

for over three decades of velocity. The measured dependence of the wall velocity on the electric field can be shown under certain conditions to be consistent with the well-known $e^{-\alpha/E}$ switching dependence of BaTiO₃. A nucleation mechanism for the wall motion is suggested by its field dependence, and the field dependence rules out the equation of motion usually applied to domain boundaries.

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Surface Transport Theory

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A theory is presented for the dependence of the galvanomagnetic parameters on the surface potential of a semiconductor. The expression for the conductivity reduces to that given by Schrieffer when the magnetic field is zero. Formal equations for the magnetoconductivity and Hall coefficient are derived. By using a constant relaxation time, and a linear space charge region potential, one can obtain closed-form expressions for the conductivity effective mobility and the Hall effective mobility. The Hall mobility is found to be 13% smaller than the conductivity mobility for large values of the surface potential.

INTRODUCTION

IN a recent paper, Petritz¹ derived a set of expressions for the Hall coefficient and magnetoresistance which depend on the surface potential of a semiconductor. His derivation was based on an unbounded solution of the Boltzmann equation. As a result, the expressions do not explicitly describe the surface potential dependence. In an earlier paper, Schrieffer² derived a formal expression for an effective conductivity mobility from a diffuse-scattering boundary condition on the solution of the Boltzmann equation. In this paper, we extend the problem to include the presence of a magnetic field. Formal expressions are found for the magnetoconductivity and Hall coefficient as functions of surface-dependent terms. By using a linear potential in the space-charge region we can evaluate the appropriate integrals for these terms when the relaxation time is independent of energy. The conductivity and Hall effective mobilities are compared with each other.

GENERAL THEORY

We shall follow the general procedure used by Schrieffer. The Boltzmann equation is assumed to have a relaxation time τ in the collision term³ so that

$$\mathbf{v} \cdot \text{grad}_v f + \mathbf{a} \cdot \text{grad}_v f = (f_0 - f)/\tau, \quad (1)$$

where f is the distribution function for the electrons

in the specimen and f_0 is their equilibrium distribution. We let

$$f = f_0 + f_1, \quad (2)$$

where f_1 is the perturbation function. Spherical energy surfaces are assumed so that the equilibrium distribution function is given by

$$f_0 = C \exp \left\{ -\frac{m(v_x^2 + v_y^2 + v_z^2)}{2kT} + \frac{q\psi(z)}{kT} \right\}. \quad (3)$$

The accelerations in the various directions are

$$\begin{aligned} a_x &= -q(E_x + v_y H)/m, \\ a_y &= -q(E_y - v_x H)/m, \\ a_z &= -qE_z(z)/m. \end{aligned} \quad (4)$$

We assume that the magnetic field is in the z direction and is constant in magnitude. Introducing Eqs. (2), (3), and (4) into Eq. (1) and neglecting products of $f_1 E_x$ and $f_1 E_y$, we obtain

$$\begin{aligned} v_z \frac{\partial f_1}{\partial z} - \frac{qE_z}{m} \frac{\partial f_1}{\partial v_z} - \frac{qH}{m} \left(v_y \frac{\partial f_1}{\partial v_x} - v_x \frac{\partial f_1}{\partial v_y} \right) \\ + \frac{f_1}{\tau} = -\frac{qf_0}{kT} (E_x v_x + E_y v_y). \end{aligned} \quad (5)$$

By Lagrange's method, we obtain a particular solution of Eq. (5):

$$\epsilon = \frac{1}{2} m v_z^2 - q\psi(z). \quad (6)$$

¹ R. L. Petritz, Phys. Rev. **110**, 1254 (1958).

² J. R. Schrieffer, Phys. Rev. **97**, 641 (1955).

³ A. H. Wilson, *The Theory of Metals* (Cambridge University Press, London, 1953).

Making use of this expression, we can transform f_1 from a function of v_z and z to a function of either ϵ and z or ϵ and v_z :

$$f_1(v_z, z) = f_1(z, \epsilon) = f_1(v_z, \epsilon). \tag{7}$$

The latter transform was used by Schrieffer. Under certain circumstances it is preferable to transform to ϵ and z . However, we shall not concern ourselves with this problem here.

