

## 1. TENSORIAL ASPECTS OF PHYSICAL PROPERTIES

$$\rho(T) = \rho_i(1 + BT^2) + AT^2. \quad (1.8.3.14)$$

The term  $\rho_i$  is the constant due to the impurity scattering. There is also a term proportional to  $BT^2$ , which is proportional to the impurity resistance. This factor is due to the Koshino–Taylor effect (Koshino, 1960; Taylor, 1964), which has been treated rigorously by Mahan & Wang (1989). It is the inelastic scattering of electrons by impurities. The impurity is part of the lattice and phonons can be excited when the impurity scatters the electrons. The term  $AT^2$  is due to electron–electron interactions. The Coulomb interaction between electrons is highly screened and makes only a small contribution to  $A$ . The largest contribution to  $A$  is caused by phonons. MacDonald *et al.* (1981) showed that electrons can interact by exchanging phonons. There are also terms due to boundary scattering, which is important in thin films: see Bruls *et al.* (1985).

Note that (1.8.3.14) has no term from phonons of  $O(T^5)$ . Such a term is lacking in simple metals, contrary to the assertion in most textbooks. Its absence is due to *phonon drag*. For a review and explanation of this behaviour, see Wiser (1984). The  $T^5$  term is found in the noble metals, where phonon drag is less important owing to the complexities of the Fermi surface.

## 1.8.3.2. Metal alloys

Alloys are solids composed of a mixture of two or more elements that do not form a stoichiometric compound. An example is  $\text{Cu}_x\text{Ni}_{1-x}$ , in which  $x$  can have any value. For small values of  $x$ , or of  $(1-x)$ , the atoms of one element just serve as impurities in the other element. This results in the type of behaviour described above. However, in the range  $0.2 < x < 0.8$ , a different type of resistivity is found. This was first summarized by Mooij (1973), who found a remarkable range of behaviours. He measured the resistivity of hundreds of alloys and also surveyed the published literature for additional results. He represented the resistivity at  $T = 300$  K by two values: the resistivity itself,  $\rho(T = 300)$ , and its logarithmic derivative,  $\alpha = d \ln(\rho)/dT$ . He produced the graph shown in Fig. 1.8.3.2, where these two values are plotted against each other. Each point is one sample as represented by these two numbers. He found that all of the results fit within a band of numbers, in which larger values of  $\rho(T = 300)$  are accompanied by negative values of  $\alpha$ . Alloys with very high values of resistivity generally have a resistivity  $\rho(T)$  that decreases with increasing temperature. The region where  $\alpha = 0$  corresponds to a resistivity of  $\rho^* = 150 \mu\Omega \text{ cm}$ , which appears to be a fixed point. As the temperature is increased, the resistivities of alloys with  $\rho > \rho^*$  decrease to this value, while the resistivities of alloys with  $\rho < \rho^*$  increase to this value.

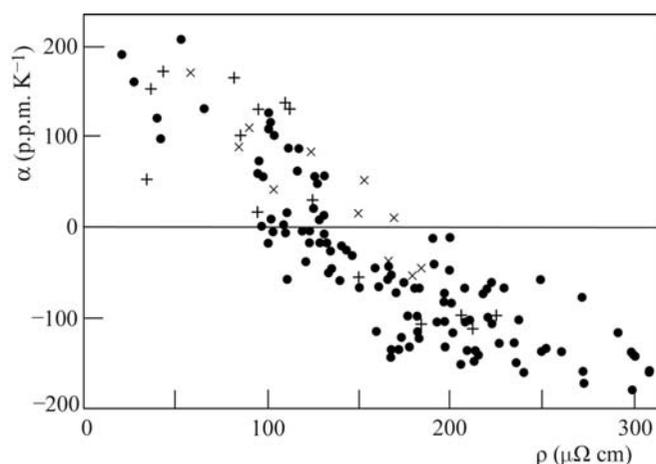


Fig. 1.8.3.2. The temperature coefficient of resistance *versus* resistivity for alloys according to Mooij (1973). Data are shown for bulk alloys (+), thin films (•) and amorphous alloys (x).

Mooij's observations are obviously important, but the reason for this behaviour is not certain. Several different explanations have been proposed and all are plausible: see Jonson & Girvin (1979), Allen & Chakraborty (1981) or Tsuei (1986).

Recently, another group of alloys have been found that are called *bad metals*. The ruthenates (see Allen *et al.*, 1996; Klein *et al.*, 1996) have a resistivity  $\rho > \rho^*$  that increases at high temperatures. Their values are outliers on Mooij's plot.

## 1.8.3.3. Semiconductors

The resistivity of semiconductors varies from sample to sample, even of the same material. The conductivity can be written as  $\sigma = n_0 e \mu$ , where  $e$  is the charge on the electron,  $\mu = e\tau/m^*$  is the mobility and  $n_0$  is the density of conducting particles (electrons or holes). It is the density of particles  $n_0$  that varies from sample to sample. It depends upon the impurity content of the semiconductor as well as upon temperature. Since no two samples have exactly the same number of impurities, they do not have the same values of  $n_0$ . In semiconductors and insulators, the conducting particles are extrinsic – they come from defects, impurities or thermal excitation – in contrast to metals, where the density of the conducting electrons is usually an intrinsic property.

