THERMAL CONDUCTIVITY

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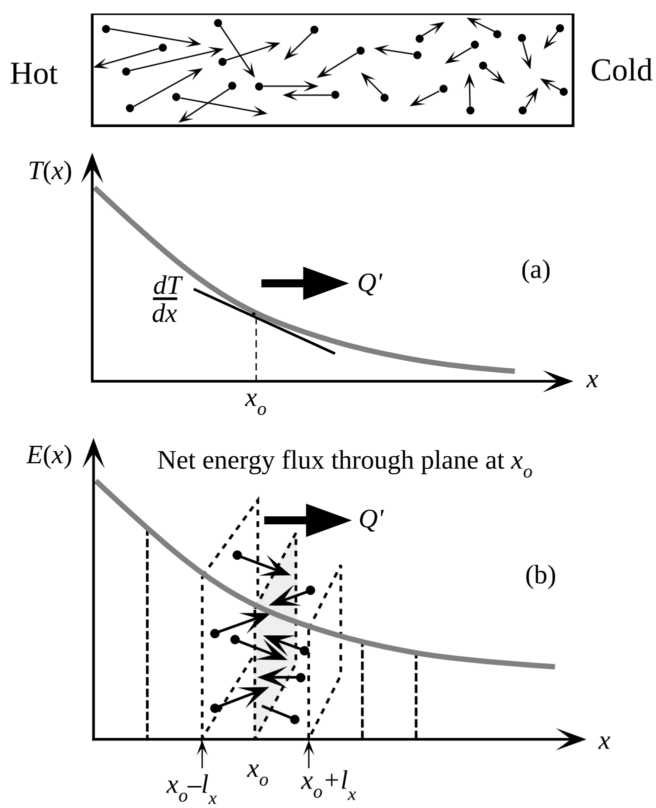
1. General Expression for Thermal Conductivity

We first consider a metallic solid in which there are nearly-free conduction electrons. When this metal is heated at one end as shown in Figure 1, the atoms vibrate more violently in this region. Electrons scattered from these atoms therefore gain energy and travel faster. Thus electrons in the hot regions are more energetic than those in the cooler regions. As a result of a temperature gradient there is therefore an electron energy gradient along the solid as illustrated in Figure 1 (a) and (b). We can represent the energy per electron as shown in Figure 1 (b) in which going towards the cooler regions, the energy decreases. Let l_x be the mean free path of an electron between scattering events along the x-direction which is the direction of heat flow. Then the electron travels a distance l_x before impacting with a vibrating lattice atom and thereby imparting some of its energy. This is how the energy is transported through the solid, by collision of fast electrons and vibrating lattice atoms. Electrons carry the energy from more energetic lattice vibrations in the hot regions to less energetic vibrations in the cold regions.



Net flux of energy from hot to cold regions of a solid. There is a net energy transfer across the area A at x_o due to the random motions of the electrons.

Figure 1

We consider an arbitrary plane at x_o and the motion of the electrons within a distance l_x on both sides of x_o. We choose a distance of l_x because within that distance, electrons suffer no randomizing collisions and we can easily follow their trajectories. Thus the x-axis is divided into equal segments of width l_x. If τ is the mean free time between collisions, then $l_x = \tau v_x$ where v_x is the mean speed along x. If E_o is the electron energy at x_o then all electrons within $x_o - l_x$ on the left side have an average energy,

$$\overline{E}_{\text{leftside}} = E_o + \left(\frac{l_x}{2}\right)\left(-\frac{dE}{dx}\right)$$

The negative sign multiplying the gradient ensures that the average energy in the left segment is greater than E_o since the gradient, dE/dx, is negative. If n is the number of electrons per unit volume, then the number of electrons in the volume l_xA is $n(l_xA)$. These electrons will reach the plane at x_o as they do not suffer collisions within l_x. Time taken to traverse l_x is τ. Stated differently, τ is the mean free time between electron scattering events. Thus, the flow of energy per unit time towards the right is given by

$$\text{Rate of energy flow towards right} = Q'_{+x} = \frac{\text{Total energy}}{\text{Time}} = \frac{n(l_xA)\left[E_o - \dfrac{l_x}{2}\dfrac{dE}{dx}\right]}{\tau}$$

The average energy of electrons in the right segment, within $x_o + l_x$, is smaller than E_o and is given by,

$$\overline{E}_{\text{right side}} = E_o - \left(\frac{l_x}{2}\right)\left(-\frac{dE}{dx}\right)$$

The corresponding energy flow per unit time towards the left is,

$$\text{Rate of energy flow towards left} = Q'_{-x} = \frac{\text{Total energy}}{\text{Time}} = \frac{n(l_xA)\left[E_o + \dfrac{l_x}{2}\dfrac{dE}{dx}\right]}{\tau}$$

The net energy flow, Q', towards the right is the difference between the above two rates:

$$Q' = Q'_{+x} - Q'_{-x} = -\frac{Anl_x^2}{\tau}\left(\frac{dE}{dx}\right)$$

Using $l_x = \tau v_x$ and $(dE/dx) = (dE/dT)(dT/dx)$ we obtain,

$$Q' = -An\tau v_x^2\left(\frac{dE}{dx}\right) = A\left(n\tau v_x^2\frac{dE}{dx}\right)\left(\frac{dT}{dx}\right)$$

