9c. Electronic Properties of Solids

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DEFINITIONS AND FORMULAS

9c-1. Energy-band Theory of Solids (refs. 1, 2, and 3). According to quantum theory an electron bound to an atom can exist in only a limited number of discrete energy states. A large number of noninteracting identical atoms will all have the same set of allowed discrete energy states. If, now, these atoms are brought closer together and finally to their actual distances in a solid, they begin to interact and the energy levels will split. In a periodic array of atoms (crystalline solid), the allowed states tend to cluster into continuous groups of energy levels called *energy bands*. These energy bands may or may not overlap. The solid may also consist of two, three, or more kinds of different atoms (compounds).

Metal: A material in which the highest occupied energy band is only partly filled. The resistivity of metals *increases* with temperature; the temperature dependence is close to linear except at low temperatures.

Semiconductor (refs. 1, 2, and 3): A material in which the highest occupied energy band (*valence band*) is completely filled at absolute zero. The *energy gap* between the valence band and the next higher band (*conduction band*) is between zero and 4 or 5 eV. The resistivity *decreases* in certain temperature ranges exponentially with increasing temperature.

Insulator: A material in which the highest occupied energy band is completely filled. The difference between insulators and semiconductors is only gradual. Materials with energy gaps larger than 4 or 5 eV are usually called insulators. The resistivity of pure insulators at room temperature is extremely high. At elevated temperature ionic conduction often dominates electronic conduction.

Effective Mass (refs. 1, 2, and 3). Near the top or the bottom of a band the energy is generally a quadratic function of the wave vectors, so that by analogy with the expression $\mathcal{E} = p^2/2m = \hbar^2k^2/2m$ for free electrons we can define an effective mass m^* such that $\partial^2\mathcal{E}/\partial k^2 = \hbar^2/m^*$ (p = momentum, k = wavevector, $\hbar$ = Planck's constant $\times 1/2\pi$). The effective mass of electrons is positive. Near the top of a band m^* is negative, so that the motion corresponds to that of a positive charge (*hole*).

9c-2. Distribution Function, Fermi Energy, etc. The probability that a given state of energy $\mathcal{E}$ is occupied is given by

$$f = \frac{1}{e^{\frac{\mathcal{E}-\mathcal{E}_F}{kT}} + 1}$$

[1] Definitions and Formulas.

[2] Bibliography of Energy Band Calculations.

This is called the *Fermi-Dirac distribution function.* $\mathcal{E}_F$ is the *Fermi energy.* At absolute zero $\mathcal{E}_F{}^0$ has the significance of a cutoff energy. All states with energy less than $\mathcal{E}_F{}^0$ are occupied, and all states with energy greater than $\mathcal{E}_F{}^0$ are vacant. The distribution is called *degenerate* when $\mathcal{E}_F \gg kT$ and *nondegenerate* when $\mathcal{E}_F \ll kT$. In the latter case the distribution function becomes

$$f = e^{\frac{\mathcal{E}_F - \mathcal{E}}{kT}} = A \cdot e^{-\frac{\mathcal{E}}{kT}}$$

This is known as the *Maxwell-Boltzmann* or *classical distribution function.* The *density of states* (or number of states with energy $\mathcal{E}$) per unit volume is given by

$$g(\mathcal{E}) = \frac{4\pi(2m^*)^{3/2}}{h^3}\,\mathcal{E}^{1/2}$$

(for spherical energy surfaces). The Fermi energy or Fermi level is determined by the total number of electrons per unit volume (n_0). One calculates for Fermi-Dirac statistics:

$$\mathcal{E}_F \cong \mathcal{E}_F{}^0\left[1 - \frac{\pi^2}{12}\left(\frac{kT}{\mathcal{E}_F{}^0}\right)^2 + \cdots\right]$$

where

$$\mathcal{E}_F{}^0 = \frac{h^2}{2m^*}\left(\frac{3n_0}{8\pi}\right)^{2/3}$$

and for Maxwell-Boltzmann statistics:

$$\mathcal{E}_F = kT \ln \frac{n_0 h^3}{2(2\pi m^* kT)^{3/2}}$$

9c-3. Transport Properties. *Electrical Conductivity.* In a solid where ohmic conduction occurs, the current density **J** is given by

$$\mathbf{J} = \sigma \mathbf{E}$$

where σ is the conductivity and **E** the applied electric field. In a homogeneous isothermal crystal σ is a tensor having the symmetry of the crystal.

