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Electrical Properties of Thin-Film Semiconductors*

Abstract: The theory of the electrical properties of metal films as given by Fuchs and Sondheimer is extended to nondegenerate semiconductors with ellipsoidal energy surfaces. A change of variables reduces the problem to a simpler one with spherical energy surfaces but with electric and magnetic fields which are tilted with respect to the film. This is solved to first order in the applied fields. The effective mobility and Hall coefficient vary with film thickness much as for a metal but show an anisotropy with film orientation, even for cubic crystals. Anisotropy is observed for both diffuse and specular surface scattering and for surface channels as well as films, and it provides a means of measuring the effective mass ratio of the carriers.

1. Introduction

Fuchs[1] has given the theory of the electrical conductivity of a thin metal film, and Sondheimer,[2,3] Chambers,[4] and MacDonald and Sarginson[5] have extended it to the galvanomagnetic effects. The present paper presents a similar analysis for a thin single-crystal film of a nondegenerate semiconductor. We shall be particularly concerned in our derivation to take proper account of the ellipsoidal shape of the surfaces of constant energy in the band structure of the film material. It will be shown that the conductivity and Hall coefficient of the film vary with the orientation of the normal to the film with respect to the crystallographic axes, even for materials of cubic symmetry such as germanium or silicon. This contrasts with the isotropic behavior of these quantities in the bulk material. This variation permits an experimental determination of the ratio of the components of the effective mass tensor.

The problem of solving the Boltzmann equation for a thin film and ellipsoidal energy surfaces with arbitrary electric and magnetic fields can be reduced by a change of variables to the simpler problem of solving the equation with spherical energy surfaces. Although many writers have used a transformation of the propagation vector **k** alone to simplify the algebra of various calculations involving ellipsoidal surfaces,[6,7] the usefulness of the complete transformation of the position vector **x** and the electric and magnetic fields as well as **k** seems not to have been pointed out.

Although our explicit results are given for diffuse surface scattering, we shall show that even with specular reflection the film conductivity can be anisotropic. We shall show too that the above transformation is also useful in the analysis of the electrical properties of a surface channel and that the anisotropy of a channel is similar to that for a film. Previous work on channels by Schrieffer[8] and Zemel[9] has assumed spherical energy surfaces.[10]

The anisotropy in the conductivity of thin metal films due to ellipsoidal energy surfaces has been derived by Englman and Sondheimer.[11] Their results are very similar to ours, apart from the difference in statistics. We also consider the Hall coefficient, and our work can be extended in a straightforward manner to the magnetoresistance.

2. Solution of the Boltzmann equation for a thin film

We assume that the surfaces of constant energy in the occupied regions of the Brillouin zone are ellipsoids of revolution centered at the extrema of the energy bands. In the neighborhood of one such extremum the energy is therefore

$$E(\mathbf{k}) = (\hbar^2/2m)[\alpha_s(k_1^2+k_2^2)+\alpha_p k_3^2], \quad (1)$$

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where m is the free electron mass and $\mathbf{k}=(k_1, k_2, k_3)$ is the propagation vector relative to the extremum. It is convenient first to solve the Boltzmann equation for electrons in the neighborhood of a single such extremum and to calculate their contribution to the current density in the film, then to add the contributions from the several extrema. Accordingly, we make use of a different coordinate system for the ellipsoids at the different extrema, choosing the 3-axis to coincide with the axis of rotation of the ellipsoid.

If the normal $\mathbf{n}$ to the film makes an angle θ with the symmetry axis of the ellipsoid, and if $\mathbf{x}=(x_1, x_2, x_3)$ denotes a point in coordinate space, we may describe the surfaces of the film by the equations

$$n_1x_1+n_3x_3=\pm d\,, \tag{2}$$

$$n_1=\sin\theta,\quad n_2=0,\quad n_3=\cos\theta\,. \tag{3}$$

The electrons are accelerated by electric and magnetic fields $\mathbf{E}=(E_1, E_2, E_3)$ and $\mathbf{H}=(H_1, H_2, H_3)$, and we assume in our calculation below that these fields are independent of position and time.

The distribution function of the electrons may be written

$$f=f_0(\mathbf{k})+f_1(\mathbf{k}, \mathbf{x})\,, \tag{4}$$

where $f_0=C\exp(-E(\mathbf{k})/k_0T)$ is the equilibrium distribution function. The Boltzmann equation then takes the form to first order in $\mathbf{E}$,

$$-\mathbf{v}\cdot\nabla_x f_1+(e/\hbar c)(\mathbf{v}\times\mathbf{H})\cdot\nabla_k f_1-f_1/\tau$$
$$=-(e/\hbar)\mathbf{E}\cdot\nabla_k f_0\,, \tag{5}$$

where $\mathbf{v}$ is the velocity of an electron and $-e$ its charge. We assume that scattering processes within the film may be represented by a term $-[f(\mathbf{k})-f_0(\mathbf{k})]/\tau(\mathbf{k})$ and that the relaxation time $\tau(\mathbf{k})$ depends on $\mathbf{k}$ only through the energy $E(\mathbf{k})$. We shall show later that the use of such a relaxation time is not strictly correct for a thin film even if it is correct for calculations of bulk conductivity. However, the error made with this assumption is small.

Scattering occurring at the surface of the film imposes boundary conditions on the solution of the Boltzmann equation. If the electrons are diffusely scattered by the surface, these are[1]

$$f_1(\mathbf{k}, +d)=0 \qquad \text{if } (\mathbf{n}\cdot\mathbf{v})<0\,,$$
$$f_1(\mathbf{k}, -d)=0 \qquad \text{if } (\mathbf{n}\cdot\mathbf{v})>0\,. \tag{6}$$

We shall indicate in Section 4 how the calculations are modified if the electrons are in part scattered specularly at the surface.

