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SCATTERING PROCESSES AND CARRIER MOBILITY IN SEMICONDUCTORS

by

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Abstract: The mobility of the carriers in semiconductors is effected by scattering processes. In this paper the theories on the effect of the different scattering mechanisms on the mobility that have been developed so far and explain the experimental results are reviewed.

The mobility μ , is defined as the magnitude of the drift velocity per unit electric field E,

 $\mu = \frac{\mid \upsilon \mid}{E}$.

The conductivity σ of a medium in terms of the mobility is given by

$$\sigma=$$
 nem .

In the classical kinetic treatment, the conductivity is given by the expression

 $\sigma = n e^{_2} \frac{\tau}{m}$

where τ is the mean free time between the collisions of the carriers with other particles. The above expressions yield the expression for the mobility

$$\mu = |e| \frac{\tau}{m} .$$

The mobility is thus a statistical quantity.

In modern physics the electrons are described by wave functions which, under many experiments will actually be wave packets. These wave packets behave like particles if the phenomena considered do not involve distances smaller than the size of the wave packet. The simplest way to study the statistical behaviour of such wave - particles under the effect of external fields is by the Boltzmann equation, that is, to study the rate of change of the local concentration of the carriers $f_k(r)$ in the state k in the neighbourhood of the point r in the k space. The Boltzmann equation says that at any point and for any value of k the net rate of change of $f_k(r)$ is zero. For a homogeneous medium under the influence only of the electric field we have:

$$\frac{\partial f_k}{\partial t} \bigg|_{\text{scattering}} + \frac{\partial f_k}{\partial t} \bigg|_{\text{field}} = 0$$

The Boltzmann equation describes a steady state. But we assume that the steady state distribution does not depart very far from equilibrium, and write that

$$q_k = f_k - f_k^o$$

where f_k^{o} is the equilibrium distribution. It can be easily shown then that the equation yields

$$\left(-\frac{\partial f_k}{\partial k}\right)\frac{e}{h} E = -\frac{\partial f}{\partial t} \quad \left| \begin{array}{c} \mathrm{scatt.} \end{array} \right.$$

0r

$$\left(-\frac{\partial f^o}{\partial \epsilon}\right) v_k \cdot e \cdot E = -\frac{\partial f_k}{\partial t} \bigg|_{\text{scatt.}}$$

where v_k is the velocity of the particle in the k state, neglecting the term

which corresponds to deviations from Ohm's law. The mobility under such conditions will be briefly discussed at the end of this presentation.

Assuming that the distribution function returns to its unperturbed form exponentially we introduce the relaxation time τ and write that

$$\left(-\frac{\partial f_{\mathbf{k}}}{\partial \varepsilon}\right) \mathbf{v}_{\mathbf{k}} \cdot \mathbf{e} \cdot \mathbf{E} = \frac{q_{\mathbf{k}}}{\tau}$$

To define the conductivity we need the electrical current density,

$$\mathbf{J} = 2 \int \mathbf{e} \mathbf{v}_{\mathbf{k}} \mathbf{f}_{\mathbf{k}} d\mathbf{k} = 2\mathbf{e}^2 \int \mathbf{v}_{\mathbf{k}} \cdot \mathbf{v}_{\mathbf{k}} \cdot \mathbf{E} \left(-\frac{\mathbf{\partial} \mathbf{f}^{\mathbf{o}}}{\mathbf{\partial} \mathbf{\varepsilon}} \right) d\mathbf{k}$$

where e denotes the magnitude of the carrier's charge.

The mobility of the carriers in Semiconductors defined from the Boltzmann equation.

So far everything that has been said holds equally well for metals, degenerate and non degerate semiconductors. The treatment however of the last equation will be different for each of these materials, since their carriers obey different distribution functions. The carriers in metals obey the fermi statistics

$$f^o = \frac{1}{e^{(\epsilon-\zeta)/k_B T} + 1}$$

In degenerate semiconductors the electrons in the conduction band are numerous, the fermi energy lies in the conduction band, and the electrons obey the Fermi statistics. Thus the solution of the Boltzmann equation, and consenquently the properties of the mobility of the carriers in such materials, will follow a similar pattern as that for the metals. For this reason the mobility of degenerate semiconductors won't be discussed here.

In nondegenerate semiconductors the electron concentration in the conduction band is so small, that only a small fraction of the band is occupied and electron distribution becomes a classical one:

$$f_{B}^{o} \approx e^{-(\epsilon - \zeta)/k_{B}T}$$

The fermi level lies below the conduction band edge in the energy gap.

On the top of the valence band the «holes», which also contribute to the electric current, also obey a Boltzmann distribution,

$$f_{h}^{o} = (1 - f_{e}^{o}) = e^{(\epsilon - \zeta_{h})/k_{B}T} = e^{-(\epsilon_{e} + \zeta_{h})/k_{B}T}$$

if their energy is measured downwards from the top of the valence band.