Mobility. The drift mobility of charge carriers is defined as the drift velocity per unit applied electric field (v_D/E). The relation to the *collision time* τ_c is given by

$$\mu^{(D)} = \frac{e\tau_c}{m^*}$$

Hall Effect. When a magnetic field is applied to a conductor carrying a current density **J**, an electric field $\mathbf{E}_H$ (Hall field) is developed given by the relation

$$\mathbf{E}_H = R\mathbf{J} \times \mathbf{B}$$

R is called the *Hall coefficient* and **B** is the magnetic induction. When the current density is in the length direction of the sample (J_x) and the field in the z direction, the Hall coefficient (for electrons *or* holes) is

$$R = \mp \frac{r}{ne} = \mp \frac{\mu}{\sigma}$$

where n = carriers/cm³
$e = 1.6 \times 10^{-19}$ coul
μ = cm²/volt-sec
σ = (ohm-cm)$^{-1}$
r = a scattering factor of the order of 1

Hence R = cm³/coul. μ is called the *Hall mobility* and is usually somewhat different from the drift mobility.

Magnetoresistance. The resistance of a metal or semiconductor is altered by the presence of a magnetic field. The relative change in resistance is

$$\frac{\Delta\rho}{\rho} = \frac{aB^2}{1 + \mu^2 B^2}$$

The theory for a single isotropic energy band gives no change in resistance for metals. For semiconductors (with one type of carrier scattered by acoustical lattice vibrations) one finds at low fields that

$$a = 0.38\mu^2 \times 10^{-16}$$

where the mobility μ is measured in cm²/volt-sec and B in oersteds.

Seebeck Effect (Thermoelectric Power). If two different conductors are joined together at both ends and the two junctions kept at different temperatures, an electromotive force is set up which is proportional to the temperature difference (for small ΔT). The thermoelectromotive force per degree centigrade is called the *thermoelectric power* (Q).

For metals: $$Q = \frac{\pi^2 k^2 T}{3e} \left(\frac{\partial \log \sigma(\mathcal{E})}{\partial \mathcal{E}} \right)_{\mathcal{E} = \mathcal{E}_F}$$

where $\sigma(\mathcal{E})$ is the electrical conductance due to charge carriers of energy $\mathcal{E}$.

For semiconductors see Sec. 9e-4.

Thomson Effect. When an electric current $\mathbf{J}$ passes between two points of a homogeneous conductor, with a temperature difference ΔT existing between these points, an amount of heat $\sigma_T \mathbf{J}\, \Delta T$ is emitted or absorbed in addition to the Joule heat. The parameter σ_T is called the *Thomson coefficient.*

Peltier Effect. If two conductors are joined together and kept at a constant temperature while a current $\mathbf{J}$ passes through the junction, heat is generated or absorbed at the junction in addition to the Joule heat. The *Peltier coefficient* Π_{12} is defined so that the heat emitted or absorbed per second at the junction is $\Pi_{12} J$.

Kelvin Relations

$$Q_{12} = \Pi_{12} T$$
$$T \frac{dQ_{12}}{dT} = \sigma_{T_1} - \sigma_{T_2}$$

Nernst Effect (ref. 4). If a temperature gradient is maintained in an electronic conductor ($\mathbf{J} = 0$) in the presence of a transverse magnetic field, a transverse electric field develops which is given by

$$\mathbf{E}_t = Q_N \nabla T \times \mathbf{B}$$

Q_N is called the isothermal *Nernst coefficient.* For semiconductors (one type of carrier, classical statistics, and acoustical lattice scattering):

$$Q_N = -\frac{3\pi}{16} \frac{k}{e} \mu$$

Ettinghausen Effect (ref. 4). If a temperature difference is maintained across an electronic conductor perpendicular to a current of density $\mathbf{J}$ in the presence of a magnetic field, a transverse temperature gradient is established given by

$$\nabla_t T = P \mathbf{J} \times \mathbf{B}$$

P is called the *Ettinghausen coefficient.* The Ettinghausen coefficient P, the Nernst coefficient Q_N, and the thermal conductivity κ are related by the expression

$$\kappa P = T Q_N$$

Righi-Leduc Effect (ref. 4). If a temperature difference is maintained in an electronic conductor in the presence of a magnetic field in which $\mathbf{J} = 0$, a transverse temperature gradient is established:

$$\nabla_t T = S\mathbf{B} \times \nabla T$$

S is called the *Righi-Leduc coefficient.*

Thermal Conductivity. If a temperature difference is maintained across a solid, the heat transported per unit time and unit cross-sectional area is

$$q = \kappa \nabla T$$

where κ is the *thermal conductivity.* The thermal conductivity of an electronic conductor can be written as the sum of two compounds; κ_l is due to heat transport via the lattice, and κ_e stems from the electronic heat transport:

$$\kappa = \kappa_l + \kappa_e = \kappa_l + L\sigma T$$

where σ is the electrical conductivity and L the *Lorenz number* or *Wiedemann-Franz ratio.* For degenerate free electrons,

$$L = \frac{\pi^2}{3}\left(\frac{k}{e}\right)^2 = 2.45 \times 10^{-8}\,\frac{\text{watt-ohm}}{\text{deg}^2}$$

For nondegenerate free electrons and acoustical lattice scattering,

$$L = 2\left(\frac{k}{e}\right)^2$$

Thermionic Emission. The current density of electrons emitted from a metal at temperature T is

$$J = AT^2e^{-\phi/kT}$$

This is the *Richardson-Dushman equation.* ϕ is the *work function,* $A = 4\pi mek^2/h^3 =$ 120 amp/cm²/deg².

