

Semiconductor Physics

P. S. Kireev

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**SEMICONDUCTOR
PHYSICS**

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by
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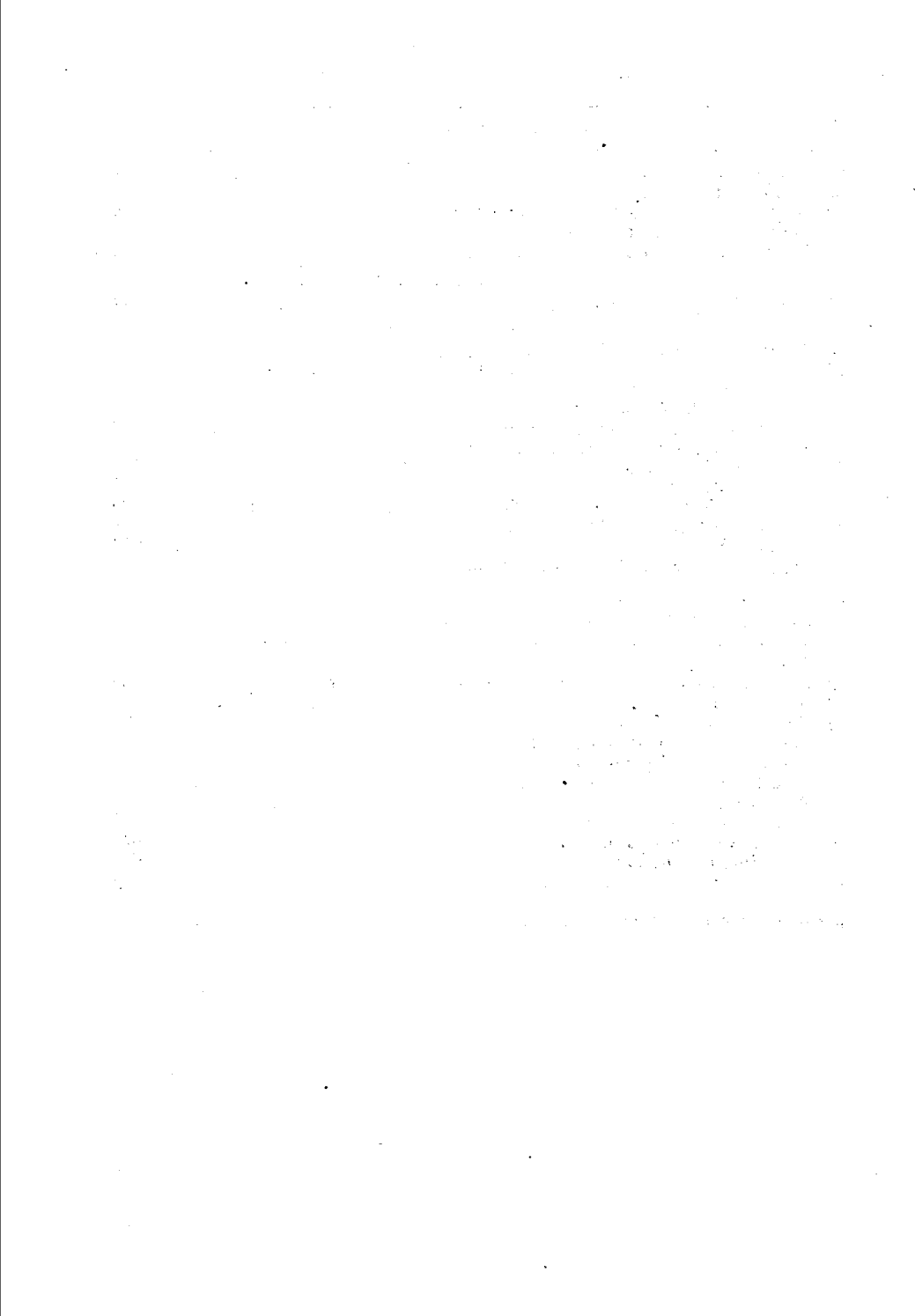
Contents. Classical Mechanics (122 problems). Electrodynamics (147 problems). Quantum Mechanics (135 problems). Statistical Physics and Thermodynamics (171 problems).

