Exercise 6.1

High-temperature thermal conductivity. At high temperature, the phonon relaxation time in a crystal is

$$\frac{1}{\tau} = \frac{k_B T}{mva}$$

where a is of the order of distance between atoms and m is the atomic weight.

a) Prove that the high-temperature thermal conductivity is proportional to $1/T$.

b) The thermal conductivity of silicon at 300 K is 145 $\mathrm{W m^{-1} K^{-1}}$. Estimate its thermal conductivity at 400 K.

Solution

(a) From the kinetic theory of phonon gas, we know that the thermal conductivity κ can be expressed as

$$\kappa = \frac{1}{3}Cv^2\tau,$$

where C and v are heat capacity and phonon group velocity, respectively. Since the inverse of relaxation time $1/\tau$ (called scattering rate) is proportional to temperature T and other properties (i.e. heat capacity and group velocity) are almost temperature-independent at high temperatures, the thermal conductivity is thus

$$\kappa = \frac{1}{3}Cv^2\tau = \frac{Cv^3 ma}{3k_B T} = \frac{A}{T},$$

proportional to $1/T$ (A is a constant). This is actually the result of Umklapp scattering of phonons which dissipate heat and the $1/T$ dependence of thermal conductivity can be the signature of the dominant Umklapp scattering in crystal.

(b) Due to the fact that the thermal conductivity at high temperatures is proportional to $1/T$, we can obtain the following relation

$$\kappa_{300} \cdot 300 = \kappa_{400} \cdot 400.$$

So the thermal conductivity of silicon at 400 K is

$$\kappa_{400} = \frac{3}{4} \times 145 = 108.75\,\mathrm{Wm^{-1}K^{-1}}.$$

Exercise 6.2

Landauer formulation for electron thermal conduction. A metallic square nanowire is placed between two thermal reservoirs at temperature T_1 and T_2. Assume that electron transmissivity is equal to one. Derive an expression for the thermal conductance of the nanowire contributed by the electron.

Solution

As electron transmissivity being 1, we can use Landauer formalism to treat the heat transfer easily. As the structure confines, we will consider strictly the 1D energy transfer by electron through the nanowire along x.

The energy transfer from reservoir 1 to 2 can be written as:

$$q_{12} = 2 \cdot \frac{1}{V} \cdot \sum_{k_x=0}^{\infty} v_x \tau_{12} (E-\mu) f_{FD}(E, T_1) = \int_0^{\infty} v_x (E-\mu) \tau_{12} D_{1D} f_{FD}(E, T_1) dE$$

This formula is similar to that of phonon, but the difference in electron case is that we consider energy $E - \mu$ and Fermi-Dirac statistic distribution of electron. Spin degeneracy, number 2 on the left equation, is implemented in the 1D density of state D_{1D} in the right equation.

Considering the detailed balance between opposite energy flows from the two reservoir, we express the flow based on the properties of one reservoir.

$$q = q_{12} - q_{21} = \int_0^{\infty} v_x (E-\mu) \tau_{12} D_{1D} (f_{FD}(E, T_1) - f_{FD}(E, T_2)) dE$$

If T_1 and T_2 are not so different,

$$q = (T_1 - T_2) \cdot \int_0^{\infty} v_x (E-\mu) \tau_{12} D_{1D} \frac{\mathrm{d} f_{FD}(E,T)}{\mathrm{d}T} dE = \Delta T \cdot K$$

$$K = \int_0^{\infty} v_x (E-\mu) \tau_{12} D_{1D} \frac{\mathrm{d} f_{FD}(E,T)}{\mathrm{d}T} dE$$

Replacing $v_x = \sqrt{\frac{2(E-E_c)}{m^*}}$,$D_{1D} = \frac{1}{\pi\hbar}\sqrt{\frac{m^*}{2(E-E_c)}}$, $\tau_{12} = 1$, $\frac{\mathrm{d} f_{FD}(E,T)}{\mathrm{d}T} = \frac{e^{\frac{E-\mu}{k_B T}}}{(e^{\frac{E-\mu}{k_B T}}-1)^2} \cdot \frac{E-\mu}{k_B T^2}$,

$$K = \int_0^{\infty} \frac{k_B^2 T}{\pi\hbar} \frac{(E-\mu)}{k_B T} \frac{e^{\frac{E-\mu}{k_B T}}}{(e^{\frac{E-\mu}{k_B T}} - 1)^2} \cdot \frac{E-\mu}{k_B T^2} dE$$

Here T can be considered as the average temperature. Setting $\chi = \frac{E-\mu}{k_B T}$, we get the final form of the 1D thermal conductance from electron,

$$K = \frac{k_B^2 T}{\pi\hbar} \int_{-\frac{\mu}{k_B T}}^{\infty} \frac{e^{\chi}}{(e^{\chi}-1)^2} \chi^2 d\chi$$

If the temperature is low, we can approximate the lower limit of integral to -∞.

$$K = \frac{k_B^2 T}{\pi\hbar} \int_{-\infty}^{\infty} \frac{e^{\chi}}{(e^{\chi}-1)^2} \chi^2 d\chi = \frac{k_B^2 T}{\pi\hbar} \cdot \frac{\pi^2}{3} = \frac{\pi k_B^2 T}{3\hbar}$$