Introducing the transformed distribution function in Eq. (5) and changing the variables by means of

$$\begin{aligned} \frac{\partial K}{\partial v_z} &= \frac{m}{q\tau(v, \epsilon)E_z(v_z, \epsilon)}, \\ v_x &= v \sin\theta, \\ v_y &= v \cos\theta, \end{aligned} \tag{8}$$

we find

$$\frac{\partial f_1}{\partial K} + \frac{q\tau H}{m} \frac{\partial f_1}{\partial \theta} - f_1 = \frac{q\tau v f_0}{kT} (E_x \sin\theta + E_y \cos\theta). \tag{9}$$

We note that

$$K = \int_0^{v_z} \frac{m dv_z}{q\tau(v, \epsilon)E_z(v_z, \epsilon)}, \tag{10}$$

and that at the surface

$$K_0 = K|_{v_z=v_{zs}}, \tag{11}$$

where v_{zs} is the z velocity of a carrier at the surface.

By making further use of Lagrange's method, it is simple to show that for a diffuse scattering boundary condition, i.e., $f_1=0$ at the surface, the distribution function becomes

$$\begin{aligned} f_1 = & -\frac{q\tau v f_0}{kT(1+\mu^2 H^2)} \{ (1 - e^{\Delta K} \cos\mu H \Delta K) (a_1 \sin\theta \\ & + b_1 \cos\theta) - e^{\Delta K} \sin\mu H \Delta K (b_1 \sin\theta - a_1 \cos\theta) \}, \end{aligned} \tag{12}$$

where

$$\begin{aligned} \Delta K &= K - K_0, \\ a_1 &= E_x - \mu H E_y, \\ b_1 &= E_y + \mu H E_x, \\ \mu &= q\tau/m. \end{aligned} \tag{13}$$

It is obvious that this solution vanishes at the surface since there $v_z=v_{zs}$ and ΔK is zero. If we assumed a specular scattering boundary condition, we would find the usual bulk distribution function. If the scattering is not entirely diffuse, the distribution function would be a weighted sum of the diffuse and specular solutions.

CALCULATION OF THE COEFFICIENTS

In order to determine the galvanomagnetic coefficients, we calculate the currents in the x and y

directions:

$$I_x = -q \int f_1 v_x dv_x dv_y dv_z dz, \tag{14}$$

$$I_y = -q \int f_1 v_y dv_x dv_y dv_z dz. \tag{15}$$

We transform the integration over (v_x, v_y, v_z, z) to an integration over $(v, \theta, \epsilon, \Delta K)$. The Jacobian of the transformation is $\tau v/m$. By using Eqs. (3) and (12), the currents can be reduced to

$$\begin{aligned} I_x = & \frac{\pi m C}{kT} \{ \langle A_H (1 - \mu^2 H^2) + 2\mu H B_H \rangle_{v, \epsilon} E_x \\ & + \langle 2\mu H A_H - (1 - \mu^2 H^2) B_H \rangle_{v, \epsilon} E_y \}, \end{aligned} \tag{16}$$

$$\begin{aligned} I_y = & \frac{\pi m C}{kT} \{ \langle A_H (1 - \mu^2 H^2) + 2\mu H B_H \rangle_{v, \epsilon} E_y \\ & + \langle 2\mu H A_H - (1 - \mu^2 H^2) B_H \rangle_{v, \epsilon} E_x \}. \end{aligned} \tag{17}$$

For convenience we use the following notation

$$\langle g \rangle_{v, \epsilon} = \int_{\epsilon} \int_0^{\infty} g(v, \epsilon) \frac{\mu^2 v^3 \exp(-mv^2/2kT)}{(1+\mu^2 H^2)^2} e^{-(\epsilon/kT)} dv d\epsilon. \tag{18}$$

$$\langle g \rangle_{\epsilon} = \int_{\epsilon} g(\epsilon) e^{-\epsilon/kT} d\epsilon. \tag{19}$$

