ON THE THEORY OF ELECTRICAL CONDUCTIVITY IN SEMICONDUCTING THIN FILMS UNDER A HIGH ELECTRIC FIELD

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Non-ohmic electrical conductivity in thin films of non-degenerate semiconductors is studied using the electron-temperature approximation. It is assumed that the distribution function f can be expressed as the sum of two functions: $f = f_0 + f_1$ where $f_1 \ll f_0$. The non-symmetrical part f_1 is calculated from the Boltzmann transport equation with the boundary condition of the diffuse scattering. The symmetrical part f_0, which is determined by the energy scattering, is of the Maxwell-Boltzmann type with an electron temperature T_e. The energy surface scattering which influences the electron temperature T_e is characterized by the phenomenological parameter. The electron temperature T_e and the non-ohmic parameter β in thin films are calculated for the case of the acoustic mode scattering inside the film.

I. INTRODUCTION

It is known [1, 2, 3] that in the ohmic region of an electric field, transport coefficients (electrical conductivity, magnetoresistance, Hall coefficient etc.) considerably depend on the thickness of the semiconductor thin films. We can expect this size effect in a high electric field, too.

We can express the distribution function of conduction electrons exposed to a high electric field in a thin film, similarly as in a bulk semiconductor, as the sum of two functions $f = f_0 + f_1$, where $f_1 \ll f_0$. The term $f_0(\epsilon, T_e)$ is the Maxwell-Boltzmann distribution function of an electron temperature T_e, but this is by no means the general case. Nevertheless, it has become customary to speak of an electron temperature for the hot electrons, meaning a measure of their average energy. In the steady state, the average energy gaines from the electric field between collisions must equal the average energy loss in a collision. If the collisions are elastic, therefore, the gain from the electric field between collisions is small. If, in addition, the collisions are not predominantly

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forward or small-angle ones, it is apparent that the energy gained from the field will have been randomized.

Thus in this electric fields the distribution function is again in the form of a small drift superimposed on a function of energy only, i. e., $f = f_0 + f_1$. There two conditions of the scattering processes required to produce a high-field distribution of the latter form are usually satisfied by the long wavelength acoustic mode scattering. In general, the elastic and inelastic scattering processes are both present, and whether or not $f = f_0 + f_1$ is a good approximation depends on their relative importance.

When the scattering is not predominantly elastic and isotropic, further terms in the expansion of the distribution function f in the Legendre polynomials $P_n(X)$, where X is the cosine of the angle between wave vector $\boldsymbol{k}$ and $\boldsymbol{E}$ (external electric field), i. e.

$$f(\epsilon, X) = \sum_{n=0}^{\infty} G_n(\epsilon) P_n(X)$$

are necessary to obtain a good approximation of the distribution function f; this leads to an infinite set of coupled differential equations for the coefficients $G_n(\epsilon)$. In practice, n may be chosen small, so that one need solve only a small number of coupled differential equations [4].

In a high electric field we have to know besides the function f_1 which is determined by the momentum scattering of conduction electrons, also the symmetric part f_0 of the distribution function f, which is determined by the energy scattering of the conduction electrons. The scattering processes have to be characterized both from the momentum and the energy point of view.

In this films besides bulk scattering processes, the surface scattering processes play an important part in electric conductivity. In theory, we can include the influence of the surface scattering processes on the momentum and energy scattering in appropriately formulated boundary conditions.

We consider a non-degenerate single crystal semiconductor thin film, which occupies a part of the space: $-\infty < x; y < \infty; -d \leqslant z \leqslant d$ ($2d$ is the thickness of the film). To this thin film there is applied a high electric field in the direction of the x-axis. We are dealing with a simple case when $\psi = 0$ (ψ is the electrostatic potential which may exist near the surface), that is, a thin film without any space charge. In general, the local density of electrons is then given by $n = n_0 \exp(-q_e \psi/k_0 T_0)$ (q_e is the electron's electric charge, k_0 the Boltzmann constant). In our case $n = n_0$ (n_0 is the thermal equilibrium density of electrons in the bulk). The model adopted in the present paper is based upon the assumption of spherical energy surfaces and the existence of a relaxation length which is independent from energy. The scattering of the momentum and the energy inside the film is predominantly due to acoustic phonons. The effective

mass m^* is taken to be a scalar quantity. Furthermore, the semiconductor is non-degenerate, the quantization of the transverse motion of the electrons is not taken into account. We use the electron-temperature approximation. We assume therefore that the quasi-equilibrium distribution function f_0 is of the Maxwell-Boltzmann type with an electron temperature T_e, which we shall calculate from an energy balance equation as an unknown parameter. The electron temperature is a function of the z-coordinate perpendicular to the surface of the film.

