by interfaces or boundaries. The phonon transmissivity from material 1 to material 2 can be obtained via [eq. (5.96) of the textbook]

$$\tau_{12}^{d} = \frac{v_1 C_1 T}{v_1 C_1 T + v_2 C_2 T} = \frac{v_1 C_1}{v_1 C_1 + v_2 C_2} = \frac{3900 \times 1.67 \times 10^6}{3900 \times 1.67 \times 10^6 + 6400 \times 1.66 \times 10^6} \approx 0.38.$$

From energy conservation, we can also get $\tau_{21}^{d} = 1 - \tau_{12}^{d} = 0.62$. Then, thermal boundary resistance [eq. (5.92) of the textbook] can be computed approximately by

$$R_e = \frac{4}{\tau_{12}^{d} v_1 C_1} = \frac{4}{0.38 \times 3900 \times 1.67 \times 10^6} \approx 1.62 \times 10^{-9}\,\mathrm{m^2 K W^{-1}}.$$

So the temperature drop at the interface is

$$\Delta T = R_e q = 10^8 \times 1.62 \times 10^{-9} = 0.162\,\mathrm{K}.$$

## Exercise 5.2

*Thermal boundary resistance at low temperature.* Thermal boundary resistance is a phenomenon that is important at low temperatures even for bulk materials and becomes important even at room temperature in nanostructures, determined by

$$\frac{1}{R_e} = \frac{1}{2}\int_0^1 \mu_1 d\mu_1 \int_0^{\omega_D} v_1 C_1(\omega)\tau_{12}(\omega,\mu_1) d\omega.$$

In the above equation, $v_1$ is sound velocity in medium 1, $C_1(\omega)$ is spectral heat capacity of medium 1, $\tau_{12}$ is phonon transmissivity from medium 1 to medium 2, $\mu_1$ is diectional cosine, and $\omega_D$ is Debye frequency. At low temperatures, it can be shown that thermal boundary resistance obeys the relation $R_e^{-1} \propto T^3$. Treating the transmissivity $\tau_{12}$ as independent of angle and frequency, derive an expression for its proportionality coefficient between $R_e^{-1}$ and $T^3$ at low temperatures.

## Solution

Considering transmissivity $\tau_{12}$ independent of angle and frequency and sound velocity $v_1$ as a constant (independent of temperature), we can simply the expression to compute thermal boundary resistance as

$$\frac{1}{R_e} = \frac{v_1\tau_{12}}{4}\int_0^{\omega_D} C_1(\omega)d\omega = \frac{v_1\tau_{12}}{4}\int_0^{\omega_D} \hbar\omega D(\omega)\frac{\partial f_{BE}(\omega,T)}{\partial T}d\omega = \frac{v_1\tau_{12}}{4}C.$$

The $C$ is total heat capacity of the system, and the spectral heat capacity $C_1(\omega)$ contributed from all the phonons with frequency $\omega$ is $\hbar\omega D(\omega)\partial f_{BE}/\partial T$, where $D(\omega)$ is the phonon density of states and $f_{BE}$ is the Bose-Einstein distribution for a phonon mode. In Debye's calculation of phonon heat capacity, lattice vibrations in solids are treated in the long-wavelength limit, having the dispersion relation $\omega(\mathbf{k}) = v|\mathbf{k}|$ with $v$ as sound velocity, and there are only three vibrational modes (one longitudinal mode and two transverse modes). So the expression for the total energy of the system $\langle E\rangle$ is

$$\langle E\rangle = 3\sum_{\mathbf{k}}\hbar\omega(\mathbf{k})f_{BE}(\omega,T) = \frac{3V}{(2\pi)^3}\int d\mathbf{k}\hbar\omega(\mathbf{k})f_{BE}(\omega,T),$$

where $V$ is the volume of the system. To make the integral easy to compute, we convert the expression above into spherical coordinate and use the dispersion relation $k = \omega/v$ to obtain

$$\begin{aligned}\langle E\rangle &= \frac{3V}{(2\pi)^3}\int_0^{2\pi} d\phi\int_0^{\pi}\sin\theta d\theta\int_0^{\infty}k^2dk\hbar\omega(k)f_{BE}(\omega,T)\\ &= \frac{12\pi V}{(2\pi)^3}\int_0^{\omega_D} d\omega\frac{\hbar\omega^3}{v^3}f_{BE}(\omega,T).\end{aligned}$$