It is inconvenient to solve (5) in its present form because of the complicated geometry introduced when the normal $\mathbf{n}$ is not along one of the principal axes of the ellipsoid. We therefore make the following transformation:

$$\begin{aligned} w_i&=\alpha_i^{\frac{1}{2}}k_i\,,\\ y_i&=\alpha_i^{-\frac{1}{2}}x_i\,,\\ u_i&=\alpha_i^{-\frac{1}{2}}v_i\,,\\ \mathfrak{E}_i&=\alpha_i^{\frac{1}{2}}E_i\,,\\ \mathfrak{H}_i&=\alpha_i^{-\frac{1}{2}}(\alpha_s^2\alpha_p)^{\frac{1}{2}}H_i\,, \end{aligned} \tag{7}$$

where $\alpha_1=\alpha_2=\alpha_s$ and $\alpha_3=\alpha_p$. The Jacobian of the transformation from $\mathbf{k}$, $\mathbf{x}$ to $\mathbf{w}$, $\mathbf{y}$ is unity, so that the distribution function f is appropriate to either set of variables, and in terms of the new variables the Boltzmann equation (5) takes the form

$$-\mathbf{u}\cdot\nabla_y f_1+(e/\hbar c)(\mathbf{u}\times\mathfrak{H})\cdot\nabla_w f_1-f_1/\tau$$
$$=(e/\hbar)\mathfrak{E}\cdot\nabla_w f_0\,. \tag{8}$$

In $\mathbf{w}$-space the energy surfaces are spherical,

$$E(\mathbf{k})=\frac{\hbar^2}{2m}(w_1^2+w_2^2+w_3^2)\,, \tag{9}$$

and $\mathbf{u}$ has the form of a velocity in the new space:

$$\mathbf{u}=(1/\hbar)\nabla_w E(\mathbf{k})\,.$$

Moreover, from (2) and (7) we obtain the equation of the film surfaces in the new variables

$$n_1'y_1+n_3'y_3=\pm d'\,. \tag{10}$$

The new direction cosines of the normal $\mathbf{n}'$ are

$$n_1'=(\alpha_s/\alpha_c)^{\frac{1}{2}}\sin\theta,\quad n_2'=0,\quad n_3'=(\alpha_p/\alpha_c)^{\frac{1}{2}}\cos\theta\,, \tag{11}$$

where

$$\alpha_c=\alpha_s\sin^2\theta+\alpha_p\cos^2\theta\,.$$

The effective thickness is

$$2d'=2d/\alpha_c^{\frac{1}{2}}\,. \tag{12}$$

The new boundary conditions are found from (6) to be

$$f_1(\mathbf{w}, +d')=0 \qquad \text{if } (\mathbf{n}'\cdot\mathbf{w})<0$$
$$f_1(\mathbf{w}, -d')=0 \qquad \text{if } (\mathbf{n}'\cdot\mathbf{w})>0\,. \tag{13}$$

The equations (8) to (13) are those encountered in calculating the response of electrons with spherical energy surfaces to electric and magnetic fields $\mathfrak{E}$ and $\mathfrak{H}$ in a film of thickness $2d'$. By means of this change of variables we have therefore transformed the problem with ellipsoidal energy surfaces into an equivalent and simpler one with spherical surfaces; however, the calculation is now more complicated than that given by Fuchs, Sondheimer, and other investigators because even if $\mathbf{E}$ lies originally in the plane of the film and $\mathbf{H}$ is perpendicular or parallel to it, $\mathfrak{E}$ and $\mathfrak{H}$ are generally tilted with respect to the film in the new space.

The general solution of (8) is a complicated function with which it is difficult to satisfy the boundary conditions except in simple situations in which $\mathfrak{H}$ either is zero or is parallel to $\mathbf{n}'$. We have therefore assumed that f_1 can be expanded in powers of the components of $\mathfrak{H}$ and have obtained all terms linear in $\mathfrak{H}$ by replacing f_1 in the second term of (8) by the solution in the absence of a magnetic field and integrating the resulting equation. This expansion is valid in an asymptotic sense in the limit of a vanishingly small magnetic field. We obtain

$$f_1=-\left(\frac{e\tau}{k_0T}\right) f_0 \sum_{i=1}^{3} \mathfrak{E}_i' \left\{\left[u_i'+\left(\frac{e\tau}{mc}\right)(\mathbf{u}\times\mathfrak{H})_i'\right]\cdot\right.$$
$$\cdot\left[1-\exp\left(\frac{-y_3'\pm d'}{\tau u_3'}\right)\right]+\left(\frac{e\tau}{mc}\right)\exp\left(\frac{-y_3'\pm d'}{\tau u_3'}\right)\cdot$$
$$\left.\cdot\left[-(\mathbf{u}\times\mathfrak{H})_i' \frac{(y_3'\mp d')}{\tau u_3'}-u_i'(\mathbf{u}\times\mathfrak{H})_3' \frac{(y_3'\mp d')^2}{2\tau^2(u_3')^3}\right]\right\}\ . \tag{14}$$

Here the components of the vectors $\mathbf{w}$, $\mathbf{y}$, $\mathbf{u}$, $\mathfrak{E}$, and $\mathfrak{H}$ are given relative to a new coordinate system, the 3-axis of which is parallel to $\mathbf{n}'$. The components (A_i) of any such vector $\mathbf{A}$ relative to the reference system of the ellipsoid axes are therefore to be obtained from those (A_1') in this new system from the relation

$$\mathbf{A}=\mathbf{S}\cdot\mathbf{A}'\ , \tag{15}$$

$$\mathbf{S}=\begin{pmatrix} n_3' & 0 & n_1' \\ 0 & 1 & 0 \\ -n_1' & 0 & n_3' \end{pmatrix}. \tag{16}$$

In (14) and the integrals to follow, wherever there is a double sign the upper one goes with the half-space $u_3'<0$, the lower with $u_3'>0$.

We could carry this iterative process one step further to obtain all terms in $(\mathfrak{H})^2$ in order to derive the magnetoresistance. However, for this procedure to be meaningful it is necessary that it be limited to small magnetic fields for which the electrical properties of the thin film have asymptotic expansions in positive powers of $\mathfrak{H}$. There is the usual restriction, which is also applicable to the bulk, that

$$|\mathfrak{H}|\ll\frac{cm}{\tau e}\equiv|\mathfrak{H}_0|\ .$$

But in the thin-film problem there is the additional requirement that the overwhelming majority of orbits intersect both surfaces, so that the boundary condition (13) remain applicable. This places a restriction on the component of magnetic field perpendicular to $\mathbf{n}'$,

$$|\mathfrak{H}\times\mathbf{n}'|\ll\frac{cm\sqrt{kT/m}}{2de}\equiv|\mathfrak{H}_1|\ .$$

In the opposite limit of $|\mathfrak{H}\times\mathbf{n}'|\gg|\mathfrak{H}_1|$, the majority of orbits intersect neither surface and the conductivity tensor goes to the bulk limit. While an investigation of the strong and intermediate magnetic field properties would be of great interest, and could be pursued along the lines of Reference 5, it is beyond the scope of the present work. We shall therefore limit ourselves to fields which are small compared with $\mathfrak{H}_0$ and $\mathfrak{H}_1$, and retain only the linear terms.