We can return now to the expression of the current density. It is not difficult from this expression to show that the conductivity is given by the simple expression of

$$\sigma = \frac{ne^2 \langle \tau \rangle}{m^*}$$

where the electon density for the semiconductor is given by:

$$n \, = \, \mathrm{e}^{-\zeta_{e} \ / k_{\mathbf{B}} \, T} \, \int_{\epsilon_{0}}^{\infty} \ \mathrm{N}(\epsilon) \, \mathrm{e}^{-\epsilon_{e} \ / k_{\mathbf{B}} \, T} \ \mathrm{d}\epsilon \ . \label{eq:n_element}$$

where $N(\varepsilon)$ is the density of states, and defining the average relaxation time $\langle \tau \rangle$ by the expression

$$\langle \tau \rangle = \frac{2}{3k_{\rm B}T} \int \epsilon \tau(\epsilon) e^{-\epsilon/k_{\rm B}T} N(\epsilon) d\epsilon / \int e^{-\epsilon/k_{\rm B}T} N(\epsilon) d\epsilon$$

Thus the mobility is now given by:

$$\mu = |e| \langle \tau \rangle / m^*$$

For the general case where both electrons and holes contribute separately to the current, the conductivity should be given by the expression

$$\sigma = n_e \left| e \right| \mu_e + n_h \left| e \right| \mu_h$$

and hole and electron mobilities should be defined by the expression

$$\mu_{h} = \frac{|\mathbf{e}| < \tau_{h} >}{m_{h}^{*}} \quad , \quad \mu_{e} = \frac{|\mathbf{e}| < \tau_{e} >}{m_{e}^{*}} \text{ respectively.}$$

The mobility is expressed in cm^2 /statvolt - sec in C.G.S. and it is 300 times higher than the mobility in practical units. It can be obtained from measurements of the conductivity or of the Hall effect. The theory of the Hall effect yields the expression

$$\mu_{\rm H} = c \left| R_{\rm H} \right| \sigma \simeq \frac{e \langle \tau \rangle}{m^*} \cdot \frac{\langle \tau^2 \rangle}{\langle \tau \rangle^2} \quad {\rm or} \quad \mu_{\rm H} = \mu \; \frac{\langle \tau^2 \rangle}{\langle \tau \rangle^2}$$

where $\mu_{\rm H}$ is the so called Hall mobility.

If the relaxation time is independent of energy, or if electrons of one energy participate in the scattering process then $\mu_{\rm H} = \mu$. More generally, the two mobilities are related through a numerical factor.

It is obvious from the above formula that the mobility depends upon the effective mass. There is a tendency for crystals with small energy gaps to have high values of electron mobilities. Small gaps lead to small effective masses which favour high mobilities. But the mobility of a carrier is mainly determined by the scattering effects which define the relaxation time. Thus the mobility will be discussed separately for each type of scattering.

Inter - and intra - valley scattering.

Most of the basic calculations, such as the transition probabilities, that will be given in the following chapters are made on the assumption that the carriers are distributed in spherical energy surfaces and thus the variation of energy with k from the center of the zone is parabolic. The band structure of many semiconductors is however rather more complicated. The valence bands of Si and Ge show a maximum at $\mathbf{k} = 0$. These could be approximated by spherical surfaces and their properties could be approximately described by the effective mass of the holes m*. But the conduction bands show minima lying at some distance from $\mathbf{k} = 0$ along the 111 direction for Ge and along the 100 direction for Si. These minima are ellipsoids with ratios of the principal axes of the order of 10. Thus the deviation from the spherical form is great. There has been a method, however, proposed by Herring (1955) to take account of the energy bands having multiple minima. The method is like this:

Let us suppose that the minima in the conduction band are distributed as shown in figure (1). Around each center the energy is given approximately by

$$\varepsilon_{\mathbf{k}} = \hbar^{2} \left| \frac{(\delta \mathbf{k}_{1})^{2}}{2m^{*}_{1}} + \frac{(\delta \mathbf{k}_{2})^{2}}{2m^{*}_{2}} + \frac{(\delta \mathbf{k}_{s})^{2}}{2m^{*}_{3}} \right|$$

where $k = k_i + \delta k$. From symmetry, k_i must provide one priucipal axis

of the ith ellipsoid, with $m_1 = m_{||}$ and the other two principal masses m_2^* and m_3^* must be equal say to m_1 .