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PREFACE

This textbook is based on lectures which the author has been reading to the students of the Semiconductor Materials and Devices Faculty of the Moscow Institute of Steel and Alloys. The course in Physics of Semiconductors is read after the students become familiar with such courses as "Crystallography", "Quantum Mechanics", etc. This is why this textbook does not treat any questions pertaining to crystal lattice structure, types of atomic bonds in the lattice, etc. Students' familiarity with the principal concepts of quantum mechanics enables its methods to be used to obtain a more rigorous solution of problems arising in the course of formulating various aspects of semiconductor physics. This applies, practically, to every section of the course, and first of all to the fundamentals of the energy band structure and to the charge carrier transition processes involving the interaction with lattice defects, phonons and photons.

Experience has shown that the rather high standards employed in formulating the material do not present undue difficulties to the students. The understanding is substantially facilitated by the presence of practically all of the intermediate calculations. The results of the calculations are sometimes illustrated by experimental data.

The use of the methods of the theory of groups simplifies the handling of many of the problems involved. However, the author bearing in mind that the theory of groups is as a rule not studied in techni-

cal colleges felt he had no right to use the theory of groups approach in formulating the material contained in the book limiting himself to an Appendix containing the fundamentals of this theory.

Treating Semiconductor Physics as a separate discipline the author shied away from anything that dealt with the operation of concrete semiconductor devices.

The author uses this occasion to thank everyone who co-operated in the work that led to the publication of this edition of Semiconductor Physics.

The author.

INTRODUCTION. ELECTRON THEORY OF CONDUCTIVITY

1. ELECTRON THEORY OF CONDUCTIVITY. OHM'S LAW

Many concepts of modern physics are based on the electron theory of metals. This is true especially of such concepts as electric conductivity and carrier mobility.

The electron theory of metals developed in the XIX century presumes the electron gas to be in thermal equilibrium with the crystal lattice. The electron gas is presumed to be analogous to the ideal gas of molecular physics in that *it occupies no volume, and there is no interaction between the electrons*. The state of motion of each particle is described by six quantities: the three co-ordinates x, y, z and three velocity components v_x, v_y, v_z (or momentum components p_x, p_y, p_z), or by two vectors \mathbf{r} and \mathbf{v} (or \mathbf{p}). The assumption of a negligible volume is apparently a correct one, since, according to the classical theory, the radius of an electron $r_e \approx 10^{-16}$ m and the volume $V_e \approx 10^{-46}$ m³. Taking the number of electrons per unit volume to be $n \approx 10^{24}$ m⁻³, we calculate the relative volume of the electrons proper b to be $b = n V_e \approx 10^{-22}$ of the volume of the body. However, the assumption of no interaction between the electrons seems to be absolutely unjustified. In fact, the charge of the electron is $e = 1.6 \cdot 10^{-19}$ C, and the force of interaction between two electrons at a distance of 10^{-10} m is $2 \cdot 10^{-8}$ N. The acceleration of an electron that would result from the application of this force would amount to $2 \cdot 10^{23}$ m/s². The energy of Coulomb interaction between two electrons at a distance of $r = 10^{-10}$ m is about 14 eV.

The total energy of Coulomb interaction (repulsion) of all the electrons should reach enormous positive values. The experiment, on the other hand, proves the energy of the electrons in metals to be negative (in relation to the energy of an electron at an infinite distance from the metal). This is due to the fact that besides the forces of repulsion between the electrons there are the forces of Coulomb attraction acting between the electrons and the atomic nuclei. The force and energy of this interaction are of the same order of magnitude as those of the electron-electron interaction. Moving in the

composite field of all electrons and nuclei each electron experiences both attraction and repulsion. Those two types of interaction together bring about the "apparent independence" of motion of the individual electron. As will be shown in Chapter II, the laws of quantum mechanics do, in fact, allow for the electrons to be considered as noninteracting particles.

The electrons move in the crystal at random. In the course of motion they "collide" with the lattice ions, and this changes their velocities both in *modulus* and *direction*. The change in velocity modulus of the electron is connected with the change in its kinetic energy. In conditions of thermal equilibrium the temperature of the electron gas should be equal to the temperature of the lattice ions. This means that, on the average, there is no energy transfer from the electrons to the lattice or vice versa.

But should the temperature of the electron gas be changed, the temperature of the lattice, too, would change as a result of the exchange of energy between the electrons and the ions. This fact is important for explaining the conductivity of metals and semiconductors and will be made use of below.

Because of the random nature of the scattering of electrons after their collisions with the lattice, the velocity and displacement of a given electron averaged over a long period of time considered as vectors should be equal to zero. The conditions are the same for all the electrons; therefore this is true of *every* electron. Since the mean displacement of the electrons taking part in random (thermal) motion is zero such random motion cannot result in an electric current which describes the transport of a charge across some cross section. To establish a current a directional motion of the electrons is needed. This may be initiated by various factors: electric field, temperature gradient, nonuniform illumination, etc.