From explicit expression of the electron temperature T_e we shall know the explicit expression of the energy distribution function f_0. We shall calculate the non-symmetric part f_1 of the distribution function f from the Boltzmann transport equation with the boundary condition of the diffuse surface scattering.

II. THE DISTRIBUTION FUNCTION

We express the distribution function of conduction electrons as the sum of two functions

$$f(\boldsymbol{p}, \boldsymbol{r}) = f_0(\epsilon, \boldsymbol{r}) + f_1(\boldsymbol{p}, \boldsymbol{r}), \qquad (1)$$

where $\boldsymbol{p}$ is the quasimomentum of an electron, $\boldsymbol{r}$ is the radius vector. The quasiequilibrium distribution function in the electron-temperature approximation is assumed to be Maxwellian with an effective electron temperature $T_e(z)$:

$$f_0 = \frac{n_0}{[2\pi m^* k_0 T_e(z)]^{3/2}} \exp(-p^2/2m^* k_0 T). \qquad (2)$$

The electron-temperature approximation, however, has no rigorous justification. This approximation was originally proposed by Fröhlich [5], who assumed that interelectronic collisions were sufficiently strong to enforce an internal equilibrium of the electron systems, thus justifying the concept of an electron temperature. Straton [6] extended the calculation of Fröhlich to include a variety of scattering processes and the lattice temperature T_0. That the strong interelectronic scattering maintains a Maxwellian distribution is only an assumption. This assumption has not been proved because of the difficulty of solving the Boltzmann transport equation for arbitrary electric fields in the presence of electron-electron collisions. In most comparisons with experiments, the electron-temperature approximation agrees well with the experiment. Even with electron densities of orders of magnitude below that required for its justification, it can give a fairly good result [7, 8].

The effective electron temperature in the thin film is considerably influenced by the surface scattering. The scattering is a new source of energy loss and a current of energy appears across the sample. When we denote by P_z the z-coordinate of the vector of energy flux density $P = \int_p \frac{p^2}{2m^*} f_1 v \, d^3p$, then the derivative dP_z/dz is the mean energy change due to the current of energy per unit volume and time.

The energy balance equation for the calculation of the effective temperature in the thin film has the following form:

$$j_x E_x + \left(\overline{\frac{\partial \varepsilon}{\partial t}}\right)_c = \frac{dP_z}{dz},$$ (3)

where the first term is the mean energy the conduction electrons gained from the external electric field per unit time, the second term is the mean energy per time which electrons transfer to the lattice within the unit volume inside the film. j_x is the x-coordinate of the vector of current density $j = q_e \int_p v f_1 d^3p$. Now we need to know the analytic expression of the distribution function f_1 on an explicit expression of the terms of energy balance equation (3).

The applied electric field effectively perturbs the distribution function f_0 of the unperturbed system by supplying an average energy $\Delta\varepsilon$ to the electrons and the energy surface scattering causes that the energy distribution function f_0 in a high electric field depends on the z coordinate. Thus we can write

$$f = f_0(\varepsilon - \Delta\varepsilon, z) = f_0(\varepsilon, z_0) - \Delta\varepsilon \frac{\partial f_0(\varepsilon, z_0)}{\partial \varepsilon} - \Delta z \frac{\partial f_0(\varepsilon, z_0)}{\partial z},$$ (4)

and the perturbation function f_1 becomes

$$f_1 = -\Delta\varepsilon \frac{\partial f_0}{\partial \varepsilon} - \Delta z \frac{\partial f_0}{\partial z}.$$ (5)

In generally $\Delta\varepsilon$ and Δz would be written by [9]

$$\Delta\varepsilon(t) = q_e \int_{-\infty}^{t} dt' \, \mathbf{E} \cdot \langle \mathbf{v}(t')\rangle,$$ (6)

$$\Delta z(t) = \int_{-\infty}^{t} dt' \langle v_z(t')\rangle,$$ (7)

$\langle \mathbf{v}(t')\rangle$ is the average velocity at the time t' of an assembly of electrons all of

the velocity $\mathbf{v}$ at the time $t' = 0$. The probability that the electron will survive from time t' to time t without collision is given (if a magnetic field is not present $H = 0$) by

$$\exp[-(t - t')/\tau],$$ (8)

where τ is the relaxation time.