We can further express it in phonon density of states $D(\omega)$ and assume there are $N$ atoms in the system. It becomes

$$\langle E\rangle = \int_0^{\omega_D} d\omega\hbar\omega D(\omega)[f_{BE}(\omega,T)+\frac{1}{2}] = \int_0^{\omega_D} d\omega\hbar\omega D(\omega)\frac{1}{e^{\frac{\hbar\omega}{k_BT}}-1},$$

and

$$D(\omega) = \frac{3\omega^2V}{2\pi^2v^3} = \frac{9N\omega^2}{\omega_D^3},$$

with the Debye frequency $\omega_D = (6\pi^2Nv^3/V)^{1/3}$. This Debye cutoff frequency sets the upper limit in doing the integral because in real materials there are finite number of vibrational modes (i.e. the freedom of system, $3N$), and we can get

$$3N = \int_0^{\omega_D} d\omega D(\omega).$$

By defining the variable $x = \hbar\omega/(k_BT)$, we can evaluate the integral at low temperatures*

$$\begin{aligned}\langle E\rangle &= \frac{9N\hbar}{\omega_D^3}\int_0^{\omega_D} d\omega\frac{\omega^3}{e^{\frac{\hbar\omega}{k_BT}}-1}\\ &= \frac{9N(k_BT)^4}{(\hbar\omega_D^3)^3}\int_0^{\infty}dx\frac{x^3}{e^x-1}\\ &= \frac{9N(k_BT)^4}{(\hbar\omega_D^3)^3}\frac{\pi^4}{15}\end{aligned}$$

Notice this derivation is similar to Planck's calculation of the $T^4$ energy of photons (also note the similarity to Exercise 4.3 which ended in the integral form). As a result, the heat capacity of the system is

$$C = \frac{\partial \langle E \rangle}{\partial T} = \frac{12\pi^4 N k_B}{5} \frac{(k_B T)^3}{(\hbar \omega_D)^3} = \frac{12\pi^4 N k_B}{5} \frac{T^3}{T_D^3} \propto T^3,$$

where $T_D$ is the so-called Debye temperature by the definition $k_B T_D = \hbar \omega_D$ (at which lattice vibrations are fully excited and heat capacity saturates to $3k_B N$). So the thermal boundary resistance is

$$\frac{1}{R_e} = \frac{v_1 \tau_{12}}{4} C = \frac{3\pi^4 N k_B v_1 \tau_{12}}{5} \frac{(k_B T)^3}{(\hbar \omega_D)^3} \propto T^3,$$

and the proportionality coefficient $P$ is

$$P = \frac{3\pi^4 N k_B^4 v_1 \tau_{12}}{5\hbar^3 \omega_D^3}.$$

*Note: in the integral with variable $x = \hbar\omega/(k_B T)$, we change the upper limit of integral to $\infty$ because we consider it at low temperatures and $x \to \infty$. Therefore, this result for heat capacity is only valid at low temperatures. At high temperatures, we should get the Dulong-Petit heat capacity as $C = \partial \langle E \rangle / \partial T = \partial(3k_B T N)/\partial T = 3k_B N$, which means each atom contributes $3k_B$ to the heat capacity.

## Exercise 5.3

*Phonon thermal conductivity at intermediate temperature* The phonon-phonon scattering relaxation time in the intermediate range of temperature (when $T < \theta_D$) can be approximated as

$$\frac{1}{\tau} = Aexp[-\frac{\Theta}{aT}]T^3\omega^2$$

On the basis of the Debye model(linear dispersion), derive an expression for the thermal conductivity and discuss its dependence on temperature.

## Solution

We start with a equation calculating thermal conductivity that considers phonon relaxation time being dependent on angular frequency, and the temperature :

$$k = \frac{1}{3}\int \tau\nu^2 C_\omega d\omega$$

where $\tau$, $\nu$, $C_\omega$ are phonon relaxation time, phonon velocity, and specific heat per unit frequency $\omega$ and temperature $T$ ($C_\omega = \hbar\omega D(\omega)\frac{\mathrm{d}f_0}{\mathrm{d}T}$, $f_0$ corresponds to Bose-Einstein distribution).