The method consists of evaluating the conductivity separately for each valley by transfering the origin of our coordinate system at the center of the ellipsoid. Because $m_{\parallel} \neq m_{\perp}$ the mobility associated with a simple ellipsoid may be very anisotropic. However when we come to



Fig. 1

study the mobility of the whole electron system, we must take the average over a cubically symmetric distribution of valleys. We obviously return to an apparently isotropic mobility except that

$$\frac{1}{\mathbf{m}^*_{\mathbf{e}}} = \frac{1}{3} \left(\frac{1}{\mathbf{m}^*_{\mathbf{1}}} + \frac{1}{\mathbf{m}^*_{\mathbf{2}}} + \frac{1}{\mathbf{m}^*_{\mathbf{3}}} \right) = \frac{1}{3} \left(\frac{1}{\mathbf{m}_{||}} + \frac{2}{\mathbf{m}_{\mathbf{1}}} \right)$$

Thus for a better agreement of the experimental results of the mobility with the theory the effective mass of the electron that appears in the formulas of the mobility should be replaced by the above expression.

Another effect of this kind of band structure is the possibility

that a scattered electron will not remain in the same valley that it was before scattering but will go in another valley. The change of the electron wave vector $k_i - k_j = q_{ij}$ is large, approximating the distance between the valleys. This is quite a large distance in the k space. The caclulations given below for the different cases of scattering assume a small change in the electron wave vector; that is they describe the so called intravalley scattering. The intervalley scattering could be approximated by the scattering of optical modes, discussed below, because it involves phonons of large wave vectors. Thus the mobility for such a scattering will be expected to follow a $T^{-3/2}$ law for $T > \Theta$ and an exponential form for $T < \Theta$.

Impurity Scattering.

A lattice imperfection acts as a scattering center because of its charge. All calculations are made on the assumption that the scattered electron is effectively free and the scattering power depends on the range and form of the potential associated with the imperfection. Conwell and Weisskopf (1950) gave a formula for scattering of electrons by impurities. They assumed a Coulomb potential associated with the imperfection to cause a Rutherford scattering of the carriers. They cut off the scattering at small angles on the basis that it is then referred to carriers that passed at a distance from the scattering center greater than the mean spacing of the impurities. A better theory which ta kes into account the screening of the charged impurities was given by Brooks and Herring. The scattering potential is treated as a perturbation on the carriers and the differential cross section is found by the Born approximation. The matrix element is, for scattering from a k to a k' state:

$$\mathbf{M}_{\mathbf{k}'\mathbf{k}} = \int \Psi_{\mathbf{k}}^{*} \, \nabla \Psi_{\mathbf{k}} \, \mathrm{d}\mathbf{r} = \int e^{\mathbf{i}(\mathbf{k}-\mathbf{k}')\mathbf{r}} \quad \frac{\mathbf{Z}e^{2}}{\mathbf{r}} \, e^{-\lambda\mathbf{r}} \, \mathrm{d}\mathbf{r} = \frac{4\pi \mathbf{Z}e^{2}}{|\mathbf{k}'-\mathbf{k}|^{2}+\lambda^{2}}$$

where the screening parameter λ is given by Brooks (1955) for the semiconductors as

$$\lambda = \frac{4\pi e^{2}}{\varkappa k_{\rm B}T} n \left(2 - \frac{n}{N_{\rm D}}\right)$$

and takes account of the dielectric constant \varkappa and the difference be tween the number of free carriers n and the number of ionized donors $N_{\rm D}$.

From the matrix element one could easily calcucate the differential cross section per unit solid angle* to find

$$\sigma(\theta) = \left(\frac{2\mathrm{mZe}^2}{\hbar^2}\right)^2 |1| / (\mathbf{k}' - \mathbf{k})^2 + \lambda^2|^2$$

and from this formula the relaxation time can be evaluated:

$$\frac{1}{\tau(\epsilon)} = N_i 2\pi \upsilon \int (1 - \cos\theta) \sigma(\theta) \sin\theta d\theta = 2\pi N_i \upsilon \left(\frac{Ze^2}{\varkappa\epsilon}\right)^2 \int_0^1 \frac{1/2 Z^3 dZ}{(Z^2 + \lambda^3 h^2 / 8m^*\epsilon)^2}$$

where use has been made of the geometry of scattering

$$k'-k=2k_e~(\sin\theta/2)=2k_eZ$$
 and $k_e^2=rac{2m_e^*}{\hbar^2}\epsilon_e$.

Evaluation of the intergal gives:

$$\frac{1}{\tau(\varepsilon)} = \frac{\pi}{\sqrt{2}} \frac{Z^2 e^4 N_i}{\varkappa^2 \varepsilon^{2/3} m^{*1/2}} F(\varepsilon) \quad \text{where} \quad F(\varepsilon) \quad \text{is}$$
$$F(\varepsilon) = \ln(1 - \frac{8m^* \varepsilon}{\lambda^2 \hbar^2}) - |1 + \frac{\lambda^2 \hbar^2}{8m^* \varepsilon}|^{-1}$$

The function $F(\varepsilon)$ does not vary much with ε and can be replaced by its value at the typical energy $\overline{\varepsilon} = 3k_B T$ which is where the maximum of the integral occurs. Thus it can be taken out of the integral when we evaluate the average $\langle \tau \rangle$. So we find

$$\langle \tau \rangle = rac{2^{7/2}}{\pi^{3/2}} \; rac{\varkappa^2}{Z^2 e^4} \; rac{m^*}{m^{*\,1/2}} \; rac{(k_B \, T)^{3/2}}{N_i} \; F(3k_B \, T) \; .$$

Thus the mobility will be like:

$$\mu \propto T^{3/2} m^{*1/2} / N_i$$

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^{*} In the pertubation theory of quantum mechanics the transmition probability is related to the differential cross section. See for example Schiff's Quantum Mechanics.