From (14) we may now calculate the current density $\mathfrak{J}'$ in $\mathbf{y}'$-space from the relation

$$\mathfrak{J}_i'=-e\int u_i'f_1 d\mathbf{w}\ . \tag{17}$$

We may write the result in the form

$$\mathfrak{J}'=\boldsymbol{\lambda}'\cdot\mathfrak{E}'\ , \tag{18}$$

where

$$\boldsymbol{\lambda}'=\begin{pmatrix} \sigma_1(y_3') & -\beta_1(y_3')\mathfrak{H}_3' & \eta(y_3')\mathfrak{H}_2' \\ \beta_1(y_3')\mathfrak{H}_3' & \sigma_1(y_3') & -\eta(y_3')\mathfrak{H}_1' \\ -\xi(y_3')\mathfrak{H}_2' & \xi(y_3')\mathfrak{H}_1' & \sigma_3(y_3') \end{pmatrix}, \tag{19}$$

and

$$\sigma_1(y_3')=\frac{e^2}{k_0T}\int f_0(u_1')^2\tau\left[1-\exp\left(\frac{-y_3'\pm d'}{\tau u_3'}\right)\right]d\mathbf{w}\ , \tag{20}$$

$$\sigma_3(y_3')=\frac{e^2}{k_0T}\int f_0(u_3')^2\tau\left[1-\exp\left(\frac{-y_3'\pm d'}{\tau u_3'}\right)\right]d\mathbf{w}\ , \tag{21}$$

$$\beta(y_3')=\frac{e^3}{k_0Tmc}\int f_0(u_1')^2\tau^2\left\{1-\left[1+\frac{(y_3'\mp d')}{\tau u_3'}\right]\right.$$
$$\left.\times\exp\left(\frac{-y_3'\pm d'}{\tau u_3'}\right)\right\}d\mathbf{w}\ , \tag{22}$$

$$\eta(y_3')=\frac{e^3}{k_0Tmc}\int f_0(u_1')^2\tau^2\left\{1-\left[\frac{(y_3'\mp d')}{\tau u_3'}\right.\right.$$
$$\left.\left.+\frac{(y_3'\mp d')^2}{2\tau^2(u_3')^2}+1\right]\exp\left(\frac{-y_3'\pm d'}{\tau u_3'}\right)\right\}d\mathbf{w}\ , \tag{23}$$

$$\xi(y_3')=\frac{e^3}{k_0Tmc}\int f_0(u_3')^2\tau^2$$
$$\times\left\{1-\left[1+\frac{(y_3'\mp d')}{\tau u_3'}\right]\exp\left(\frac{-y_3'\pm d'}{\tau u_3'}\right)\right\}d\mathbf{w}$$
$$+\frac{e^3}{k_0Tmc}\int f_0(u_1')^2\tau^2\,\frac{(y_3'\mp d')^2}{2\tau^2(u_3')^2}$$
$$\times\ \exp\left(\frac{-y_3'\pm d'}{\tau u_3'}\right)d\mathbf{w}\ . \tag{24}$$

We may now transform the tensor $\boldsymbol{\lambda}'$ to the coordinate system of the ellipsoid with use of (16) and

$$\boldsymbol{\lambda}=\mathbf{S}\cdot\boldsymbol{\lambda}'\cdot\mathbf{S}^{-1} \tag{25}$$

so that

$$\mathfrak{J}=\boldsymbol{\lambda}\cdot\mathfrak{E}\ .$$

Then using (7) and comparing (17) with the equation for the current density $\mathbf{J}$ in $\mathbf{x}$-space

$$J_i=-e\int v_i f_1 d\mathbf{k}=\alpha_i^{\frac{1}{2}}(\alpha_s^2\alpha_p)^{-\frac{1}{2}}\mathfrak{J}_i\ , \tag{26}$$

we may obtain the conductivity tensor $\boldsymbol{\sigma}'$ satisfying the relation $\mathbf{J}=\boldsymbol{\sigma}'\cdot\mathbf{E}$. It is finally convenient to transform once more to a coordinate system (r, s, t) with the t-axis parallel to the normal $\mathbf{n}$ of the film, the r- and s-axes in the plane of the film such that the projection of the ellipsoid symmetry axis upon the plane of the film makes an angle ϕ with the r-axis:

$$\begin{aligned}&\mathbf{J}=\boldsymbol{\sigma}\cdot\mathbf{E}\\&\boldsymbol{\sigma}=\mathbf{T}\cdot\boldsymbol{\sigma}'\cdot\mathbf{T}^{-1}\,,\end{aligned}\tag{27}$$

$$\mathbf{T}=\begin{pmatrix}-\cos\theta\cos\phi & \sin\phi & \sin\theta\cos\phi\\ -\cos\theta\sin\phi & -\cos\phi & \sin\theta\sin\phi\\ \sin\theta & 0 & \cos\theta\end{pmatrix}.\tag{28}$$

We obtain the following expressions for the elements of the conductivity tensor $\boldsymbol{\sigma}$ with respect to the (r, s, t) coordinate system, the components of $\mathbf{H}$ having been expressed with respect to this same set of axes.

$$\sigma_{rr}=\sigma_1(y_3')\rho[\alpha_s\sin^2\phi+\alpha_s\alpha_p\alpha_c^{-1}\cos^2\phi]$$
$$+\sigma_3(y_3')\rho\alpha_c^{-1}(\alpha_s-\alpha_p)^2\cos^2\theta\sin^2\theta\cos^2\phi\,,\tag{29a}$$

$$\sigma_{ss}=\sigma_1(y_3')\rho[\alpha_s\cos^2\phi+\alpha_s\alpha_p\alpha_c^{-1}\sin^2\phi]$$
$$+\sigma_3(y_3')\rho\alpha_c^{-1}(\alpha_s-\alpha_p)^2\cos^2\theta\sin^2\theta\sin^2\phi\,,\tag{29b}$$

$$\sigma_{tt}=\sigma_3(y_3')\rho\alpha_c\,,\tag{29c}$$

$$\sigma_{rs}=\sigma_1(y_3')\rho\sin\phi\cos\phi[-\alpha_s+\alpha_s\alpha_p\alpha_c^{-1}]$$
$$+\sigma_3(y_3')\rho\sin\phi\cos\phi\alpha_c^{-1}(\alpha_s-\alpha_p)^2\sin^2\theta\cos^2\theta$$
$$-\beta(y_3')\rho\alpha_s^2\alpha_p\alpha_c^{-1}H_t$$
$$-\eta(y_3')\rho\alpha_s(\alpha_s-\alpha_p)\sin\theta\cos\theta[H_r\cos\phi+H_s\sin\phi$$
$$+H_t\alpha_c^{-1}(\alpha_s-\alpha_p)\sin\theta\cos\theta]\,,\tag{29d}$$