If we consider $\tau$ and $\nu$ are independent of frequency $\omega$ for above equation, we get the kinetic theory of gas equation $k = \frac{1}{3}C\nu^2\tau$. When $\tau$ is dependent with frequency as given in the exercise, the calculation is difficult but can be approximated by introducing Debye model.

Specific heat of Debye model per given frequency $\omega$ is written as.

$$C_w = \hbar\omega \cdot \frac{3\omega^2 V}{2\pi^2\nu^3} \cdot \frac{\hbar\omega}{k_B T^2} \frac{\exp\left\{\frac{\hbar\omega}{k_B T}\right\}}{(\exp\left\{\frac{\hbar\omega}{k_B T}\right\} - 1)^2}$$

Replacing $C_w$ with Debye model of specific heat in the above thermal conductivity equation and considering constant phonon velocity, the lattice thermal conductivity can be written as,

$$k = \frac{1}{2\pi^2\nu}\int_0^{\omega_D} \tau \cdot \frac{\hbar^2\omega^4}{k_B T^2} \cdot \frac{\exp\left\{\frac{\hbar\omega}{k_B T}\right\}}{(\exp\left\{\frac{\hbar\omega}{k_B T}\right\} - 1)^2} d\omega$$

Inputting $\frac{1}{\tau} = Aexp[-\frac{\Theta}{aT}]T^3\omega^2$ ($\Theta$=Debye temperature) and replacing $\omega$ with x ($x = \frac{\hbar\omega}{k_B T}$), thermal conductivity becomes,

$$k = \frac{k_B^2}{2A\pi^2\hbar\nu} \cdot e^{\frac{\Theta}{aT}} \cdot T^{-2} \cdot \int_0^{\frac{\Theta}{T}} \frac{x^2 e^x}{(e^x - 1)^2} dx$$

By numerically plotting above equation wrt. temperature, it is possible to see that :

if $a > 0$, thermal conductivity is approximately inversely proportional to the temperature.

if $a < 0$, thermal conductivity shows a dome shape with a peak at certain temperature value.

## Exercise 5.4

*Heat generation distribution due to absorption.* A plane wave with an intensity of $10^4$ $Wm^{-2}$ at $\lambda_0 = 0.517$ $\mu m$ meets a gold surface at $30^o$ of incidence. Determine the heat generation distribution inside the gold specimen. The refractive index at 0.517 $\mu m$ is $N = n + i\kappa = 0.608 + 2.12i$.

## Solution

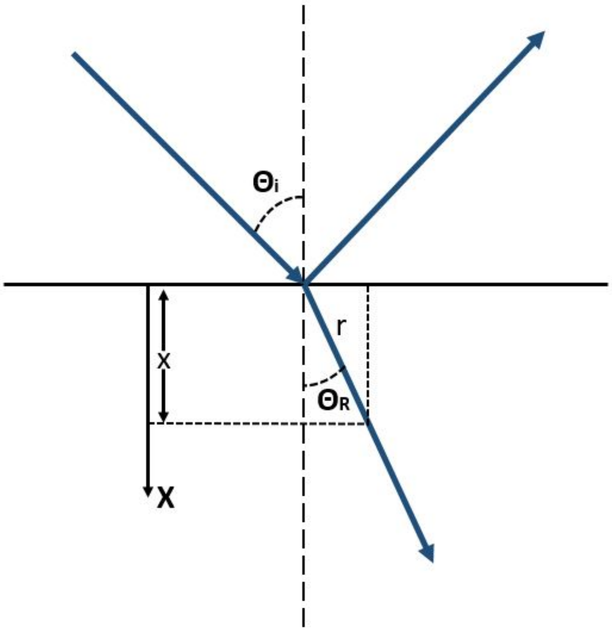

Figure 1: Incident, reflected and transmitted waves with incidence and refracted angle $\Theta_i$ *amd* $\Theta_R$ respectively.