In semiconductors, instead of talking about the conductivity, the more fundamental transport quantity (Rode, 1975) is the mobility  $\mu$ . It is the same for each sample at high temperature if the density of impurities and defects is low. There is an intrinsic mobility, which can be calculated assuming there are no impurities and can be measured in samples with a very low density of impurities. We shall discuss the intrinsic mobility first.

Fig. 1.8.3.3 shows the intrinsic mobility of electrons in silicon, from Rode (1972), as a function of temperature. The mobility generally decreases with increasing temperature. This behaviour is found in all common semiconductors. The mobility also decreases with an increasing concentration of impurities: see Jacoboni *et al.* (1977).

The intrinsic mobility of semiconductors is due to the scattering of electrons and holes by phonons. The phonons come in various branches called TA, LA, TO and LO, where T is transverse, L is longitudinal, A is acoustic and O is optical. At long wavelengths, the acoustic modes are just the sound waves, which

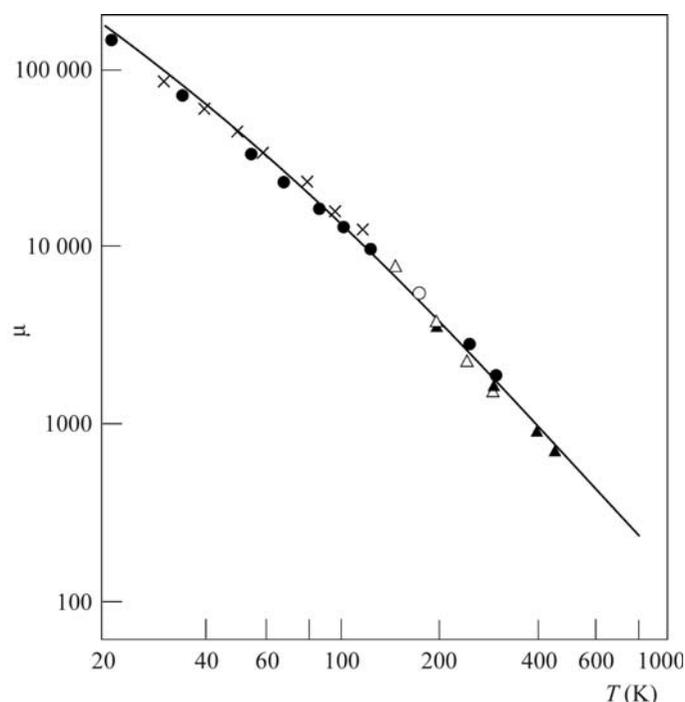


Fig. 1.8.3.3. The intrinsic mobility of electrons in silicon. Solid line: theory; points: experimental. After Rode (1972).

## 1.8. TRANSPORT PROPERTIES

can be modelled by a Debye model,  $\omega_j(\mathbf{q}) = c_j q$ , where  $c_j$  is the speed of sound for the mode  $j$ . At long wavelengths, the optical modes have a constant frequency which is represented by an Einstein model,  $\omega_j(\mathbf{q}) = \omega_0$ .

The intrinsic mobility is that for a low density of electrons or holes. The existing conducting particles are then confined to the lowest wavevector states near the minimum of the conduction band (electrons) or near the maximum of the valence band (holes). The phonons scatter the particles locally, so that the wavevector changes by small amounts, which can only be done by phonons of long wavelength. The above approximations, of using a Debye model for A modes and an Einstein model for O modes, is accurate. This is because one only needs to consider phonons of long wavelength: the approximations are inaccurate for phonons of short wavelength, but they are irrelevant.

The exception to this general behaviour is where the conduction band has several equivalent minima and the phonons scatter an electron from one minimum to another. This is called intervalley scattering. If the minima of the two electron pockets are separated by a wavevector  $\mathbf{q}_m$ , then one needs phonons of energy  $\omega_j(\mathbf{q}_m)$ . Again, these are a fixed set of constants, so one can assume an Einstein model with these phonons as the frequency. For the calculation of the intrinsic mobility of a semiconductor, one does not need to know all of the phonon modes in the solid, as one does for a metal. Instead, one needs to know only the phonons at selected points in the Brillouin zone.

The inverse lifetimes for each scattering process are simply added:

$$\frac{1}{\tau(k)} = \frac{1}{\tau_A(k)} + \frac{1}{\tau_O(k)} + \frac{1}{\tau_I(k)}. \quad (1.8.3.15)$$

The three terms are acoustic, optical and intervalley. First, we discuss the scattering by optical phonons. The inverse lifetime is proportional to the density of optical phonons  $N_0$ :

$$\frac{1}{\tau_0} = \frac{N_0}{\tau}, \quad (1.8.3.16)$$

$$N_0 = \frac{1}{\exp(\hbar\omega_0/k_B T) - 1}. \quad (1.8.3.17)$$

The lifetime  $\tau_0 \propto N_0^{-1} = \exp(\hbar\omega_0/k_B T) - 1$ . This shows that the mobility increases exponentially at lower temperatures according to the factor  $\exp(\hbar\omega_0/k_B T) - 1$ . This feature is common to nearly all semiconductors.