Further,

$$A_H = \exp\{-2K_0\} \cos 2\mu H K_0 + 2K_0 - 1, \tag{20}$$

$$B_H = \exp\{-2K_0\} \sin 2\mu H K_0 - 2\mu H K_0. \tag{21}$$

Upon setting $I_y=0$, and using the usual definitions, the Hall coefficient is

$$R = \frac{1}{H\sigma} \left(\frac{\langle 2\mu H A_H - (1 - \mu^2 H^2) B_H \rangle_{v, \epsilon}}{\langle 2\mu H B_H + (1 - \mu^2 H^2) A_H \rangle_{v, \epsilon}} \right), \tag{22}$$

and the magnetoconductivity is

$$\sigma = \frac{\pi m C (1 + R^2 \sigma^2 H^2)}{kT} \langle A_H (1 - \mu^2 H^2) + 2\mu H B_H \rangle_{v, \epsilon}. \tag{23}$$

If we assume that $\mu H \ll 1$, we can expand Eqs. (20) and (21). Keeping terms of order $\mu^2 H^2$ only, we find

$$\begin{aligned} A_H &= (e^{-2K_0} + 2K_0 - 1) - \mu^2 H^2 (2K_0^2 e^{-2K_0}) \\ &= A - \mu^2 H^2 G, \end{aligned} \tag{24}$$

$$B_H = \mu H (2K_0 - 2K_0 e^{-2K_0}) = \mu H B. \tag{25}$$

Equations (22) and (23) then become

$$\sigma = \frac{\pi m C (1 + R^2 \sigma^2 H^2)}{kT} \langle A - \mu^2 H^2 (A + G - 2B) \rangle_{v, \epsilon}, \tag{26}$$

$$R = \frac{\pi m C (1 + R^2 \sigma^2 H^2)}{kT \sigma^2} \langle \mu (2A - B) \rangle_{v, \epsilon}. \tag{27}$$

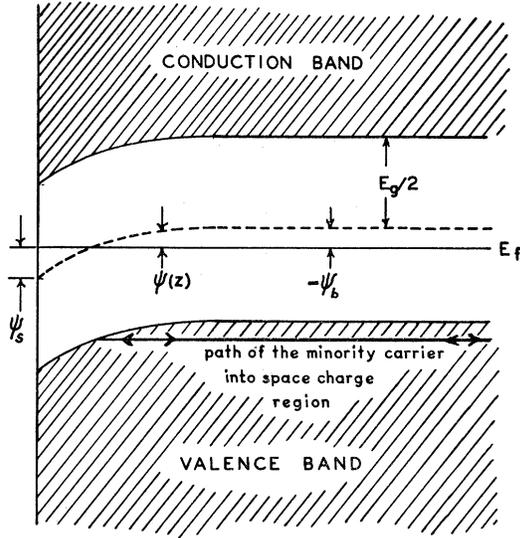


FIG. 1. Variation of the potential $\psi(z)$ at the surface of a semiconductor. ψ_s and ψ_b are the surface and bulk potentials, respectively, E_f is the Fermi level and E_g is the band gap. The specular reflection of minority carriers in the space-charge region is indicated by the arrows on the path of the minority carrier.

There are several things to be noted at this point. First, the expressions derived represent the sheet conductivity and Hall coefficient. As such they yield the conductivity and Hall coefficient per square of surface for a sample of arbitrary thickness. In order to demonstrate the effect of the surface potential on these quantities, a scheme must be devised to separate surface and bulk effects. Recently, the author has obtained such a separation.⁴ The second point is that the assumption of an energy-dependent relaxation time introduces a serious computational problem: it has been impossible so far to find a closed form solution of the appropriate integrals using $\tau(v, \epsilon)$. Without this assumption, the magnetoresistance will vanish. In the remainder of the paper we assume an energy-independent relaxation time and treat the Hall coefficient exclusively. The third point concerns the form of the solution when H vanishes. Comparison with Schrieffer's paper indicates that our formal expression for the conductivity differs from his. However, this is due to our use of a negative rather than a positive surface field.