If an electric field of intensity E is established in a metal the electrons will be accelerated by this field. The acceleration of the electron in this field is

$$a = \frac{e}{m} E. \quad (1.1)$$

In time t the electron attains the velocity

$$v = at = \frac{et}{m} E, \quad (1.2)$$

directed against the field. If the initial velocity of the electron is v_T , its speed at the moment t will be equal to

$$at + v_T = \frac{et}{m} E + v_T \quad (1.3)$$

As we see from here, the electron velocity component in the direction of the field decreases, and that against the field increases. As a result the electron ensemble attains an appropriate directional velocity. The electrons moving at random at the same time take part in the motion against the field. *The directional motion of the electron ensemble in an electric field is termed drift, and the velocity of directional motion is termed drift velocity and is designated by v_d .* Acted upon by the field E the electron in time t will be displaced to a distance

$$l(t) = \frac{et^2}{2m} E. \quad (1.4)$$

The classical electron theory presumes the change in velocity to result from an instant interaction of the electron with the lattice (with the atoms or ions of the lattice). In other words, it is assumed that the electron-lattice interaction is analogous to the impact phenomenon in mechanics. Between two collisions the electron moves as a particle free from the action of the field of the lattice and of the other electrons.

To describe the motion of the electrons the concepts of *mean free transit time* (the mean time between two collisions) τ and of *mean free path* l are introduced.

The mean free path l is related to the mean free transit time τ by the expression

$$l = v_T \tau. \quad (1.5)$$

Here v_T is the mean velocity of thermal motion of the electrons, i.e. the mean value of the velocity modulus.

Let us determine the mean electron drift velocity in an electric field. If at $t=0$ the velocity of directional motion of the electron is zero, at $t=\tau$ it will be equal to

$$a\tau = \frac{e\tau}{m} E. \quad (1.6)$$

The drift velocity will be equal to the mean velocity of directional motion, i.e. to the half-sum of the initial and the final velocities

$$v_d = \frac{0 + a\tau}{2} = \frac{e\tau}{2m} E. \quad (1.7)$$

It follows from (1.7) that the mean velocity of directional motion is proportional to the electric field intensity E . *The coefficient in the relation between the drift velocity and field intensity is termed electron mobility and is denoted by the letter μ .*

$$\mu = \frac{e\tau}{2m}; \quad v_d = \mu E. \quad (1.8)$$

Numerically, electron mobility is equal to electron drift velocity in an electric field of unit intensity.

If electron concentration is n , then per unit time a charge will pass through a unit cross section which is contained in a parallelepiped of unit base and height equal to $1 \cdot v_d$. The charge passing through unit cross section per unit time is termed current density j , and we may write

$$j = en v_d = en \mu E = \sigma E. \quad (1.9)$$

Equation (1.9) is the expression of Ohm's law in differential form. With the aid of (1.9) and (1.8) we obtain the electric conductivity

$$\sigma = en \mu \quad (1.10)$$

and

$$\sigma = \frac{e^2 n \tau}{2m}. \quad (1.11)$$

Expression (1.11) was first obtained by Drude. Expressing τ out of (1.5) we may write (1.11) in the form

$$\sigma = \frac{e^2 n l}{2m v_T}. \quad (1.12)$$

Ohm's law is valid as long as the electric field does not change electron concentration n or mobility μ . However, as the field E increases, the concentration and mobility of the electrons may change under its influence. Here, for example, is what happens to mobility.

In deducing Ohm's law we made the assumption that the energy of directional motion of the electron as a result of every collision is fully transferred to the lattice. In case of weak electric fields the drift velocity is much smaller than the thermal velocity and for this reason τ is independent of the field intensity E . But as the field increases the drift velocity grows to become comparable to the thermal velocity, and this will lead to a decrease in the free transit time, since now

$$\tau = \frac{l}{v_T + v_d} \quad (1.13)$$

The electron mobility and the conductivity of the metal will decrease accordingly. The critical field E_{cr} at which the effect sets in will be the smaller, the smaller is v_T , i.e. the temperature of the body, and the greater is the electron mobility in weak fields E .

There is another way in which the concept of the free transit time may be interpreted. If at some moment we turn the electric field off, the electron ensemble will continue its directional motion until it, as a result of collisions, transfers all its kinetic energy accumulated in the field to the lattice.