The variation of the mobility with impurities is in agreement with the experimental results generally.

The physical explanation of the above formula is that, at high temperatures the carriers have more energy and thus the average carrier goes faster, and it is less easily scattered by the impurity. The Born approximation overestimates the scattering cross section, and the experimental values of the mobility do not agree with the T dependance very well. Another analysis was made by Blatt (1957) using partial



Fig. 2 A', the normalized scattering cross section for scattering of charge carriers by ionized impurities as a function of $k^{\prime 2}$, for value of the screening parameter R' = 500

waves. In this method the cross section is different for scattering by a repulsive and by an attractive potential while in the Born approximation it is the same. This difference indicates that the minority

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impurities are less effective than the majority impurities in scattering carriers.

Fig. (2) shows the total scattering cross section for scattering of charge carriers by ionized impurities as calculated by Blatt (1957) in the Born approximation, curve labeled B, and the total scattering cross section in the partial wave method, curves labeled + and - for an attractive and a repulvive potential respectively. The curve is given in parametric form suitable for arbitrary choices of effective mass m^{*}, dielectric constant \times and charge Z. The scaling factor is

$$Q = 2.8 \ (\kappa/Zm^*).$$

The calculations were made on the assumption of spheroidal energy surfaces and corrections of the effective mass in case of ellipsoid surfaces should be applied.



Fig. 3. Hall and drift mobilities as functions of temperature.

Fig. (3) shows the dependence of the mobility on the temperature calculated by Blatt on the basis of these cross sections. The B curves were obtained using the Born approximation and the P ones using the partial wave method. The linear T dependence and the $T^{3/2}$ dependence are also shown in this figure. The departure from the $T^{3/2}$ law arises

mainly from the temperature dependence of the screening parameter in the case of the Born approximation. The screening radius increases with increasing temperature and produces increasing cross sections. Therefore the average relaxation time increases less rapidly with the temperature than it would if λ were independent of temperature. The additional reduction in the temperature dependence in the case of the partial waves is because the energy dependence of the cross section is now less rapid than in the Born approximation.

As for the agreement of the observed values of mohility with theory, Debye and Conwell (1954) found that for impurity scattering in N type Ge from 20 - 300 K the exponent of T starts from 1 and increases to reach the value of 1.5 asymptotically at higher temperatures.

The experiments of Morin and Maita (1954) in Si and Ge are also in favor of an exponent nearer to unity than 1.5 for the temperature dependence. Thus it seems that the mobility is given correctly by the Born approximation at higher temperatures (higher than 100 K).

As the temperature is lowered more and more of the impurities become unionized and the case of scattering by neutral impurities should be taken into account. This case was studied by Erginsoy (1950) who assumed that scattering of carriers in semiconductors by neutral impurities is equivalent to hydrogen - atom scattering. He gave the formula of the mobility for such a scattering as:

$$\mu = \frac{1}{20} \ \frac{\mathbf{m^*}}{\mathbf{N_N}} \ \frac{\mathbf{e^3}}{\mathbf{\kappa h^3}}$$

which is independent of the temperature. Al though this formula was found to agree with the experimental results of Debye and Conwell (1954) at liquid helium temperature it was pointed out by Temkin and Lemkin (1961), Temkin (1962) and Drnkarev (1963) that it needed to be corrected. This was done by Blagosklonskaya *et al* (1970) who took account of the polarization of a hydrogen atom by the electric field of a scattered electron. Their experimental results agreed with their theory.

The inhomogeneous impurity distributions can greatly affect the observed mobility in semiconductors. This is due to the formation of large space - charge regions surrounding local inhomogeneities. The scattering cross section of Coulombic centers can be increased by over an order of magnitude when inhomogeneously distributed. Assuming that inhomogeneities can occur frequently, various anomalous mobility effects cau be explained such as «mobility killers» in GaAs InAs, giant scattering cross sections in GaAs, InP, Cds and CdSe.

Electron - Electron Scattering.