Finally, in this paper we do not attempt to treat the question of the minority carrier in the space-charge region. As this carrier approaches the surface, it encounters a repulsive potential so that when the momentum is sufficiently low, the carrier will not reach the surface but will be specularly reflected at the surface barrier. This is indicated schematically in Fig. 1. As a result only some of the minority carriers will suffer a scattering collision with the surface. Thus, for this case our treatment is inadequate.

⁴ J. N. Zemel, Bull, Am. Phys. Soc. Ser. II, 3, 255 (1958).

LINEAR SPACE CHARGE REGION
POTENTIAL MODEL

Using the assumption that τ is independent of energy, Eqs. (26) and (27) reduce to

$$\sigma = \frac{2\pi kT \mu_b^2 C}{m} \langle A \rangle_\epsilon, \tag{28}$$

$$R = \frac{1}{\sigma^2} \frac{2\pi kT \mu_b^3 C}{m} \langle 2A - B \rangle_\epsilon, \tag{29}$$

where μ_b is the bulk mobility of the carrier defined as $q\tau/m$ and where terms of order H^2 and higher are neglected. If the potential in the z direction varies linearly with distance, the field is constant and equal to E_{zs} . Introducing this into Eq. (11) and noting that at the surface $v_{zs} = (2\epsilon/m)^{1/2}$, and assuming that the surface potential $\psi_s = \psi_b$, we find

$$K_0 = \left(\frac{\epsilon}{kT} \right)^{1/2} \frac{(2mkT)^{1/2}}{q\tau E_{zs}}. \tag{30}$$

If we set $y = (\epsilon/kT)^{1/2}$ and $\alpha = (2mkT)^{1/2}/q\tau E_{zs}$, then Eqs. (28) and (29) can be integrated in closed form, leading to

$$\sigma = Nq\mu_b [1 - \exp(\alpha^2) \operatorname{erfc}\alpha], \tag{31}$$

$$R = \frac{1}{\sigma^2} Nq\mu_b^2 \left[1 - \frac{2\alpha}{\pi^{1/2}} - (1 - 2\alpha^2) \exp(\alpha^2) \operatorname{erfc}\alpha \right], \tag{32}$$

where N is the number of carriers per square. N is obtained from

$$N = \int f_0 dv_x dv_y dv_z dz = \frac{2\pi kT \mu_b}{m} C (kT (\pi)^{1/2} \alpha). \tag{33}$$

Following the procedure suggested by Petritz, the effective conductivity and Hall mobilities are respectively

$$(\mu_{\text{eff}}/\mu_b)_\sigma = 1 - \exp(\alpha^2) \operatorname{erfc}\alpha, \tag{34}$$

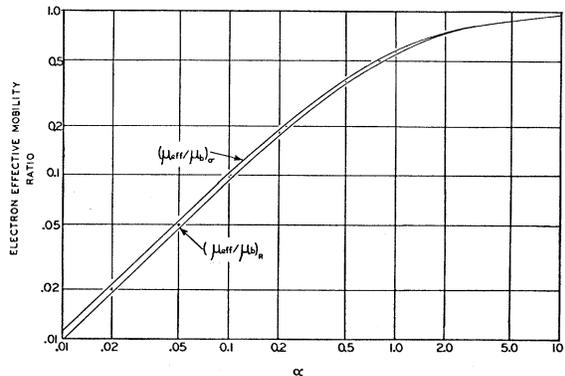


FIG. 2. The effective mobilities as a function of α , where $\alpha = (2mkT)^{1/2}/q\tau E_{zs}$. $(\mu_{\text{eff}}/\mu_b)_\sigma$ is the conductivity effective mobility and $(\mu_{\text{eff}}/\mu_b)_R$ is the Hall effective mobility.