This directional motion will cease after a mean time τ (for all the electrons). After that the electrons will return to the state of random thermal motion.

We see from here that collisions tend to bring the electron ensemble into thermal equilibrium with the lattice, while the electric field tends to disturb that equilibrium. The passage of a system from the state of non-equilibrium to the state of equilibrium is termed relaxation process or relaxation, and the time in which equilibrium previously disturbed is recovered is termed relaxation time. Thus, we may say that the free transit time is actually the relaxation time.

The SI unit for electrical conductance is siemens (S), and that for specific conductance or conductivity, S/m. The dimensions of mobility in SI may be obtained from (1.8)

$$[\mu] = (\text{A} \cdot \text{s}^2) \text{ kg}^{-1}.$$

Mobility may also be expressed as velocity in a unit field, i.e. as a quantity having the dimensions m/s: $\text{V/m} = \text{m}^2/(\text{V} \cdot \text{s})$. In practice the most widely used units are those that do not belong to the system, i.e. cm, V, s, and mobility is measured in $\text{cm}^2/(\text{V} \cdot \text{s})$ and conductivity in $\text{ohm}^{-1} \cdot \text{cm}^{-1}$ ($\Omega^{-1} \cdot \text{cm}^{-1}$). Evidently,

$$1 \text{ m}^2/(\text{V} \cdot \text{s}) = 10^4 \text{ cm}^2/(\text{V} \cdot \text{s}),$$

$$1 \text{ S/m} = 10^{-3} \frac{1}{\text{ohm} \cdot \text{cm}} \left(\frac{1}{\Omega \cdot \text{cm}} \right).$$

Summary of Sec. 1

1. Main features of the classical electron theory of conductivity are as follows:

(a) Electrons make up an ideal (electron) gas and take part in random thermal motion which is described by the mean free path l and the mean free transit time τ .

(b) Electrons exchange energy and momentum with lattice ions and this causes thermal equilibrium between the electron gas and the lattice to be maintained.

(c) The electric field imparts directional velocity to the electrons thereby causing electric current to flow.

2. The current density is proportional to electric field intensity

$$\mathbf{j} = \sigma \mathbf{E}. \quad (1.1s)$$

3. Conductivity is related to electron concentration n and mobility μ

$$\sigma = en\mu. \quad (1.2s)$$

4. Mobility is determined by the behaviour of the electron and by the nature of its random motion in weak fields

$$\mu = \frac{e\tau}{2m} = \frac{el}{2m\nu_T}. \quad (1.3s)$$

5. Numerically, the mobility is equal to the electron drift velocity in a unit field

$$\mu = \frac{v_d}{E}. \quad (1.4s)$$

6. Ohm's law ceases to be valid in strong electric fields.

7. Free transit time may be regarded as relaxation time.

2. MEAN-FREE TIME AND FREE-PATH DISTRIBUTION FUNCTIONS

The above expressions for mobility and conductivity which were obtained in the assumption that mean transit times for all the electrons are equal should be rewritten to take account of the fact that the values of mean free time are not the same for all the electrons but vary from 0 to ∞ . To do this one should know the probabilities of definite mean free time values assumed to be random quantities. Let us find the distribution function for mean free times.

Let us make the assumptions that

(1) *the probability for an electron to be involved in a collision (scattering) during the time interval dt is proportional to its duration;*

(2) *collision probability per unit time is independent of time.*

These two assumptions suffice for the mean-free time distribution function to be obtained. Let us denote the probability of a particle to move without collision during the time from t to $t+dt$ by

$$dw = dw(dt). \quad (2.1)$$

The quantity $w(t)$ is the probability of free motion during the time interval $(t, t+1)$, and $w(t+dt)$, the probability of free motion during the time from $t+dt$ to $t+dt+1$. The quantity $w(t+dt)$ can be expressed in two different ways. On the one hand,

$$w(t+dt) = w(t) + \frac{dw}{dt} dt. \quad (2.2)$$

On the other hand, the fact of free motion of the electron during the time $t+dt$, the event C , may be regarded as a product of two events—one A which is the fact of free motion during time t , and the other B , the fact of free motion during dt , so that

$$C = AB. \quad (2.3)$$

The probability of the product of two events is equal to the product of the probability of the first by the conditional probability of the second:

$$w(C) = w(A) w\left(\frac{B}{A}\right) = w(B) w\left(\frac{A}{B}\right) \quad (2.4)$$