

1.8. TRANSPORT PROPERTIES

$$\frac{1}{\tau_i(k)} = \frac{4\pi n_i \hbar}{m^* k} \sum_l l \sin^2[\delta_l(k) - \delta_{l-1}(k)]. \quad (1.8.3.5)$$

Although this expression appears complicated, one can view it as consisting of three parts:

$$\frac{1}{\tau_i} = n_i v_k \sigma_c(k), \quad (1.8.3.6)$$

$$v_k = \frac{\hbar k}{m^*}, \quad (1.8.3.7)$$

$$\sigma_c = \frac{4\pi}{k^2} \sum_l l \sin^2[\delta_l(k) - \delta_{l-1}(k)]. \quad (1.8.3.8)$$

The three factors are the concentration n_i of impurities, the electron velocity v_k and the cross section σ_c . For each impurity, the cross section is a function of k . The lifetime is the density of impurities multiplied by a simple function of electron energy and is independent of temperature. A careful analysis shows that there is a temperature dependence to the scattering by impurities. However, this dependence is rather slight, and is dwarfed by the large temperature dependence of the electron scattering by phonons (Bass *et al.*, 1990). It is a common approximation to treat τ_i as a constant independent of temperature. It is easy to determine this constant experimentally: the resistivity in the limit of zero temperature contains just the contribution from impurities and defects.

It is possible to add a known amount of impurities intentionally. Then a measurement of the impurity resistance provides a measurement of the cross section σ_c , since the Fermi velocity v_F is usually known.

(2) *Phonons in metals.* Crystals are composed of atoms, which vibrate. As the temperature increases, they vibrate with larger amplitude. These vibrations provide a noise spectrum for the electrons and cause the electrons to scatter. The scattering of electrons by phonons is an intrinsic process. For most solids, this process is the dominant contribution to the electrical resistivity at temperatures above 100 K.

Ziman (1962) first derived the following expression for the resistivity due to the scattering of electrons by phonons in a metal:

$$\rho(T) = C' \sum_{\lambda} \int q d^3 q |M_{\lambda}(\mathbf{q})|^2 (\hat{\xi}_{\lambda} \cdot \mathbf{q})^2 \left[-\frac{\partial n_B(\omega)}{\partial \omega} \right]_{\omega=\omega_{\lambda}(\mathbf{q})} \quad (1.8.3.9)$$

$$C' = \frac{3\hbar v_0}{Me^2 16v_F^2 k_F^4}. \quad (1.8.3.10)$$

The constant C' collects numerous constants including the Fermi wavevector k_F , the Fermi velocity v_F , the ion mass M and the unit-cell volume v_0 . The phonons have wavevector \mathbf{q} and different phonon bands (e.g. TA, LA, TO) are denoted by λ . The phonon frequencies are $\omega_{\lambda}(\mathbf{q})$ and the matrix element for scattering the electron by wavevector \mathbf{q} is $M_{\lambda}(\mathbf{q})$.

Equation (1.8.3.9) is easy to evaluate using a computer code that generates all of the phonons at different points in the Brillouin zone. It is the formula used most often to calculate the temperature dependence of the resistivity of metals. However, the reader is warned that this formula is not exact, as it represents an approximate solution of the Boltzmann equation. In the only case in which the accuracy of equation (1.8.3.9) has been tested against numerically accurate solutions of the Boltzmann equation, Wu & Mahan (1984) found that (1.8.3.9) had an error of a few per cent. However, the formula is useful because it gives an answer that only errs by a few per cent and is relatively easy to calculate.

Equation (1.8.3.9) has one feature that is simple and important. At high temperature, the resistivity becomes proportional to

temperature. The Bose–Einstein occupation number $n_B(\omega) \simeq k_B T / \hbar \omega$ and then the derivative with respect to ω is simple. This gives the expression

$$\rho(T) = \frac{m^*}{n_0 e^2} \frac{1}{\tau(T)} \quad (1.8.3.11)$$

$$\frac{1}{\tau} = \frac{2\pi}{\hbar} \lambda_i k_B T \quad (1.8.3.12)$$

$$\lambda_i = \frac{m}{M} \frac{v_0}{16\pi^2 k_F^3} \int q d^3 q \frac{|M_{\lambda}(\mathbf{q})|^2 (\hat{\xi}_{\lambda} \cdot \mathbf{q})^2}{[\hbar \omega_{\lambda}(\mathbf{q})]^2}. \quad (1.8.3.13)$$

At high temperature, which in practice is above half of the Debye temperature, the inverse lifetime of the electron is proportional to the temperature. The coefficient is the dimensionless constant λ_i , which is called the ‘transport form of lambda’ (see Grimvall, 1981). This parameter gives the strength of the interaction between the electrons and the phonons. It ranges from very small values ($\lambda_i \sim 0.1$) for the noble metals to values above 4 for heavy metals such as lead and mercury (see Grimvall, 1981).

Now we give some examples of the resistivity of common metals and show that the above formulas give a good account of the resistivity. Fig. 1.8.3.1 shows the intrinsic resistivity as a function of temperature for a simple metal (sodium). The data are taken from Bass *et al.* (1990). The impurity resistivity has been subtracted away. The resistivity is lowest at low temperature, increases at higher temperature and becomes linear at very high temperatures. In actual crystals, the low-temperature value is determined by scattering from impurities and is different for each piece of metal. If one subtracts the constant value and plots $\rho(T) - \rho(0)$, then the curve is the same for each crystal of sodium. This is just the phonon contribution to the resistivity.

At very high temperatures, the resistivity is found to deviate from being linear with temperature. This deviation is due to the thermal expansion of the crystal at high temperature. This can be suppressed by taking measurements at constant volume, as is the case for the results shown in Fig. 1.8.3.1. If the crystal is put under pressure to maintain constant volume, then the high-temperature resistivity is highly linear with temperature.

Also interesting is the behaviour of the resistivity at very low temperatures, say less than 1 K. For the alkali metals, the temperature dependence was found by Bass *et al.* (1990) to be

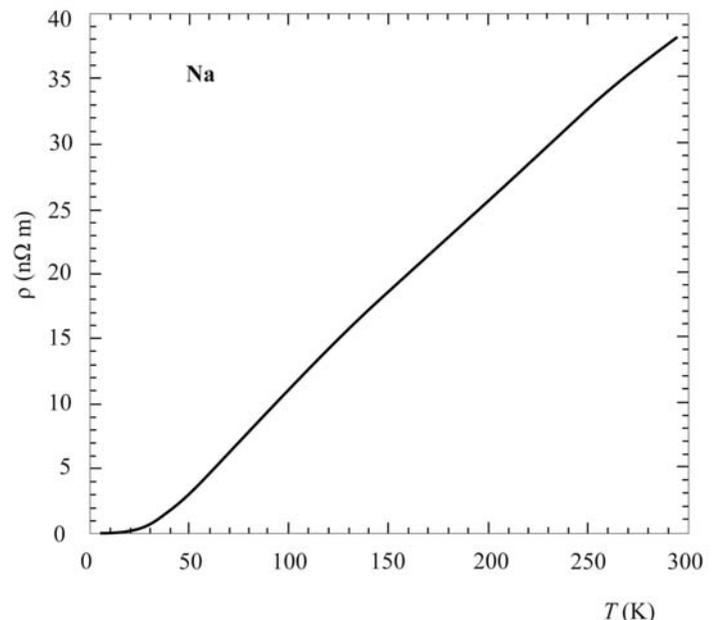


Fig. 1.8.3.1. The temperature dependence of the intrinsic electrical resistivity of sodium at constant density. The data are taken from Bass *et al.* (1990).