At first it would seem that electron - electron scattering could not affect the mobility since the total momentum is unaltered. However, this process influences the mobility indirectly. In determining the mobility of electrons and holes scattered by impurities we have seen that electrons of high energy are scattered less effectively by the impurities than those of low energy. Thus these electrons tend to acquire large momentum from the field. If, however, the mean free path for an electron - electron collision is smaller than the mean free path of these fast electron - impurity collisions then the mobility will tend to decrease because the electron - electron collision tends to equalize their momenta. It has been pointed out that in the region where impurity scattering is dominant the mobility should decrease by a factor of 0.6 while in the region where the lattice scattering is important the mobility should decrease by a factor of 0.88, (Spitrer and Harm, 1953).

Electron - Hole scattering also reduces the mobility. However, as pointed out by Morin and Maita, (1954) is negligible in Si below 1200 K and in Ge below 1000 K.

Dislocation scattering.

Dislocations in Ge and in Si can scatter electrons in two ways. The first is due to elastic properties of dislocations. They give rise to elastic strains, thus there is dilatation and the deformation potential can be determined (Dexter and Seitz). This kind of scattering is expected to be small and uniportant in good quality crystals. The temperature dependence of mobility is linear with T.

The other mechanism is due to the fact that dislocations act as electron acceptors, thus reducing the electron concentration in n type specimens, and even converting it to p type (Read 1954, 1955). Thus the dislocation becomes negatively charged. This negative line should be surrounded by an extensive cylindrical region of equal positive space charge. Thus, the dislocation line can give rise to a strong, perturbing potential, and can scatter electrons quite effectively. However, this scattering should not appear in p - type specimens which is in fact in agreement with the experimental observations.

In Fig. 4 the triangles present the T dependence of the mobility due to lattice scattering and the dotted line the T dependence due to dislocation scattering. When the two are added in the form

$$\frac{1}{\mu_{I}}$$
 + $\frac{1}{\mu_{2}}$

the so calculated mobility (solid line) fits the observed one (dotts) (Logan et al, 1959).

Lattice scattering.

The carriers in semiconductors are thought as being concentrated near an energy minimum in the k space. This makes the calculations of electrons scattered by phonons easier in a semiconductor than in



Fig. 4. Temperature variation of mobility in germanium with and without udded dislocations.

metals, because the change of the wavevector of electrons is small and the phonon vector q_1 has to be near a center of a zone. Thus

we can assume that the occupancy of the phonon is given by

$$n_q = k_B T / \hbar v_q$$

where v_q is the phonon frequency.

Another characteristic of this interaction is that the energy change of the electron is very small and can be neglected which in classical scattering corresponds to scattering by an ion of infinite mass.

In the lattice vibrations the ions move about their lattice sites, so that the potential energy in the lattice is changed by the amount δV from its value in the undistorted crystal. This change of the potential is seen by the electrons as a pertubation and has the effect of scattering them into new states. Admitting that the extra potential is a linear function of the displacement we can say that

$$\delta V = \sum_{l,q} \frac{\partial V}{\partial u_{l,q}} \cdot e_q$$

where $u_{l,q} = U_q e^{-iql} \bar{e}_q$ is the lattice vibration and \bar{e}_q is the unit vector for the displacement.

This potential δV is treated by time dependent pertubation theory to give the matrix element for the transition probability for an electron from the k to k', by the phonon $|n_q >$

$$\begin{split} \mathbf{M}_{\mathbf{k}'\mathbf{k}} &= \left< \mathbf{n}_{\mathbf{q},\mathbf{p}} \mid \int \Psi_{\mathbf{k}'}(\mathbf{r}) \ (\delta \mathbf{v}) \ \Psi_{\mathbf{k}}(\mathbf{r}) \mathrm{d}\mathbf{r} \mid \mathbf{n}_{\mathbf{q},\mathbf{p}} - 1 \right> \\ &= -\mathbf{i} \ \sum_{\mathbf{l}} \ \upsilon_{\mathbf{q}} \mathrm{e}^{-\mathbf{i}\mathbf{q}\mathbf{l}} \ \int \Psi_{\mathbf{k}'} \ (\mathbf{r}) \ (\delta \mathbf{v}) \ \Psi_{\mathbf{k}}(\mathbf{r}) \mathrm{d}\mathbf{r} \\ &= -\mathbf{i} \upsilon_{\mathbf{q}} \ \delta_{\mathbf{k}'-\mathbf{k}-\mathbf{q},\mathbf{g}} \int \Psi_{\mathbf{k}'} \ (\mathbf{r}) \ (\delta \mathbf{v}) \ \Psi_{\mathbf{k}}(\mathbf{v}) \mathrm{d}\mathbf{r} \end{split}$$

The phonon $|n_q \rangle$ is described by its amplitude v_q and occupancy n_q .