$$\sigma_{st}=-\sigma_3(y_3')\rho(\alpha_s-\alpha_p)\cos\theta\sin\theta\sin\phi$$
$$-\eta(y_3')\alpha_s\rho\{H_r[\alpha_p+(\alpha_s-\alpha_p)\sin^2\theta\cos^2\phi]$$
$$+H_s(\alpha_s-\alpha_p)\sin^2\theta\sin\phi\cos\phi$$
$$+H_t(\alpha_s-\alpha_p)\cos\theta\sin\theta\cos\phi\}\,,\tag{29e}$$

$$\sigma_{rt}=-\sigma_3(y_3')\rho(\alpha_s-\alpha_p)\cos\theta\sin\theta\cos\phi$$
$$+\eta(y_3')\rho\alpha_s\{H_r(\alpha_s-\alpha_p)\cos\phi\sin\phi\sin^2\theta$$
$$+H_s[\alpha_p+(\alpha_s-\alpha_p)\sin^2\theta\sin^2\phi]$$
$$+H_t(\alpha_s-\alpha_p)\sin\theta\cos\theta\sin\phi\}\,,\tag{29f}$$

where $\rho=(\alpha_s^2\alpha_p)^{-\frac{1}{2}}$, and $\alpha_c=(\alpha_s\sin^2\theta+\alpha_p\cos^2\theta)$. The components σ_{sr}, σ_{ts}, σ_{tr} may be obtained from σ_{rs}, σ_{st}, σ_{rt}, respectively, by changing the sign of all terms containing $\mathbf{H}$.[12]

We have indicated in (29) that the quantities $\sigma_1(y_3')$, $\sigma_3(y_3')$, et cetera, depend on $y_3'=\mathbf{y}\cdot\mathbf{n}'$. Since $x_t=\mathbf{x}\cdot\mathbf{n}$, we may show from (11) that $y_3'=\alpha_c^{-\frac{1}{2}}x_t$. Thus the components (29) of the conductivity tensor depend on x_t, and, as should be expected, are independent of position in the plane of the film.

The expressions (29) represent the contribution to the film conductivity from the electrons located near a single extremum of the energy bands. To obtain the total conductivity we may now add the contributions to each σ_{ij} from the different extrema, using the correct θ, ϕ, and $y_3'=[\alpha_c(\theta)]^{-\frac{1}{2}}x_t$ for each. The total current flowing in the film is now found by integrating the resulting expression for the current density, as in (27), over the thickness of the film.

Evaluation of this current requires that we specify the energy dependence of the collision time τ. The simplest choice is that τ is proportional to $E^{-\frac{1}{2}}$, as is the case if electrons in a semiconductor are scattered by lattice vibrations and if the simple deformation potential theory of scattering holds.[7] With this choice, we obtain

$$\bar{\sigma}_1=(2d)^{-1}\int_{-d}^{d}\sigma_1(y_3')dx_t=\frac{4n_ie^2l}{3\rho(2\pi mk_0T)^{\frac{1}{2}}}\left\{1-\frac{3}{2a}\left[\frac{1}{4}-F_1(a)+F_3(a)\right]\right\},$$

$$\bar{\sigma}_3=(2d)^{-1}\int_{-d}^{d}\sigma_3(y_3')dx_t=\frac{4n_ie^2l}{3\rho(2\pi mk_0T)^{\frac{1}{2}}}\left\{1-\frac{3}{a}\left[\frac{1}{4}-F_3(a)\right]\right\},$$

$$\bar{\beta}=(2d)^{-1}\int_{-d}^{d}\beta(y_3')dx_t=\frac{n_ie^3l^2}{3\rho mk_0Tc}\left\{1-\frac{3}{a}\left[\frac{1}{4}-F_3(a)\right]\right\},$$

$$\bar{\eta}=(2d)^{-1}\int_{-d}^{d}\eta(y_3')dx_t=\frac{n_ie^3l^2}{3\rho mk_0Tc}\left\{1-\frac{9}{2a}\left[\frac{1}{4}-F_1(a)+F_3(a)\right]\right.$$
$$\left.+3\left[F_0(a)-F_2(a)\right]+\frac{3a}{4}\left[\mathrm{F}_{-1}(a)-F_1(a)\right]\right\}.\tag{30}$$

Here

$$l=\tau u=\tau(2E(\mathbf{k})/m)^{\frac{1}{2}}\tag{31}$$

corresponds to a constant mean free path in the case of spherical energy surfaces, and

$$n_i=\int f_0(\mathbf{k})d\mathbf{k}\tag{32}$$

is the equilibrium number of electrons per unit volume obtained from (4) for a *single* extremum. The functions

$$F_m(a)=\int_0^1 x^m\exp(-a/x)dx\tag{33}$$

may be evaluated from tables[13] of the exponential integral

$$F_{-1}(a)=-Ei(-a)\tag{34}$$

with use of the relation

$$F_m(a)=\frac{e^{-a}}{a}-\left(\frac{m+2}{a}\right)F_{m+1}(a)\,.\tag{35}$$

Finally in (30) we have used $\rho=(\alpha_s{}^2\alpha_p)^{-\frac{1}{3}}$, and

$$a=2d'/l \tag{36}$$

is a parameter specifying the ratio of the effective film thickness (12) to the length l. We note that a depends on θ through the effective thickness and is therefore different for the ellipsoids at different extrema.

In the limit of very thick films ($a\rightarrow\infty$), $\bar{\sigma}_1$ and $\bar{\sigma}_3$ become equal, as do $\bar{\beta}$ and $\bar{\eta}$, and these quantities assume their bulk values, σ_{1B} and β_B respectively, given by the expressions multiplying the curly brackets in (30). In Fig. 1 we have plotted the ratio of these quantities to their bulk values as a function of a.