9c-4. Specific Heat. The specific heat of an electronic conductor consists of two terms

$$C_v = \gamma T + BT^3$$

where the first term is the electronic and the second the lattice contribution. The former can usually be observed only at very low temperatures.

For degenerate free electrons:

$$\gamma = \frac{\pi^2 k^2}{\mathcal{E}_F}\ \text{ergs/deg}^2\ \text{per electron}$$

For nondegenerate free electrons:

$$\gamma = \frac{3}{2}\frac{k}{T}\ \text{ergs/deg}^2\ \text{per electron}$$

9c-5. Magnetic Properties of Electrons. *Cyclotron Resonance.* Current carriers in a solid when accelerated by a microwave electric field perpendicular to an externally applied static magnetic field H will spiral about the magnetic field. For sufficiently large mean free path l or collision time τ—the condition is $\omega_c\tau > 1$—a resonance absorption is observed for a frequency

$$\omega_c = \frac{eH}{m^*c}$$

where c is the velocity of light. This technique provides a direct measurement of the effective mass electrons (or holes) m^*.

Magnetic Susceptibility of Charge Carriers. Charge carriers contribute a diamagnetic effect through their translational motion and a paramagnetic effect due to their spin. For nondegenerate conductors (semiconductors),

$$\chi_e = \frac{n\mu_B^2}{kT}\left(1 - \frac{m^2}{3m^{*2}}\right)$$

where n is the concentration of free carriers and μ_B the Bohr magneton. If m^* is small (Ge), the susceptibility is mainly diamagnetic. If m^* is large (TiO_2), the paramagnetic effect dominates.

For degenerate conductors (metals, semimetals, and impure semiconductors) at low temperature,

$$\chi_e = \frac{3n\mu_B^2}{2\mathcal{E}_F}\left(1 - \frac{m^2}{3m^{*2}}\right)$$
$$= \frac{4m^*\mu^2}{h^2}(3\pi^2 n)^{\frac{1}{3}}\left(1 - \frac{m^2}{3m^{*2}}\right)$$

Transition metals have a large m^*, and consequently they show a high magnetic susceptibility (*Pauli paramagnetism*); semimetals with small m^* (e.g., Bi) have a diamagnetic susceptibility.

Knight Shift. Polarization of conduction electrons will produce a shift in frequency at which nuclear magnetic resonance absorption will occur for a given type of nucleus in a metal relative to a particular nonmetallic solid.

9c-6. Optical Properties of Electrons. *Optical Absorption.* Electromagnetic radiation of wavelengths in the ultraviolet, visible, or infrared region will be absorbed by a semiconductor or metal through the excitation of electrons and phonons.

As far as the electronic excitation is concerned, three mechanisms can be distinguished:

1. Electronic transition between different energy bands
2. Electronic transitions within an energy band ("free carrier absorption")
3. Electronic transitions between a localized state of an imperfection and an energy band

The absorption coefficient α is deduced from the measured transmission by means of the following expression:

$$T = \frac{I}{I_0} = \frac{(1 - R^2)e^{-\alpha d}}{1 - R^2 e^{-2\alpha d}}$$

where I_0 = incident light intensity
I = transmitted light intensity
d = thickness of sample
R = reflectivity = $[(n-1)^2 + k^2]/[(n+1)^2 + k^2]$
n = refractive index
k = extinction coefficient = $\alpha \times$ wavelength/4π

Photoconductivity: An increase of electrical conductivity under illumination due to excitation of electrons or holes into conducting states.

The resulting current is given by

$$J = \frac{eIV\mu\tau}{L^2}$$

where I = absorbed light intensity
V = applied voltage
μ = carrier mobility
τ = carrier lifetime
L = length of sample

Photovoltaic Effect: The generation of a voltage (due to optical excitations) when a semiconductor is illuminated at the electrodes or at internal barriers or *p-n* junctions.

Carrier Lifetime: The length of time that an electron (hole) spends in conducting states before being captured by a hole (electron) or imperfection. The decay of excess carriers follows the law

$$\frac{dn}{dt} = \frac{n_0 - n}{\tau}$$

where n_0 is the equilibrium density of carriers and τ the *carrier lifetime.*

Exciton: A bound electron-hole pair in an insulator or a semiconductor. The exciton energy levels are states in the forbidden energy gap, below the conduction band. The exciton may move through the crystal, transporting energy but no electrical charge, because it is neutral.

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