The factor  $N_0$  occurs because the electrons must absorb an optical phonon in order to scatter. The density of optical phonons in the crystal is proportional to the factor  $N_0$ . Since usually  $k_B T < \hbar\omega_0$  at room temperature, the thermally excited electrons have less energy than an optical phonon. In this case, the electrons cannot emit a phonon, since they are unable to lose that much energy: the process has no final state.

Notice that we have not yet discussed the mechanism by which the electron couples to the optical phonons. In general, there are two: the polar interaction and the deformation potential interaction. Polar interactions are found in crystals with different atoms and where there is some ionic bonding. When the charged ions vibrate, it results in oscillating dipoles that create long-range electric fields. Polar interactions are important in III-V and II-VI semiconductors such as GaAs or CdS. Polar interactions are not present in elemental semiconductors such as silicon and germanium, since each ion is neutral. However, the deformation potential interaction is present in these and could scatter strongly.

Next we discuss the intervalley scattering, where an electron moves between equivalent conduction-band minima. Here the phonons have a discrete energy  $\hbar\omega_j(\mathbf{q}_m)$ . At low temperatures, the electron can only absorb this phonon and the process is proportional to  $N(\omega_j(\mathbf{q}_m))$ . This behaves, in many ways, like the scattering by optical phonons. However, since  $\omega_j(\mathbf{q}_m) < \omega_0$ , the

temperature at which phonon emission can occur is lower. At low temperatures, the intervalley scattering also contributes exponential factors to the inverse lifetime. These contributions are usually lower than the optical phonon scattering. However, in silicon, Rode (1972) showed that the intervalley scattering dominates over the optical phonon scattering.

The scattering by acoustic phonons only is important at low temperature. For most semiconductors, the interaction between electrons and acoustic phonons is due to the deformation potential interaction. The standard calculation gives the inverse lifetime as proportional to  $T^{3/2}$ , which becomes smaller at low temperature. However, since the other phonon contributions become smaller with an exponential dependence upon temperature, at small enough temperatures the acoustic phonon term makes the largest contribution to the inverse lifetime. Therefore, at low temperatures, the scattering by acoustic phonons limits the mobility of the electron. Of course, this presumes that there is no contribution from the scattering by impurities. Since this contribution is a constant at low temperature, it is always the dominant contribution at low temperatures. Only in samples with a small concentration of impurities can one actually observe the limitation by acoustic phonons. For most samples, with a moderate density of impurities, the optical-phonon part forms the limit at intermediate temperatures, the impurity scattering forms the limit at low temperatures and one never observes the limit from acoustic phonons.

The discussion above covers the behaviour in the majority of cases. There are special types of crystal that show special behaviour. One of these is crystals that are strongly piezoelectric. The size of the electron-phonon interaction due to piezoelectricity is governed by the electromechanical coupling constant. In crystals where this number is relatively large, the scattering of electrons by acoustic phonons gives  $\tau \propto T^{1/2}$  at low temperature, as shown by Mahan (1990). So far, the only class of crystals where this is found is the II-VI semiconductors with the wurtzite structure: ZnO and CdS. These are the most piezoelectric crystals found so far. They both show a dependence of the mobility upon  $T^{1/2}$  at low temperature.

Finally, we should mention that semiconductors have an intrinsic conductivity that provides an absolute minimum to the conductivity of any sample. The value of this conductivity depends upon temperature. An electron is thermally excited above the energy gap, creating an electron and a hole. The density of electrons or holes is usually determined by the density of the various impurities or native defects, such as vacancies or interstitials. However, in a perfect crystal without defects, there will still be electrons and holes. The density of electrons ( $n$ ) and holes ( $p$ ) obeys the relationship

$$np = 4N_c N_v \left( \frac{2\pi\hbar^2}{m_c k_B T} \right)^{3/2} \left( \frac{2\pi\hbar^2}{m_v k_B T} \right)^{3/2} \exp(-E_G/k_B T), \quad (1.8.3.18)$$

where  $E_G$  is the energy gap between the electron and hole bands, and  $N_j$  and  $m_j$  are the number of equivalent bands and their effective masses. This formula comes from chemical equilibrium: the recombination of electrons and holes is controlled by phase space and the energy gap. The absolute minimum number of electrons and holes is where  $n = p$ , so that each is equal to the square root of the right-hand side of (1.8.3.18). If this minimum value is called  $n_m = p_m$ , then the minimum conductivity is  $\sigma_m = n_m(\mu_c + \mu_v)$ , where  $\mu_c$  and  $\mu_v$  are the mobilities of the electrons and the holes, respectively. The conductivity is never lower than this value.

### 1.8.3.4. The Hall effect

Measurement of the Hall effect is simple and often useful. One takes a crystal and applies a magnetic field  $B_z$  along the  $z$  axis.