Since each collision is assumed to randomize the electron velocity completely, it follows that only unscattered electrons contribute to $\langle \mathbf{v}(t')\rangle$ in (6, 7), so that

$$\langle \mathbf{v}(t')\rangle = \mathbf{v}(t') \exp[-(t - t')/\tau],$$ (9)

and

$$\Delta\varepsilon(t) = q_e \int_{-\infty}^{t} \mathbf{E} \cdot \mathbf{v}(t') \exp[-(t - t')/\tau] dt =$$
$$= q_e E_x v_x \int_{-\infty}^{t} dt' \exp[-(t - t')/\tau],$$ (10)

$$\Delta z(t) = \int_{-\infty}^{t} v_z(t) \exp[-(t - t')/\tau] dt' = v_z \int_{-\infty}^{t} dt' \exp[-(t - t')/\tau].$$ (11)

If $H = 0$, then $\mathbf{v}(t') = \mathbf{v} = \text{const}$.

The equations (10, 11) may be generalized to include the effect of the diffuse scattering.

If the electron path intersects the surface at the time $t - t_s$ and if the surface scattering is diffuse, an electron will start at the time $t - t_s$ with $\Delta\varepsilon = 0$ and will carry no current. The excess energy at the time t is therefore equal to the energy acquired since the time $t - t_s$ and to take this into account we have to replace the lower limit of integration in (10, 11) by $t - t_s$.

The perturbation distribution function f_1, which is the exact solution of the Boltzmann transport equation in the relaxation time approximation for the case of a constant high electric field, parabolic energy band and diffuse scattering, by using (5), has the following form:

$$f_1 = -q_e \frac{\partial f_0}{\partial \varepsilon} E_x v_x \int_{-t_s}^{0} dt' \exp(t'/\tau) - v_z \frac{\partial f_0}{\partial z} \int_{-t_s}^{0} dt' \exp(t'/\tau) =$$

$$= -q_e \frac{\partial f_0}{\partial \varepsilon} E_x v_x \tau [1 - \exp(-d_s/l)] - v_z \tau \frac{\partial f_0}{\partial z} [1 - \exp(-d_s/l)],$$ (12)

where $d_s = v t_s$ is the distance that an electron travels in moving form the

surface to a point **r** inside the film, and $l = v\tau$ is the mean free path. The distance d_s for those electrons with $v_z < 0$, which are leaving the surface $z = d$ is $d_s = (d-z)/\cos\vartheta$ (ϑ is the angle between the vector **v** and the z-axis) and the distance d_s for those electrons with $v_z > 0$, which are leaving the surface $z = -d$ is $d_s = (d+z)/\cos\vartheta$.

Clearly, two analytic forms of the distribution function are needed in order to describe the system. f_1' will describe the electrons in that half of the momentum space where $v_z > 0$, and $f_1^<$ will describe the electrons in the other half, where $v_z < 0$. When we are dealing with a sample where $\psi = 0$ through-out, that is, a thin film without any space change, then simply $f_1^< = 0$ at $z = -d$ and $f_1' = 0$ at $z = d$. The analytic expressions of the functions f_1' and $f_1^<$ are:

$$f_1' = \frac{q e f_0 E_x \tau v_x}{k_0 T_e}\left[1 - \exp\left(-\frac{d+z}{\tau v_z}\right)\right] - \frac{\partial f_0}{\partial z}\tau v_z\left[1 - \exp\left(-\frac{d+z}{\tau v_z}\right)\right],$$ (13)

$$f_1^< = \frac{q e f_0 E_x \tau v_x}{k_0 T_e}\left[1 - \exp\left(-\frac{d-z}{\tau v_z}\right)\right] - \frac{\partial f_0}{\partial z}\tau v_z\left[1 - \exp\left(-\frac{d-z}{\tau v_z}\right)\right].$$ (14)