The electron wave functions are thought as Bloch functions:

$$\Psi(\mathbf{k} + \mathbf{l}) = \Psi(\mathbf{k}) e^{i\mathbf{k}\mathbf{l}}$$

The simplest way to evaluate the integrals of those matrices is to think that the potential field surrounding each ion is rigidly at-

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tached to it and moves with it. Thus we can assume that the potential is a sum of atomic potentials

$$V_{(r)} = \sum_{l} V(r - R_l)$$

The detailed calculation of the integral was done by Mott and Jones who also used the Wigner Seitz model to take for it:

$$\mathfrak{L}(\mathbf{k}' \ \mathbf{k}) = -i \mid e_q \cdot (\mathbf{k}' - \mathbf{k}) \mid \{ u(r) - \varepsilon_o \} \smallint \Psi_{\mathbf{k}}'^* \ \Psi_{\mathbf{k}} \ \mathrm{d}r \ ,$$

where ε_0 is the enery of the bottom of the band and u is the potential energy of the electron on the cell boundary.

The factor $e_q \cdot (k'-k) = \overline{e}_q \cdot \overline{q}$ tells us that the electrons are scattered by longitutinal phonons only. However, this would be true only in the case of N process. The factor $\{u(r)-\varepsilon_0\}$ can be evaluated by a method proposed by Hunder and Nabaro of the so called deformational potential. They said that when a crystal is uniformaly expanded or compressed; the radius of each cell changes from r to $r(1+\frac{1}{3}\Delta)$, where Δ is the dilatation. Then the wave function for the bottom of the band Ψ_0 must satisfy new boundary conditions and thus it is changed to Ψ_1 . By substraction of the Schrödinger equations for Ψ_0 and Ψ_1 we can get:

$$-\frac{\hbar^2}{2m} |\Psi_0 \nabla^2 \Psi_1 - \Psi_1 \nabla^2 \Psi_0| = \Psi_0 \Psi_1 \delta\varepsilon$$

This equation is integrated over the volume of the unexpanded cell, and saying that the product Ψ_0 Ψ_1 is approximately integrated to unity we have

$$\delta\epsilon_{o}=-\ \frac{\hbar^{2}}{2m}\ \int\ \Psi_{0}(r)\ \nabla\ \Psi_{1}(r)\ \mathrm{d}s$$

But $\nabla \Psi_1$ vanishes at the boundary of the expanded Winger Seitz cell. By Taylor expansion we have

$$\nabla \Psi_{\mathbf{i}} \mathrm{d}\mathbf{s} = -\frac{1}{3} \mathbf{r} \Delta \nabla^{\mathbf{s}} \Psi_{\mathbf{0}} \mathrm{d}\mathbf{s}$$

On the boundary of the Wigner Seitz cell we have that:

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$$\frac{\hbar^{2}}{2m} \Delta^{2} \Psi_{0} = \{ u(r) - \epsilon_{0} \} \Psi_{0} (r)$$

Thus we come to have that:

$$\delta \varepsilon_0 \approx \{ u(\mathbf{r}) - \varepsilon_0 \} \Delta$$
.

In other words $u(r) - \varepsilon_0$ is the rate of change with dilatation of the energy of the bottom of the conduction band. It is called the deformation potential. The method of deformation potential has been proved by Overhauser (1953) and Gibson and Keller (1957).

The integral

$$\int \Psi_k \ast \Psi_k \ dr = 2\pi \int\limits_0^\pi \int\limits_0^r \ e^{i(k'-k)r\cos\theta} r^2 sin\theta d\theta dr \;,$$

when evaluated, is a function of the form



The value of this function is shown in figure 5 from which it is detected that large angle scattering is rather avoided.

It should be mentioned that there have been other ways of evaluating the integrals $\mathfrak{L}(\mathbf{k'}-\mathbf{k})$ such as that of the deformable ion by

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Bloch or the Bardeen's self consistent calculations, but the discussion of them would go out of the scope of this work. It seems that this method is suitable for application to semiconductors having the advantage that the deformation potential can be detected by independent measurements, such as changes in the energy gap with pressure and temperature. It has been the most used method when we come to determine a scattering cross section of electrons scattered by phonons and explain the observed mobility of the electrons in many semiconductors.

The calculations presented ended with a matrix form, (if we substitute the value of v_a)

$$M_{\mathbf{k}'\mathbf{k}} = \left(\frac{\hbar^2 k_B T}{2 D \nu_q \hbar v_q}\right)^{1/2} q \cdot \epsilon_{\mathbf{i}} \ .$$

The square of it is

$$|M_{k'k}|^2 = \frac{k_B T}{2Ds^2} \epsilon_1^2$$

From this matrix element we can evaluate $\tau_{L}(\varepsilon)$

$$\tau_{L}\left(\epsilon\right) = \frac{\hbar D s^{2}}{\pi \epsilon_{1}{}^{2}k_{B}T} - \frac{1}{N(\epsilon)}$$

But N(ε) $\propto \varepsilon^{1/2}$, thus $\tau_{\rm L}(\varepsilon) \propto T^{-3/2}$

Now we have to evaluate the mean value $\langle \tau_L(\varepsilon) \rangle$. For a spherical band with effective mass m^* we obtain a temperature dependent mobility:

$$m_{L} = \frac{2^{3/2}\pi}{3} \quad \frac{Ds^{2}\hbar^{4}}{\epsilon_{1}^{2}m^{*5/2}} \quad \frac{1}{(k_{B}T)^{3/2}}$$

Since the calculations are based on a simple model it is obvious that deviations from this simple formula should be expected, when we come to explain experimental results.