The following are asymptotic expressions for these ratios for thin and thick films:[14]

Thin films:

$$\begin{aligned}&(\bar{\sigma}_1/\sigma_{1B})\sim(3a/4)ln(1/a)\\&(\bar{\sigma}_3/\sigma_{1B})=(\bar{\beta}/\beta_B)\sim(3a/4)\\&(\bar{\eta}/\beta_B)\sim(3a/8).\end{aligned} \tag{37}$$

Thick films:

$$\begin{aligned}&(\bar{\sigma}_1/\sigma_{1B})\sim1-(3/8a)\\&(\bar{\sigma}_3/\sigma_{1B})=(\bar{\beta}/\beta_B)\sim1-(3/4a)\\&(\bar{\eta}/\beta_B)\sim1-(9/8a).\end{aligned} \tag{38}$$

When the total current flowing in the film is found in this manner upon summing the contributions from the ellipsoids at the different extrema, the resulting average mobility of the electrons is found to depend on the orientation of the film even if the bulk material has cubic symmetry. A similar anisotropy is found for the Hall coefficient. These results contrast with the electrical properties of bulk material, for in a bulk material of cubic symmetry the different ellipsoids combine to make both the mobility and Hall coefficient isotropic. The film anisotropy is illustrated in Figs. 2 and 3, for values of the inverse effective mass components $\alpha_s=12.5$, $\alpha_p=0.77$ and ellipsoids oriented along the [111] axes as in n-germanium.[15,16] In Fig. 2 we plot the ratio of the average effective electron mobility in the film, μ_{eff}, to its bulk value, μ_B, for several orientations for which the current is parallel to the applied field. We obtain μ_{eff} by summing over all extrema the appropriate element, say σ_{rr}, of the conductivity tensor (29), and integrating this sum over the film thickness with use of (30) to form $(2d)\bar{\sigma}_{rr}$. Finally, we have in this case

$$(\mu_{\mathrm{eff}})_{rr}=\frac{(2d)\bar{\sigma}_{rr}}{(2d)Ne}, \tag{39}$$

where N is the total number of electrons per unit volume in the film. The same procedure for the bulk conductivities leads to

$$\mu_B=\frac{4el}{3(2\pi mk_0T)^{\frac{1}{2}}}\left(\frac{2\alpha_s+\alpha_p}{3}\right). \tag{40}$$

The ratio $(\mu_{\mathrm{eff}}/\mu_B)$ is plotted against the parameter

$$z=(2d/l). \tag{41}$$

In Fig. 3 the ratio of the Hall coefficient R to its bulk value R_B is plotted when the magnetic field is normal to

Figure 1 **Conductivity parameters vs film thickness.** *The ratio of the film conductivity parameters defined by Eq. (30) of text to their bulk values, for $\tau=(ml^2/2E)^{\frac{1}{2}}$, as a function of the ratio of the effective film thickness 2d' to the length l.*

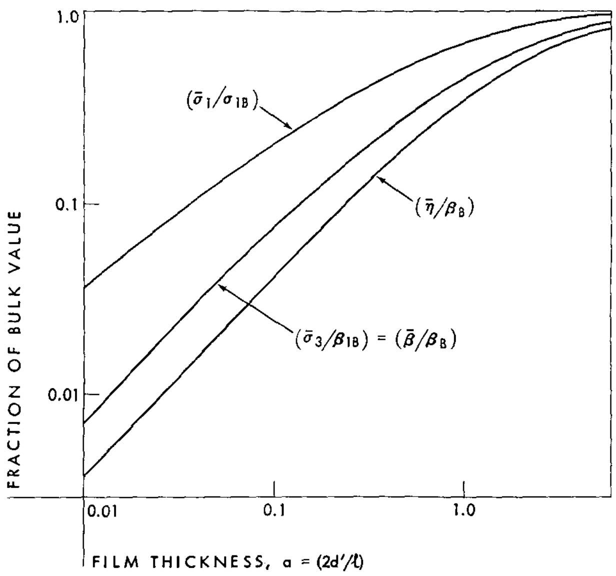
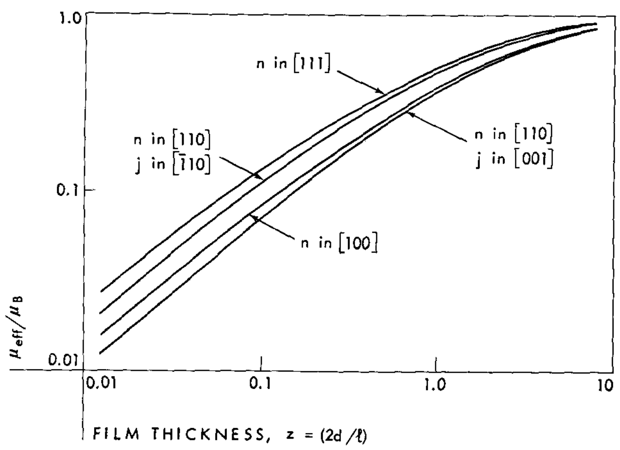


Figure 2 **Thin-film anisotropy of mobility.** *The ratio of the effective mobility to bulk mobility for carriers in a film with band structure similar to n-germanium and inverse effective mass components $\alpha_s=12.5$, $\alpha_p=0.77$, as a function of film thickness $z=2d/l$. The curves are labeled according to the direction of the film normal* **n** *and the current* **J**.



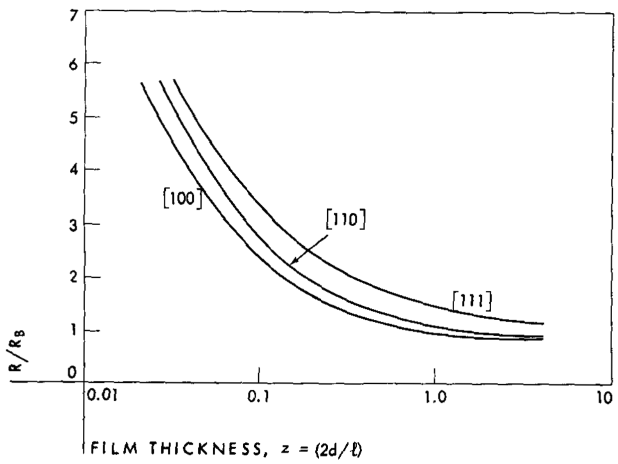
the film. In these cases R is isotropic in the plane of the film, and we have, to first order in the magnetic field,

$$\frac{R}{R_B}=\left(\frac{\bar{\sigma}_{rs}}{\sigma_{rsB}}\right)\left(\frac{\sigma_{rrB}}{\bar{\sigma}_{rr}}\right)\left(\frac{\sigma_{ssB}}{\bar{\sigma}_{ss}}\right), \tag{42}$$

where σ_{rrB} is the bulk value of $\bar{\sigma}_{rr}$.