III. THE EFFECTIVE ELECTRON TEMPERATURE

We determine the effective temperature of electrons for the lattice temperature, the thickness of the film, the external electric field from the energy balance equation (3). The current density j_x for the case of the diffuse surface scattering and the case when the mobility inside the film is milited by acoustic modes (the relaxation length l_a is energy independent) is determined

$$j_x = \frac{q_e^2 E_x l_a n_0}{[2\pi m^* k_0 T_e(z)]^{1/2}} A(\xi),$$ (15)

where

$$A(\xi) = 4/3 - \Phi_2(\eta+\xi) - \Phi_2(\eta-\xi) + \Phi_4(\eta+\xi) + \Phi_4(\eta-\xi)$$ (16)

and

$$\eta = d/l_a, \quad \xi = z/l_a, \quad \Phi_n(\alpha) = \int_1^\infty \frac{dt}{t^n}\exp(-\alpha t).$$ (17)

The integral $\Phi_n(\alpha)$ may be expanded in series:

$$\Phi_n(\alpha) = (-1)^n \frac{\alpha^{n-1} E_i(-\alpha)}{(n-1)!} + e^{-\alpha}\sum_{k=0}^{n-2}\frac{(-1)^k \alpha^k}{(n-1)(n-2)\ldots(n-1-k)}.$$ (18)

For thin films ($\xi \ll 1$) $A(\xi)$ has this simplified form:

$$A(\xi) = 2\eta(\eta - \ln\eta) + 2\xi^2(1 + 1/2\eta).$$ (19)

The z-coordinate of the vector of the energy flux density **P** and its derivative are expressed, after substituting the function f_1 into the expression for the vector **P**, as follows:

$$P_z = -3k_0\eta\omega l_a\left(\frac{2k_0 T_e}{\tau m^*}\right)^{1/2}\frac{dT_e}{dz}B(\xi),$$ (20)

$$\frac{dP_z}{dz} = -3k_0\eta\omega l_a\left(\frac{2k_0 T_e}{\tau m^*}\right)^{1/2}\left\{\frac{d^2 T_e}{dz^2}B(\xi) + \frac{B(\xi)}{2T_e}\left(\frac{dT_e}{dz}\right)^2 + \frac{dT_e}{dz}\frac{dB}{dz}\right\},$$ (21)

where

$$B(\xi) = 2/3 - \Phi_4(\eta+\xi) - \Phi_4(\eta-\xi).$$ (22)

Again, after the expanding of the integral $\Phi_4(\alpha)$ in series (18) up to quadratic terms, we get for $B(\xi)$ the following expression:

$$B(\xi) = \eta(1 - \eta) - \xi^2.$$ (23)

The explicit expressing of the last term $(\partial e/\partial t)_c$ of the balance equation depends on the kind of the energy scattering processes inside the film. The mean energy transferred from electrons to the lattice by the scattering on the deformation potential can be expressed for a non-degenerate semiconductor as follows [10]:

$$\overline{\left(\frac{\partial e}{\partial t}\right)_a} = -\left(\frac{2k_0 T_e}{\tau m^*}\right)^{1/2}\frac{8m^* s^2}{k_0 T_0}\frac{k_0}{l_a}(T_e - T_0),$$ (24)

where s is the velocity of longitudinal sound waves.

Now, we can write the energy balance equation by using the relations (15, 21, 24) as follows:

$$[\eta(1 - \eta) - \xi^2]\frac{d^2 u}{d\xi^2} - 2\xi\frac{du}{d\xi} - \frac{8m^* s^2}{3k_0 T_0}u = \frac{1}{3}\left(\frac{q_e E_x l_a}{k_0 T_0}\right)^2$$
$$\times [\eta(\eta - \ln\eta) + \xi^2(1 + 1/2\eta)],$$ (25)

where $u = T_e/T_0 - 1$.