So far the case of scattering electrons by optical modes has not been considered. The energy of an optical quantum is much larger than that of an acoustical mode, corresponds to a temperature of several hundred degrees and hence the change of the energy of the carrier during such a collision should be taken into account. The problem is studied by the variational method and it is divided into two parts according to whether we have to deal with a polar or covalent semiconductor. The latter was studied by Seitz (1948) who gave, for high temperatures, a temperature dependent mobility of the form

$$\mu \propto (k_B T)^{-3/2} m^{*-5/2}$$

At lower temperatures the occupancy of phonons is given by the Plank distribution which makes the calculations still more complicated. However, in explaining the experimental results we could say that, if a proportion of the scattering which governs the mobility at high temperatures is by optical modes, then we expect this scattering to disappear more rapidly than the acoustic phonon scattering at lower temperatures and hence the mobility is expected to rise more rapidly than $T^{-s/s}$.

In an actual sample both impurities and lattice scattering will be present since no actual sample is absolutely free from impurities and not at zero temperature. Even more the samples of semiconductors have to be dopped for special purposes. Combining the two different relaxation times is roughly done by Mathiessen's law. A more accurate combination will be like this. The relaxation time because of lattice and impurity scattering is:

$$\frac{1}{\tau(\varepsilon)} = \frac{1}{\tau_{\rm L}(\varepsilon)} + \frac{1}{\tau_{\rm i}(\varepsilon)}$$

when the effect of dislocation and electron - electron scattering is neglected. For spherical surfaces of constant energy the mobility depends on relaxation time

$$\mu = \frac{e}{m^*} \stackrel{\langle \upsilon^2 \tau(\epsilon) \rangle}{\langle \upsilon^2 \rangle}$$

The substitution of $\tau(\varepsilon)$ in the above formula and the evaluation of the mean values, results in a rather complicated integral of ε which has been solved by approximate methods (Johnson et al (1951), Debye and Conwell (1954). Conwell (1952) has also published a graph of $\mu/\mu_{\rm L}$ as a function of $\mu_{\rm L}/\mu_{\rm I}$ where $\mu_{\rm I}$ is the maximum observed mobility when both lattice and impurity scattering is present. (See fig. 6).

For more quantitative comparison of experiment and theory, the

data taken is usefully divided into the following parts.

1) Data for the range of temperatures and impurity concentrations for which impurity scattering is neglibigle. These will give a check on the theory of lattice scattering.

2) Data for the range of temperatures where impurity concentration is known and neutral impurity will be negligible. From such a data check of the impurity scattering can be made. Such a discussion has already been made.

A number of experiments have been conducted measuring the temperature dependence of mobility of electrons in Ge and Si. In n-type



Fig. 6. Mobility in specimens of Si containing various amounts of B impurity.

Si, in the lattice scattering region, the temperature dependence of mobility is $T^{-2,5}$. The deviation from $T^{-1.5}$ law is great and can not be attributed to intervalley scattering. However, this deviation was attributed to scattering by optical modes. The optical mode temperature Θ was computed by Herring to be 1200 K. Since the experiments

that gave the above results were performed at the temperature regions below 700 K, the part of the lattice scattering due to optical modes has to obey an exponential from.

For n-type Ge the experimental law is $T^{-1.06}$. The deviation can be attributed to intervalley scattering, although the change of the effective mass with temperature could also provide a temperature dependence.

The mobilities of holes in Ge and Si exhibit a $T^{-2\cdot3}$ dependence. Intervalley scattering can occur in this case. The deviation has been attributed to scattering by optical modes as well as by shear modes. Shokley found that the aconstic mode temperature for Ge is $\Theta = 520$ K. The observed deviation from $T^{-3/2}$ law for Ge can be explained by the scattering by acoustical modes up to the temperature of 500 K. In the experiment done up to 1000 K the observed deviation was explained by electron - hole scattering using the Brooks and Herring formula.