In our derivation above we have assumed that the electric field is uniform, and we have not imposed the usual requirement that the total current shall flow in the plane of the film. Since the off-diagonal components σ_{rt}, σ_{st} of the one-ellipsoid conductivity tensor (29) are zero only for special orientations of the ellipsoid and of the magnetic field, a current density normal to the film will usually be induced in a single ellipsoid by a uniform electric field along the film. Adding the current densities arising from the different sets of ellipsoids will cancel this normal component for certain orientations, such as those for which Figs. 2 and 3 have been plotted for a cubic material. But otherwise if the current is to flow along the film, a component E_t of the electric field must be induced normal to the film such that the normal total current density is zero throughout the film. Since the total conductivity tensor depends on position within the film through the dependence of $\sigma_1(y_3')$, $\sigma_3(y_3')$, etc., in (20) to (24) on x_t, evidently E_t must itself vary with x_t.[17] Furthermore, E_t must satisfy Poisson's equation if the density of electrons is not uniform across the film, and we find by integrating the distribution function $f(\mathbf{k},\mathbf{x})$ given by (4) and (14) that the density is indeed not uniform. This observation has the further complication that the collision term in the Boltzmann equation should not be $[f(\mathbf{k},\mathbf{x})-f_0(\mathbf{k},\mathbf{x})]/\tau$ as in (5) but more suitably

Figure 3 **Thin-film anisotropy of Hall effect.** *The ratio of the Hall coefficient of a film to its bulk value, for a band structure similar to n-germanium and inverse effective mass components $\alpha_s=12.5$, $\alpha_p=0.77$, as a function of film thickness $z=2d/l$. The magnetic field is along the film normal* **n**.



$$\left\{f(\mathbf{k},\mathbf{x})-f_0(\mathbf{k},\mathbf{x})\left[1+\frac{\int f_1(\mathbf{k},\mathbf{x})d\mathbf{k}}{\int f_0(\mathbf{k},\mathbf{x})d\mathbf{k}}\right]\right\}\frac{1}{\tau}. \tag{43}$$

The integral term in this expression, summed over all ellipsoids, is related to (dE_t/dx_t) by Poisson's equation.

A rigorous solution taking account of these complications has not been given and would be quite difficult. MacDonald and Sarginson[5] considered the problem for the transverse magnetoresistance of a metal in the case of a spherical energy surface with $\mathbf{H}$ in the plane of the film. They concluded that the error was not serious if one neglected the non-uniformity of E_t, omitted the integral term in (43), and averaged the contributions to the normal current density over the film thickness in determining E_t. For a metal film in the presence of only an electric field, Englman and Sondheimer[11] found a non-uniform expression for $E_t(x_t)$ which leads to a solution of the Boltzmann equation (5) that produces no normal component of current density. However, they overlooked the conditions imposed on $E_t(x_t)$ by Poisson's equation and did not consider the modification (43), so that their solution of the problem is not complete. For most thin-film problems it probably suffices to follow MacDonald and Sarginson in neglecting the non-uniformity of E_t.

A further difficulty in our analysis is the use of a relaxation time τ in the Boltzmann equation even if this is a good approximation for the bulk material. If $S(\mathbf{w}_1,\mathbf{w}_2)\,d\mathbf{w}_2$ is the probability per unit time that an electron is scattered by anything other than the film surface from the state $\mathbf{w}_1$ to a state in $d\mathbf{w}_2$, the collision terms in the Boltzmann equation (8) *should* be

$$-f_1(\mathbf{w}_1)\int S(\mathbf{w}_1,\mathbf{w}_2)d\mathbf{w}_2+\int S(\mathbf{w}_2,\mathbf{w}_1)f_1(\mathbf{w}_2)d\mathbf{w}_2\,. \tag{44}$$

In the simple case of isotropic scattering, $S(\mathbf{w}_2,\mathbf{w}_1)$ is a constant if $\mathbf{w}_1$ and $\mathbf{w}_2$ lie on the same energy surface, and use of a relaxation time

$$(1/\tau)=\int S(\mathbf{w}_1,\mathbf{w}_2)d\mathbf{w}_2 \tag{45}$$

requires only that

$$\int f_1(\mathbf{w}_2)d\mathbf{w}_2=0\,. \tag{46}$$

This is trivially true in bulk material. From (14) (setting $\mathfrak{H}=0$) we see for a film that (46) holds for terms in f_1 proportional to the components of $\mathfrak{E}$ in the plane of the film (in the transformed variables) but not for the normal component. Thus with isotropic scattering use of a relaxation time is correct in calculating $\sigma_1(y_3')$ in (19), but not for $\sigma_3(y_3')$. On transforming back to the original coordinates, $\sigma_3(y_3')$ enters the expressions (29) for the conductivity in the plane of the film, so that use of a relaxation time introduces an error through this term.

To estimate the correction to $\sigma_3(y_3')$ obtained for isotropic scattering by retaining the second term in (44), we have evaluated this term using f_1 as previously evaluated in (14). Treating this term as an additional inhomogeneous term on the right of the Boltzmann equation (8), we find that for thick films the asymptotic expression (38) for $\bar{\sigma}_3/\sigma_{1B}$ becomes $[1-(3/4a)-(0.12/a)]$, whereas for thin films the correction to $\bar{\sigma}_3/\sigma_{1B}$ in (37) is of order a^2 and therefore negligible. Since $\bar{\sigma}_3$ makes a smaller contribution to μ_{eff}/μ_B than does $\bar{\sigma}_1$, especially for very thin films, we conclude that use of a relaxation time does not introduce an error of practical importance.

3. Channel conductivity in anisotropic crystals

Schrieffer[8] has calculated the effective mobility of carriers in a channel at a semiconductor surface, and Zemel[9] has extended his analysis to obtain the Hall coefficient for a magnetic field normal to the surface. Both have assumed spherical energy surfaces.

In the space-charge region at the surface, there is a strong electric field $\mathbf{E}_c$ normal to the surface. With ellipsoidal energy surfaces we may again use the transformation (7), and the space-charge field $\mathcal{E}_c=\alpha_c^{\frac{1}{2}}E_c$ remains normal to the surface in the new variables. Schrieffer's analysis is now directly applicable to the calculation of the quantity corresponding to $\sigma_1(y_3')$ in the transformed conductivity tensor (19) for the thin film. The quantity corresponding to $\sigma_3(y_3')$ may be derived in a similar way. In the special case of a constant space charge field $\mathcal{E}_c$ and constant τ, we obtain

$$s_1=1-[\exp(z^2)](1-\operatorname{erf} z)$$

$$s_3=1-[\exp(z^2)](1-\operatorname{erf} z)(1-2z^2)-2z\pi^{-\frac{1}{2}}\,, \qquad (47)$$

where $z=(e\mathcal{E}_c\tau)^{-1}(2mk_0T)^{\frac{1}{2}}$ and s_1 and s_3 correspond to $(\bar{\sigma}_1/\sigma_{1B})$ and $(\bar{\sigma}_3/\sigma_{1B})$ in the analysis of the thin film. The derivation of the actual channel conductivity in terms of these quantities now makes use of the same algebraic manipulations as in the case of a film of the same orientation, and the conductivity shows a similar anisotropy.