If we compare this expression with the definition of thermal conductivity κ that is

$$Q' = \pm A\kappa\frac{dT}{dx}$$

then we obtain

$$\kappa = n\tau v_x^2\frac{dE}{dx} \tag{1}$$

It is useful to take Equation (1) one step further to derive a general expression for the thermal conductivity κ. In a collection of particles (electrons or atoms) moving around randomly, the speed v at any instant has components v_x, v_y, and v_z so that

$$v^2 = v_x^2 + v_y^2 + v_z^2$$

When averaged, $\overline{v_x^2} = \overline{v_y^2} = \overline{v_z^2}$ because all the particles are moving around randomly. Then

$$\overline{v_x^2} = \frac{1}{3}\overline{v^2} \approx \frac{1}{3}u^2$$

where u is simply the mean speed which is roughly $(\bar{v})^2$. Moreover, the mean free path $l = u\tau$, so that can substitute for v_x and t in Equation (1) to obtain

$$\kappa \approx \frac{1}{3}nlu\frac{dE}{dT}$$

But, dE/dT is the heat capacity per electron, and $n(dE/dT)$ is the heat capacity per unit volume, C_v so that the final expression for κ is

$$\kappa = \frac{1}{3}luC_v \qquad \textit{Thermal conductivity} \qquad (2)$$

We note that the thermal conductivity is intimately related to the mean free path of the thermal energy carriers (whether electrons in a conductor or molecules in a gas), their mean speed and their heat capacity per unit volume. Equation (2) can also be applied to solids in which thermal conduction involves lattice vibrations or *phonons*. Then, l is the mean free path of phonons between scattering events, u is their mean speed (of the order of sound velocity) and C_v is the heat capacity.

2. Wiedemann-Franz-Lorenz Law, A Classical Treatment

Suppose that we assume we can treat the collection of conduction electrons in the metal as if they were "free" and obeying the kinetic molecular theory of matter. Then their mean energy per electron and the kinetic energy along x are

$$E = \frac{3}{2}kT \qquad \text{and} \qquad \frac{1}{2}m_e v_x^2 = \frac{1}{2}kT$$

so that substituting for dE/dT and v_x in the expression for κ in Equation (1) we get,

$$\kappa = n\tau\left(\frac{kT}{m_e}\right)\left(\frac{3}{2}k\right) \qquad (3)$$

We can now use the expression for the conductivity in terms of the mean scattering time, that is $\sigma = e^2 n\tau/m_e$, and divide κ by σ to obtain,

$$\frac{\kappa}{\sigma} = \frac{3}{2}\left(\frac{k}{e}\right)^2 T \qquad (4)$$

which is the Wiedemann-Franz-Lorenz law in that $\kappa/\sigma \propto T$. The Lorenz number from Equation (4) is $C_{\text{WFL}} = {}^3/_2(k/e)^2 = 1.1 \times 10^{-8}$ W Ω K^{-2} which is at least a factor of 2 lower than typical experimental values.

Although we derived the Widemann-Franz-Lorenz law by using the kinetic theory of matter, based on classical physics, a much more rigorous quantum mechanical analysis also arrives at the same conclusion, albeit a different coefficient. Quantum mechanics predicts that

$$\frac{\kappa}{\sigma} = \frac{\pi^2}{3}\left(\frac{k}{e}\right)^2 T \qquad \textit{Wiedemann-Franz-Lorenz Law} \qquad (5)$$

where the coefficient has the value 2.45×10^{-8} W Ω K^{-2} in good agreement with experiments and twice that of the classical theory.

NOTATION

A	cross-sectional area	n	concentration of electrons (number of electrons per unit volume)
C_v	heat capacity per unit volume	Q'	rate of heat flow; net rate of energy flow
C_{WFL}	Wiedemann-Franz-Lorenz coefficient	Q'_{+x}	rate of energy flow in the $+x$ direction
e	electronic charge (magnitude only) (1.602×10^{-19} C)	T	temperature (absolute temperature)
E	energy of an electron	u	mean speed of electrons
E_o	energy of an electron at position $x = x_o$	v	velocity
k	Boltzmann's constant (1.3807×10^{-23} J K^{-1})	v_x	velocity along x
l	mean free path ($l = u\tau$)	κ	thermal conductivity
l_x	mean free path along x	σ	electrical conductivity
m_e	mass of the electron	τ	mean free time between collisions of conduction electrons with lattice vibrations

USEFUL DEFINITIONS

Lattice is a regular array of points in space with a periodicity. There are fourteen distinct lattices in three-dimensional space. When an atom or molecule is placed at each lattice point the resulting regular structure is the crystal structure.

Mean free path is the mean distance traversed by an electron between scattering events. If τ is the mean free time between scattering events, and u is the mean speed of the electron, then the mean free path, $l = u\tau$.

Mean free time is the average time it takes to scatter a conduction electron. If t_i is the free time between collisions (between scattering events) for an electron labeled as i, then $\tau = \overline{t_i}$ averaged over all the electrons. The drift mobility is related to the mean free time by $\mu_d = e\tau / m_e$. The reciprocal of the mean free time is the mean probability per unit time that a conduction electron will be scattered, or, put differently, the mean frequency of scattering events.

Phonon is a quantum of energy associated with the vibrations of the atoms in the crystal, analogous to the photon.

Thermal conductivity (κ) is a property of a material that quantifies the ease with which heat flows along a material from higher to lower temperature regions. Since heat flow is due a temperature gradient, κ is the rate of heat flow across a unit area per unit temperature gradient.

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