The differential equation (25) is solved for the following boundary conditions:

1. On the surface the electrons lose a part of their energy by the scattering caused by the surface vibration of the lattice, by the vibration of the insulator which is in a contact with the film, by absorbed molecules and atoms. Then the mean energy of the conduction electrons is proportional to a difference of the effective temperature T_e and T_0. The proportional coefficient W characterizes the rate of energy recoil on the surface and is the same for both surfaces. Then for $P_z(\pm d)$ we get:

$$P_z(d) = -3k_0 n_0 l_a \left(\frac{2k_0 T_e(d)}{\pi m^*}\right)^{1/2}\left[\frac{dT_e}{dz}\right]_{z=d}[\eta(1-\eta) - \xi]^2 = W n_0 k_0 [T_e(d) - T_0]$$ (26)

and hence

$$\left[\frac{du}{d\xi}\right]_{\xi=\eta} = -w\,\frac{u(d)}{\eta(1-2\eta)}; \quad w = \frac{W}{3}\left(\frac{\pi m^*}{2k_0 T_0}\right)^{1/2}.$$ (27)

2. We can assume from the assumption $P_z(+d) = P_z(-d)$ that the electron effective temperature is a symmetric function of the z-coordinate. The necessary condition for this is

$$\left[\frac{du}{d\xi}\right]_{\xi=0} = 0.$$ (28)

The terms (27, 28) represent two boundary conditions of the differential equation (25). The solution of equation (25) with the help of these boundary conditions is

$$u = \frac{(q_e l_a)^2}{8m^* s^2 k_0 T_0}(\eta^2 - \eta \ln \eta)E_x^2 + C\left[\xi^2 + \frac{3k_0 T_0}{4m^* s^2}(\eta - \eta^2)\right]E_x^2$$ (29)

where

$$C = \frac{1}{6}\left(\frac{q_e l_a}{k_0 T_0}\right)^2 \times$$

$$\times \frac{-\dfrac{w}{\eta(1-2\eta)}\left(\dfrac{3k_0 T_0(\eta - \ln \eta)}{4m^* s^2} - \dfrac{\eta(1+2\eta)}{12(1-\eta)} + \dfrac{1+2\eta}{3(1-\eta)}\right)}{\dfrac{w}{\left(\dfrac{8m^* s^2}{3k_0 T_0} + 6\right)\eta} + \dfrac{\eta\left(\dfrac{8m^* s^2}{3k_0 T_0} + 6\right)}{12(1-2\eta)(1-\eta)} + 2 + \dfrac{2w(1-\eta)}{3(1-\eta)} + \dfrac{8m^* s^2}{3k_0 T_0}\eta(1-2\eta)} + \frac{w}{(1-2\eta)}.$$ (30)

We can see that the effective electron temperature in a thin film depends on its thickness 2d and on the z-coordinate as well, in the case when no energy recoils on the surface. For the mean value of the effective electron temperature we get:

$$\bar{u} = \frac{(q_e l_a)^2}{8m^* s^2 k_0 T_0}(\eta^2 - \eta \ln \eta)E_x^2 + C\left[\frac{\eta^2}{3} + \frac{3k_0 T_0}{4m^* s^2}\eta(1-\eta)\right]E_x^2.$$ (31)

IV. NON-OHMIC ELECTRICAL CONDUCTIVITY

The electrical conductivity of a thin film is determined by the relation:

$$\sigma = \frac{1}{2dE_x}\int_{-d}^{d} dz\, j_x(z).$$ (32)

We use for the sake of simplicity the following notation:

$$u = u_1 E_x^2 + C\xi^2 E_x^2,$$ (33)

where

$$u_1 = \frac{(q_e l_a)^2}{8m^* s^2 k_0 T_0}(\eta^2 - \eta \ln \eta) + C\,\frac{3k_0 T_0}{4m^* s^2}\eta(1-\eta).$$ (34)

By putting equation (33) into the relation for the current density j_x and integrating over the thickness of the film we shall get the following relation for the conductivity [under the assumption $u \ll 1$ (warm electrons)]:

$$\sigma = \frac{q_e l_a n_0}{(2\pi m^* k_0 T_0)^{1/2}}\left[2\eta\left(\eta + \ln \frac{1}{\eta}\right) + \frac{\eta(2\eta + 1)}{3}\right]\left(1 - \frac{3u_1 - C\eta^2}{6}E_x^2\right).$$ (35)