Calculation of the channel Hall coefficient for ellipsoidal energy surfaces would require a similar generalization of Zemel's work, with the complication that the magnetic field in the transformed variables is no longer normal to the surface.

4. Specular surface scattering

Experiments on metals have supported the view that electrons are scattered diffusely at the surface,[3] and similar conclusions for germanium have been found by Bardeen et al[18] and by Zemel and Petritz.[19] This is the boundary condition we have imposed in the derivation of Section 2. However, Koenig's recent studies of bismuth films indicate that specular surface scattering occurs in this substance at low temperatures.[20]

In a semiconductor or semi-metal, one would expect that specular surface scattering might be more appropriate if the surface is not badly disordered, so that it is of interest to consider this alternative boundary condition in the theory of films with anisotropic energy surfaces. Wave functions in a crystal must fall to zero amplitude at the crystal surface, and the Bloch-type functions that must be combined to achieve this condition must have the same phase relationship at all points of the surface. This requires that the **k**-vectors of these Bloch-type functions have the same components parallel to the surface. This condition and the requirement that the functions have the same energy define the relation between **k**-vectors corresponding to specular reflection. When the **k**-vectors so related differ by a small fraction of the reciprocal lattice constant, as within a single ellipsoid in a semiconductor, the wave function obtained by combining these Bloch-type functions has a relatively small amplitude to a depth of several lattice spacings into the crystal. An electron described by such a function is accordingly less likely to be scattered by atomic disorder at the surface than is one described by a wave function that rises in the first atomic layer or two to its bulk amplitude. Diffuse surface scattering is more likely for a metal than for a semiconductor on this account and also because the density of final states for scattering is greater for a metal. However, other differences in the scattering matrix elements may outweigh these effects.

For an ellipsoidal energy surface (1) the conditions of specular reflection lead to complicated relations between the components of the incident and reflected **k**-vectors. It is easy to show that after the transformation (7) these are equivalent to the usual relations for specular reflection with spherical energy surfaces,

$$(w_1')_i=(w_1')_r; \qquad (w_2')_i=(w_2')_r;$$

$$(w_3')_i=-(w_3')_r\,, \qquad (48)$$

whereas in (14) we use a coordinate system with its 3-axis normal to the film in the transformed coordinates. If a fraction p of the electrons incident on the surfaces at $y_3'=\pm d'$ is scattered specularly, the boundary conditions on f_1 are then [1,3]

$$f_1(u_1',u_2',u_3';-d')=pf_1(u_1',u_2',-u_3';-d')$$

$$f_1(u_1',u_2',-u_3';+d')=pf_1(u_1',u_2',u_3';+d')\,, \qquad (49)$$

where the $u_i'=(\hbar w_i'/m)$ are velocity components, and $u_3'>0$. The solution of the Boltzmann equation (8) in the absence of a magnetic field is

$$f_1=-\frac{e\tau}{k_0T}f_0\left\{(\mathfrak{E}_1'u_1'+\mathfrak{E}_2'u_2')\left[1-\frac{(1-p)\exp\left(\dfrac{-y_3'\pm d'}{\tau u_3'}\right)}{1-p\exp(\pm 2d'/\tau u_3')}\right]\right.$$
$$\left.+\mathfrak{E}_3'u_3'\left[1-\frac{(1+p)\exp\left(\dfrac{-y_3'\pm d'}{\tau u_3'}\right)}{1+p\exp(\pm 2d'/\tau u_3')}\right]\right\}, \qquad (50)$$

where we have made a simple extension of Fuchs' result[1,3] and use the same notation as in (14). A magnetic field can be treated by the iteration procedure used earlier.[21]

The further analysis for partial specular reflection proceeds precisely as with diffuse scattering, except that the integrals $\sigma_1(y_3')$ and $\sigma_3(y_3')$ in (20) and (21) are now more complicated.

In the special case of total specular reflection, p is unity and the terms in f_1 proportional to the components of $\mathfrak{E}$ parallel to the film are the same as for bulk material. However, this is not true for the term proportional to the component of $\mathfrak{E}$ normal to the film, and in the limit of very thin films ($2d' \to 0$) this term is zero. Thus in this limit $\sigma_3(y_3')$ is zero while $\sigma_1(y_3')$ has its bulk value σ_{1B}. When we transform back to the original variables as in (29) and add the contributions of the different ellipsoids we find that the effective mobility in this limit approaches a finite value less than its bulk value (40) and that this limiting value depends on the film orientation. For spherical energy surfaces, of course, we obtain $\mu_{\text{eff}} = \mu_B$ for all film thicknesses with specular scattering.

The following values of μ_{eff}/μ_B for total specular reflection are obtained for the band structure of n-germanium,[16] with $\alpha_s/\alpha_p = 19.3$, in the limit of very thin films for several orientations of the film normal **n** and the current **J**: 0.79 (**n** in [100]); 0.95 (**n** in [111]); 1.00 (**n** in [110], **J** in [$\bar{1}$ 1 0]); 0.60 (**n** in [110], **J** in [001]). The corresponding values for n-silicon, with $\alpha_s/\alpha_p = 5.1$, are 1.00, 0.87, 0.76, and 1.00, respectively.

For certain film orientations and band structures such as those of n-germanium or n-silicon, the conditions for specular reflection could be satisfied by a process in which an electron is scattered from the neighborhood of one extremum to that of another. We have neglected such intervalley processes in our derivation.

5. Determination of the effective mass ratio

The anisotropy in the conductivity of a film or channel permits an experimental determination of the ratio of the effective mass components if the nature of the surface scattering and the general features of the band structure are known. For a crystal of cubic symmetry, one needs to measure only the ratio of the conductivities in the direction of the principal axes of the conductivity tensor for a film with normal in the [110] direction,

$$\chi = \frac{\sigma[\bar{1}\ 1\ 0]}{\sigma[0\ 0\ 1]}. \tag{51}$$

If the ellipsoids have their symmetry axes along the [111] directions, as in n-germanium, we find with $\xi = \alpha_s/\alpha_p$

$$\chi = \frac{(\xi+2)[3\xi\bar{\sigma}_1 + \bar{\sigma}_1^*(\xi+2)]}{9\xi\bar{\sigma}_1 + \bar{\sigma}_1^*(\xi+2)(2\xi+1) + 2\bar{\sigma}_3(\xi-1)^2}. \tag{52}$$

Here $\bar{\sigma}_1$, $\bar{\sigma}_1^*$, and $\bar{\sigma}_3$ are the averages defined by (30) or the corresponding quantities for a channel. Both $\bar{\sigma}_1$ and $\bar{\sigma}_3$ are for the ellipsoids with $\cos\theta = (2/3)^{\frac{1}{2}}$, and $\bar{\sigma}_1^*$ is for those with $\cos\theta = 0$. For diffuse surface scattering we find in the limit of very thin films that $(\bar{\sigma}_1^*/\bar{\sigma}_1)$ approaches $[(\xi+2)/3\xi]^{\frac{1}{2}}$ and $(\bar{\sigma}_3/\bar{\sigma}_1)$ approaches zero. For total specular reflection in the same limit $(\bar{\sigma}_3/\bar{\sigma}_1) = 0$, $(\bar{\sigma}_1^*/\bar{\sigma}_1) = 1$. Thus in both cases the ratio χ approaches limiting values which depend only on the mass ratio ξ.