The time averaged Poynting $< S >= \frac{1}{2} Re(\mathbf{E} \times \mathbf{H}^*)$vector gives the average energy flow into the volume. For a plane wave, it can be simplified to the following expression:

$$< S >= \frac{1}{2}\frac{n}{\mu c_0} e^{-\alpha r} E^2$$

where,

$$r = \frac{x}{cos\Theta_R} \ and \ \alpha = \frac{4\pi\kappa}{\lambda_0}$$

As intensity is proportional to Poynting vector, we can express intensity of the transmitted wave in terms of Poynting vector of the incident wave and Reflectivity.

$$I = I_i(1-R)e^{-\frac{\alpha x}{cos\Theta_R}}$$

The decrease in intensity with the penetration depth is converted to volumetric heat generation. So the heat generation rate is given by:

$$\dot{q} = -\frac{dI}{dx} = I_i(1-R)\frac{\alpha}{cos\Theta_R} e^{-\frac{\alpha x}{cos\Theta_R}}$$

where,

$$R = \left| \frac{-N_2 cos\Theta_i + N_1 cos\Theta_R}{N_2 cos\Theta_i + N_1 cos\Theta_R} \right|^2$$

and from Snell's law,

$$N_1 sin\Theta_i = N_2 sin\Theta_R$$

We can simplify the expression for $\dot{q}$, or use a simple matlab code to determine heat generation for different values of incidence angles.

$$\dot{q} = 1.9505 \times 10^{11} Re \left[ e^{-\frac{\alpha x}{cos\Theta_R}} \right] [Wm^{-3}]$$

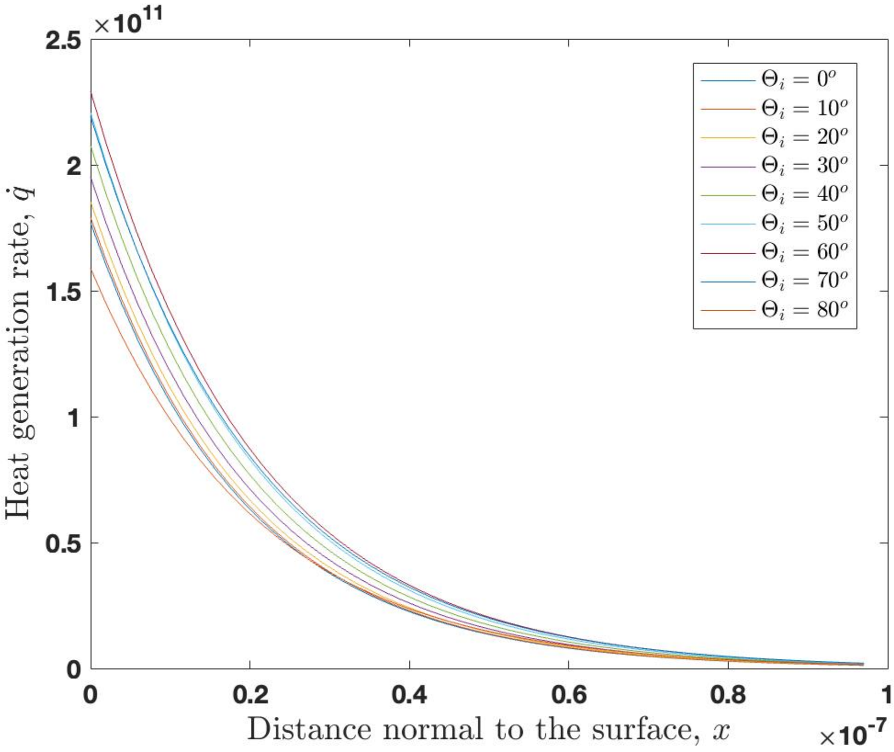

Figure 2: Volumetric heat generation rate as a function of distance normal to the surface, for various values of incidence angles.

**Note:** The value of $\Theta_R$ obtained from the Snell's law is a complex angle. What does a complex angle mean? In order to understand the significance of complex angle, one can substitute the value of $\Theta_R$ in the expression for transmitted wave and notice that the constant amplitude and constant phase surface doesn't coincides. Such a wave with different constant amplitude and phase surfaces is called an **inhomogeneous wave.**