From the assumption $u \ll 1$, we obtain the condition for the external electric field in the region of warm electrons, when the electrical conductivity can be expressed by the relation $\sigma = \sigma_0(1 + \beta E_x^2)$, where σ_0 is the ohmic conductivity of the thin film, β is the non-ohmic parameter, representing a deflection from Ohm's law:

$$E_x \ll \left(\left\{\frac{(q_e l_a)^2}{8m^* s^2 k_0 T_0}(\eta^2 - \eta \ln \eta) + C\left[\frac{\eta^2}{3} + \frac{3k_0 T_0}{4m^* s^2}\eta(1-\eta)\right]\right\}\right)^{-1/2}.$$ (36)

From equation (35) we get for the parameter β the following expression:

$$\beta = -\frac{1}{6}\left[\frac{3(q_e l_a)^2}{8m^* s^2 k_0 T_0}(\eta^2 - \eta \ln \eta) + C\left(\frac{9k_0 T_0(\eta^2 - \eta)}{4m^* s^2} - \eta^2\right)\right].$$ (37)
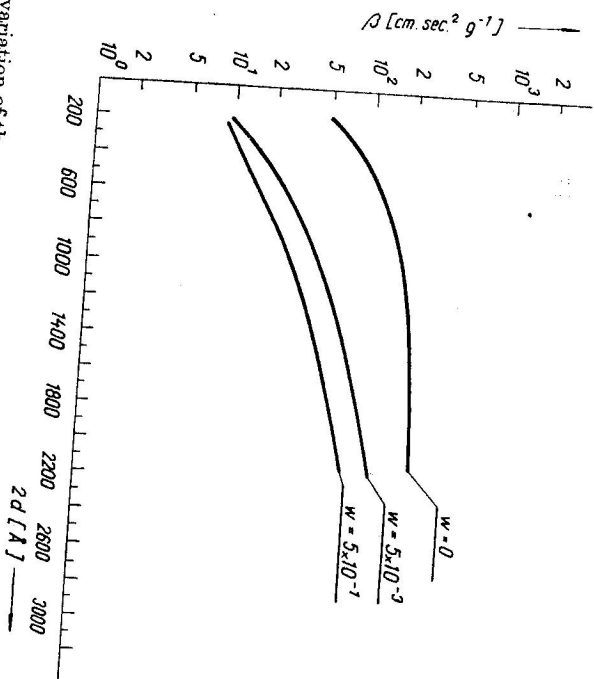
Fig. 1. The variation of the non-ohmic parameter β in dependence on the thickness of the film $2d$ at different values of the parameter w.

β [cm. sec.^{2} g^{-1}] — $2d$ [Å] —

$w = 0$ $w = 5 \times 10^{-3}$ $w = 5 \times 10^{-1}$

Fig. 1 illustrates the variation of the parameter β with the thickness of the film and Fig. 2 with the parameter w. From Fig. 1 we can see that the parameter β is larger for thicker films, i. e. a deflection from Ohm's law by applying the same electric field decreases with decreasing thickness of the film. The more perfect from the stand point of energy the thickness. The smaller the film thickness is, the less the non-ohmic behaviour depends on the film surface (characterized by parameter W) influences the electrical conductivity. We assume, in our paper, no concrete surface scattering. We characterize the surface energy scattering only by the phenomenological parameter W.

When we assume a square-law dispersion, an energy independent mean free path, and a small enough external electric field, the effective temperature for bulk material is [11]:

$$T_e = T_0 \left[1 + \frac{3\pi}{32} \left(\frac{\mu_0 E_x}{s} \right)^2 \right],$$ (38)