For the band structure of n-silicon, with ellipsoids oriented in the [100] directions, we find

$$\chi = \frac{4\bar{\sigma}_1\xi + \bar{\sigma}_3(\xi-1)^2 + \bar{\sigma}_1^*\xi(\xi+1)}{(\xi+1)(2\bar{\sigma}_1\xi + \bar{\sigma}_1^*)}, \tag{53}$$

where $\bar{\sigma}_1$ and $\bar{\sigma}_3$ are for the ellipsoids with $\cos\theta = (1/\sqrt{2})$, and $\bar{\sigma}_1^*$ is for those with $\cos\theta = 0$. For diffuse scattering we find in the limit of very thin films that $(\bar{\sigma}_1^*/\bar{\sigma}_1)$ approaches $[(\xi+1)/2\xi]^{\frac{1}{2}}$, and the other ratios have the same limiting values as for n-germanium.

One cannot distinguish between oblate and prolate ellipsoids by means of a single measurement of this sort, but measurements of the anisotropy in films of suitably different orientation will yield consistent values of ξ only if the proper choice is made for this and other general features of the band structure. The choice between specular and diffuse surface scattering will require that the effective mobility be measured as a function of decreasing film or channel thickness.

In order to observe the anisotropy predicted for the limiting case of very thin films, one would need film or channel thicknesses one-tenth or less of the length l defined by (31). Since l is 3×10^{-6} cm for electrons in germanium or silicon at room temperature, measurements on these materials must be made at low temperature, or one must use the general formula (52) or (53) for χ together with estimates of the ratios $(\bar{\sigma}_3/\bar{\sigma}_1)$ and $(\bar{\sigma}_1^*/\bar{\sigma}_1)$. Channels have been formed with thickness as small as 1×10^{-6} cm,[22,23] but the lower limit presently attainable for the thickness of uniform single crystal films is about 5×10^{-5} cm.[24]

6. Discussion

The general features of our results for the effective mobility and Hall coefficient of thin semiconductor films are in agreement as to their dependence on film thickness with the results of Fuchs, Sondheimer, and Chambers on metal films with spherical Fermi surfaces.[1-4] The anisotropy in the effective mobility arising from ellipsoidal energy surfaces is of the same character as that found for metals with diffuse surface scattering by Englman and Sondheimer.[11] The decrease in the effective mobility with specular reflection, to a finite limiting value for very thin films, and the consequent anisotropy are novel features which do not occur for spherical energy surfaces. This has been noted also by Price.[25]

It is not quantitatively quite precise, however, to describe the variation with film thickness of the effective mobility and Hall coefficient for a film with ellipsoidal energy surfaces as being the same as for spherical surfaces with an appropriate effective mass. Thus, $\sigma_3(y_3')$ usually makes an appreciable contribution to the components σ_{rr} and σ_{ss} of the conductivity tensor for ellipsoidal surfaces, as in (29), and it has a very different variation from that of $\sigma_1(y_3')$, as indicated by (37) and (38). Only $\sigma_1(y_3')$ contributes to σ_{rr} and σ_{ss} for spherical surfaces. Also, we note from Fig. 3 that (R/R_B) for thick films is slightly less than unity for some orientations, and greater than unity for others, while for spherical surfaces we find that for a semiconductor and our assumed form for τ the former is true. However, these differences are small compared with probable experimental uncertainties, so that use of the spherical model with a suitable effective mass should in practice be quite satisfactory, except of course for the case of total specular reflection.

We have found that the geometric and algebraic complications introduced by ellipsoidal energy surfaces into the theory of the electrical properties of thin films and channels can be simplified greatly by a change of variables for the **k**-vectors, position vectors, velocities, and electric and magnetic fields. This reduces the problem to one for a film with spherical energy surfaces, except that in the transformed problem the electric and magnetic fields do not have simple orientations with respect to the film. Simple extensions of previous theories permit the solution of this problem, although a minor approximation must be made in using a relaxation time. We have used the further reasonable approximation of neglecting the spatial variation of the component of the electric field normal to the film.

The anisotropy in the effective mobility, particularly in perpendicular directions on the same specimen, should permit a determination of the effective mass ratio for the carriers in a film or surface channel. Such a measurement would be of interest in order to see if the band structure of the bulk material is distorted in films or near surfaces. However, there is a complication that we have not considered that could change the predicted anisotropy, namely, an anisotropic collision time. Herring and Vogt[7] have shown that to a good approximation the current components along the different principal axes of an ellipsoid can be described as decaying with different relaxation times and that the anisotropy in τ can be appreciable for lattice scattering. A similar anisotropy for ionized impurity scattering in semiconductors was calculated by Ham.[26] Such a tensor form for τ can be included approximately in the thin-film theory by inserting the appropriate component of τ in the Boltzmann equation (8) obtained by using in the inhomogeneous term the component of the transformed electric field along the direction of one principal axis of the original ellipsoid. After solving the equation for each principal axis in turn with the different τ, the results can be combined to give the total distribution function. The algebra is straightforward but tedious.

We have suggested that specular surface scattering is more likely for semiconductors than for metals because the difference between the **k**-vectors related by the conditions for specular reflection on the occupied part of a single ellipsoid in a semiconductor is much smaller than the diameter of the Fermi surface in a metal. This has the consequence that the semiconductor wave function has a relatively small amplitude in several atomic layers beneath the surface, and consequently the probability of random scattering by surface disorder is reduced. This discussion also suggests that in a metal with a complicated Fermi surface, electrons in small pockets may be scattered specularly if the film surface is relatively perfect, while those on the main Fermi surface undergo diffuse scattering. The contribution of the latter to the conductivity of a very thin film would be suppressed, while the former would provide the principal conduction. However, if scattering occurs between different parts of the Fermi surface under specular reflection, rather than within a single pocket, the mobility of all the electrons would be reduced more nearly equally, and no such preferential conduction would occur.

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