$$(\mu_{\text{eff}}/\mu_b)_R = \left[1 - \frac{2\alpha}{\pi^{1/2}} (1 - 2\alpha^2) \exp(\alpha^2) \operatorname{erfc}\alpha \right]^{1/2}. \quad (35)$$

In Fig. 2, these two terms are plotted for comparison. For large values of α , corresponding to a shallow well, the two mobilities are the same, i.e., approximately unity. As the well deepens, the Hall term drops below the conductivity term and quickly reaches a constant fraction of the effective conductivity mobility. The amount is readily calculated. When $\alpha \rightarrow 0$, the effective conductivity mobility becomes

$$(\mu_{\text{eff}}/\mu_b)_\sigma |_{\alpha \rightarrow 0} = 2\alpha/\pi^{1/2}, \quad (36)$$

and the effective Hall mobility becomes

$$(\mu_{\text{eff}}/\mu_b)_R |_{\alpha \rightarrow 0} = \alpha. \quad (37)$$

Thus the effective Hall mobility is some 13% less than the effective conductivity mobility.

CONCLUSIONS

In this paper, we have derived formal expressions for the one-carrier magnetoconductivity and Hall coefficient. By choosing a simple model for the space-charge potential, an effective Hall mobility expression is found which is comparable to that for the effective conductivity mobility.

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Mechanical Resonance Dispersion in Quartz at Audio-Frequencies

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Measurements of the complex shear compliance ($J^* = J' - iJ''$) of single crystals of quartz and fused quartz at frequencies from 100 to 5000 cps have resulted in the discovery of sharp resonances in the compliance similar to those recently found in polycrystalline metals and crystalline polymers. The number, locations, and magnitudes of the resonances depend on crystal orientation with respect to the applied dynamic stress and vary with temperature, external static stress, and, in some cases, with time. The presence of numerous resonances in fused quartz may result from the existence of regions of long-range order (100 to 200 Å) in this material. Analysis of the data on the basis of a generalized stress-strain relation involving a linear combination of strain and its first and second time derivatives gives a close fit to the experimental curves. An explanation of the resonances is suggested by calculations of Fermi, Pasta, and Ulam for nonlinear systems in which no tendency toward equipartition of energy among modes was found. Accordingly it is proposed that (1) crystalline solids with nonlinear forces between atoms do not share their vibrational energy among all of the available modes, but pass energy back and forth among relatively few modes, (2) the frequency of the energy exchange among modes may be low, and in particular, much lower than the frequencies of the lattice vibrations, and (3) the resonance dispersions observed in the dynamic mechanical compliance of quartz and other materials occur at these various acoustic exchange frequencies. This lack of energy equipartition will not necessarily be noticed in specific heat measurements of solids, but can be expected to have some consequences in other areas.

I. INTRODUCTION

THE existence of multiple-dispersion regions of the resonance type at audio-frequencies has been demonstrated in previous investigations of the dynamic shear compliance of polycrystalline metals¹ and crystalline polymers.^{2,3} These measurements of complex shear compliance ($J^* = J' - iJ''$) now have been extended to single crystals of quartz and to fused quartz.

While a number of investigators have previously studied the dynamic mechanical properties of quartz, their measurements have not been made at closely

spaced intervals in the audio-frequency range. Determinations of logarithmic decrement ($\propto J''/J'$) as a function of temperature at frequencies in the neighborhood of 21 and 42 kcps have revealed a maximum in the vicinity of 250°C for quartz crystal bars in longitudinal vibration.^{4,5} The temperature variations of the Q ($Q^{-1} \propto J''/J'$) of quartz bars in torsional and longitudinal oscillation have also been studied at fundamental frequencies near 36 kcps and at the third and fifth overtones.^{6,7} A maximum in Q^{-1} was observed at

⁴ R. A. Artman, *J. Appl. Phys.* **23**, 475 (1952).

⁵ G. A. Alers, *J. Appl. Phys.* **24**, 324 (1953).

⁶ R. K. Cook and P. G. Weissler, *Phys. Rev.* **80**, 712 (1950).

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