where μ_0 is the mobility in the ohmic region.
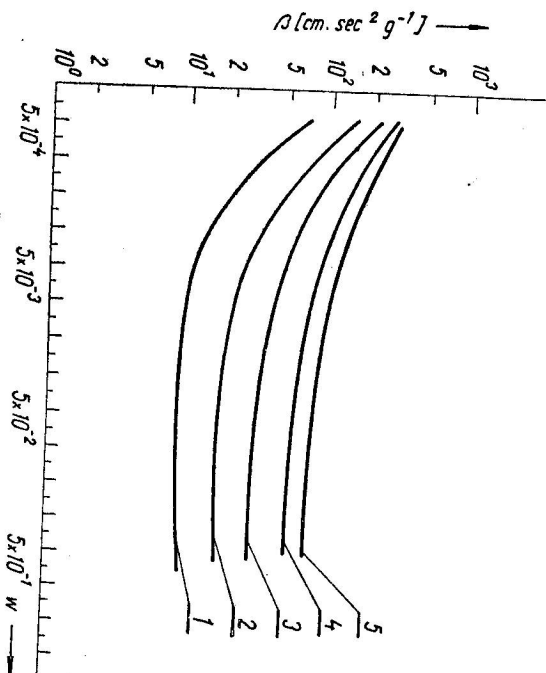The mobility μ in the region of warm electrons in the electron-temperature

Fig. 2. The variation of the parameter β with the parameter w with a different film thickness. Curve 1: $2d = 200$ Å; curve 2: $2d = 400$ Å; curve 3: $2d = 600$ Å: curve 4: $2d = 800$ Å; curve 5: $2d = 1000$ Å.

β [cm. sec.^{2} g^{-1}] — w —

approximation (the mobility limiting mechanism will be assumed to be the acoustic mode scattering) is expressed as

$$\mu = \mu_0 \left(\frac{T_0}{T_e} \right)^{1/2}; \quad \mu_0 = \frac{4 q_0 l_a}{3 (2\pi m^* k_0 T_0)^{1/2}}.$$ (39)

From the formulae (38) and (39) we get

$$\mu = \mu_0 (1 + \beta E_x^2), \text{ where } \beta = -\frac{3\pi \mu_0^2}{64 s^2}.$$ (40)

The relations (38) and (40) enable us to compare the effective temperature T_e in thin films (relationship (31)) and the non-ohmic parameter β in thin films (relationship (37)) with corresponding quantities in bulk material. This comparison is illustrated in Fig. 3 for n-Ge, $T_0 = 100$ °K, $E_x = 10$ V/cm. We can see that the heating of the conduction electrons is smaller in thin films than in some bulk material, with the same electric field. It is the evident result, because the conduction electrons gain a smaller energy from the electric field in thin films, than in bulk materials (it is expressed by the product $j_x E_x$). Similarly, a deviation from Ohm's law is smaller in thin films than in bulk materials, with the same electric field.
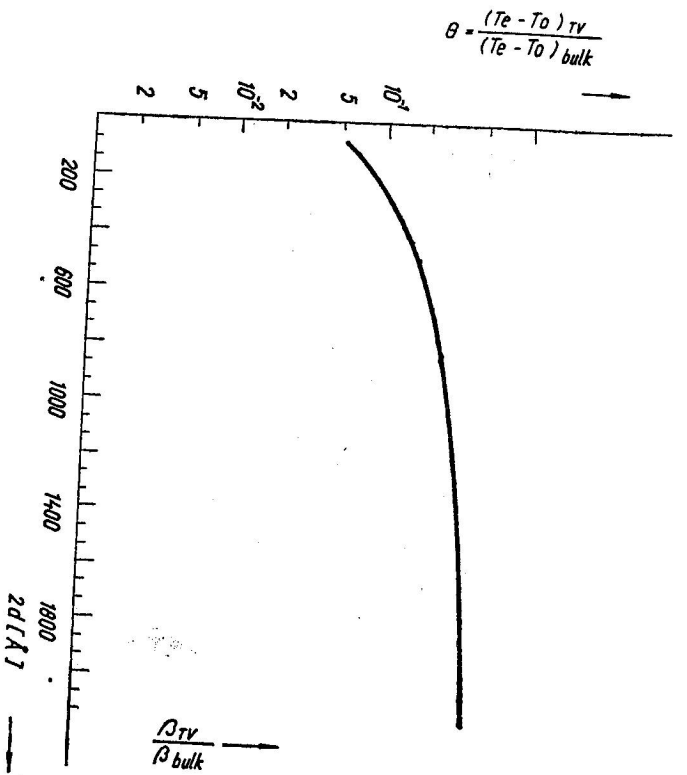
Fig. 3. The variation of the quantity $\Theta = (T_e - T_0)_{TV}/(T_e - T_0)_{bulk}$ with the thickness of the film.

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