Scattering by optical modes in polar crystals has been studied more explicitly theoretically. Because of the strong dipole moment set up by the optical modes in polar crystals the coupling between an electron and an optical mode is likely to be stronger than in non polar crystals. The matrix elements for the transition of an electron from the state k to k' by an optical mode q has been studied and the Boltzmann equation is solved by the variational theory. The temperature dependence of the mobility is of the form:

$$\mu \propto m^{*-3/2} (k_B T)^{-1/2}$$
 for high temperatures,
 $\mu \propto m^{*-3/2} (e^{\hbar\omega/k_B T} - 1)$ for lower temperatures

The above relations were found using pertubation theory to find the matrix elements for the transition. In order for pertubation theory to be applicable the coupling constant

$$\alpha = \frac{e^2}{\ln} \left(\frac{m}{2\hbar\omega_{\rm L}} \right)^{1/2} \left(\frac{\varkappa - \varkappa_0}{\varkappa_0 \varkappa} \right) \left(\frac{m_0^*}{m_o} \right)^{1/2}$$

should be smaller than unity. Thus it would be expected for the results of pertubation theory not to be applicable to all types of polar crystals. For such cases, the polaron theory of mobility has been developed (Law and Pines, 1955) to replace the perturbation theory. This theory for law temperatures $(T < \Theta)$ gives a temperature dependent mobility of the form

$$\mu \propto \frac{1}{m_e^*} e^{\hbar \omega / k_B T} \left(\frac{m_e}{m_p} \right)^{2/4}$$

where m_p is the polaron mass.

The perturbation method was applied by Rozhdestveskaya et al (1970) in the observed mobility in Strodium titanite and found to be in agreement with $\Theta = 600$ K. The slight disagreement was attributed to lattice distortion.



Fig. 7 Current denelty in n type Ge as a function of electric field.

On the other hand the polaron theory was used by Frederikse and Hosler (1967) to explain the observed mobility in SrT_1O_3 in the temperature region from 1 - 1000 K.

Concluding the discussion on the comparison of the theoretical mobility and observed mobility it should be mentioned that part of the observed disagreement should be attributed to the mischoises of proper constants such as dielectric constant, effective mass, polaron mass, etc. Hot Electron. For a complete discussion of the topic the scattering mechanisms in the case of «Hot electrons» will be briefly discussed.

In solving the Boltzmann equation a basic assumption was made, that the energy that a charge carrier gains from the applied field is sufficiently small that collision processes bring the carrier distribution into thermal equilibrium with the lattice. This is why only terms linear to the applied field were retained. At sufficiently high fields however this won't be true and the current density will no longer be proportional to the electric field. The current density versus the electric field are shown in figure 7. It appears that the curves could be divided into 3 regions (Ryder 1953).

At low fields Ohm's law is obeyed. Beyond a fairly well-defined field strength which is a function of temperature the current is proportional to E^{1/2} and at very high fields it becomes independend of the field. This behavior can be explained in the following way. As the field increases, the electrons gain more and more energy between collisions with phonons. The rate at which this energy can be transfered to the lattice is determined by the relaxation time for electron - phonon collisions, and by the maximum energy of the phonon which can be created in such a collision and which is very small compared to the energy of the electron. Thus at a critical electic field the transfer of energy to the latrice becomes too slow to establish thermal equilibrium and the electron distribution becomes hot. However, as the electron energy increases the probability of electron-phonon scattering increases until the electron - phonon interaction is again sufficiently strong to establish a steady state. The situation is very similar to that of gas discharges. Through that theory one can easily show that the mobility is like

$\mu \propto E^{-1/2}$

The current saturation at very high fields is interpreted in terms of the interaction of electrons with optical phonons. Because the energy of the optical phonon is orders of magnitude greater than of the acoustical phonon, once optical phonons can be emitted the energy of the electrons is limited and saturation arises.

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ΠΕΡΙΛΗΨΙΣ

ΦΑΙΝΟΜΈΝΑ ΣΚΈΔΑΣΜΟΥ ΤΩΝ ΗΛΕΚΤΡΙΚΩΝ ΦΟΡΕΩΝ ΚΑΙ ΕΥΚΙΝΗΣΙΑ ΑΥΤΩΝ ΕΙΣ ΤΟΥΣ ΗΜΙΑΓΩΓΟΥΣ

Υπό

ΣΕΜΙΡΑΜΙΔΟΣ ΔΙΟΝΥΣΙΟΥ - ΚΟΥ Ι ΜΤΖΗ ('Egyaστήριον Γ' "Έδρας Φυσικής, Πανεπιστημίου Θεσσαλονίκης)

'Η εὐχινησία τῶν φορέων εἰς τοὺς ἡμιαγωγοὺς ἐπηρεάζεται ὑπὸ τῶν φαινομένων σκεδάσεως. Ἐπὶ τοῦ θέματος τοὑτου ἀνασκοποῦνται αἱ θεωρίαι αἱ ὁποῖαι ἀνεπτύχθησαν τελευταίως ἐπὶ τοῦ τρόπου ἐπιδράσεως ἑκάστου μηχανισμοῦ σκεδάσεως ἐπὶ τῆς εὐκινησίας καὶ δύνανται νὰ ἑρμηνεύσουν τὰ πειραματικὰ δεδομένα.