

Simple Derivation of the Hall Anisotropy Factors for Cubic and Octahedral Constant-Energy Surfaces

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An elementary method is described for the derivation of the weak-field Hall anisotropy factor (r in $R_0=r/ne$) for the cases of cubic and octahedral energy surfaces. The magnetoconductivity approach is used (i.e., an electric field which is fixed in direction and magnitude, and a current which rotates when the magnetic field is turned on). The method simply computes the longitudinal current due to the electric field and the transverse current due to the magnetic force. The latter results entirely from carriers which drift across an edge of the energy surface, thereby changing the direction of their velocity. Then the Hall angle, Hall field, and finally the Hall coefficient are easily determined, and the results agree with the results of the much more complicated approach (the kinetic method of Shockley, McClure, and Chambers) previously used to derive the Hall anisotropy factor for these two cases.

INTRODUCTION

THIS article describes a simple method for deriving the weak-field Hall anisotropy factors for a cubic and for an octahedral constant-energy surface. By the Hall anisotropy factor we mean the quantity r in the expression for the weak-field Hall coefficient,

$$R_0=r/ne, \tag{1}$$

where n is the carrier density and e the carrier charge. We work in the metallic approximation, i.e., we compute r for the constant-energy surface at the Fermi level, and do not consider contributions from carriers on other energy surfaces.

The Hall anisotropy factor r equals $\frac{1}{2}$ for a cubic surface¹ and $\frac{2}{3}$ for an octahedral one.² These results were obtained using the method of Shockley,³ McClure,⁴ and Chambers.⁵ This method is described by Beer,⁶ and is quite mathematical and tedious. The derivation assumes that the scattering time is constant on a given energy surface. The fact that the complicated mathematics ultimately leads to the simple numbers $\frac{1}{2}$ and $\frac{2}{3}$ suggests that there should be some more elementary method of obtaining these results.

The traditional Jones-Zener⁷ series solution of the Boltzmann equation in ascending powers of the magnetic field breaks down when applied to a constant-energy surface with sharp corners. The source of the difficulty becomes clear when we consider the behavior of carriers on, for example, a cubic surface. The magnetic field causes the carriers to move along the constant-energy surface in momentum space. If they remain on one face of the surface, their velocity is unaltered by the

magnetic field; i.e., their Hall angle is zero. But for those carriers which drift across an edge of the cube, the Hall angle becomes 90° ; consequently, the weak-field approximation breaks down.

DERIVATION FOR THE CUBIC SURFACE

Figure 1 shows the cubic surface in momentum space, aligned so that its faces are parallel to the planes formed by the coordinate axes. The states are occupied within the volume bounded by the planes $p_x, p_y, p_z = \pm p$. Within the square pyramid having an apex at the origin and base $p_x = +p$ [with corners at $(p, \pm p, \pm p)$], the relation between energy and momentum is $\mathcal{E} = p_x^2/2m$. The same relation holds within the pyramidal region with base $p_x = -p$, and the corresponding relations for the pyramids with bases in the x - z and x - y planes are of course $\mathcal{E} = p_y^2/2m$ and $\mathcal{E} = p_z^2/2m$. The magnitude of the carrier velocity on all faces is $v = p_x/m = p_y/m = p_z/m = p/m$.

We now apply an electric field E along the x axis and a magnetic field H along the z axis (in the positive sense in both cases). We use the magnetoconductivity approach, i.e., we imagine a sample without transverse boundaries. Then we may keep E fixed in magnitude and direction. The current, rather than E , will rotate through the Hall angle, and will change its magnitude, when the magnetic field is turned on.

As suggested in Fig. 2, the occupied region of momentum space will then shift a certain distance along

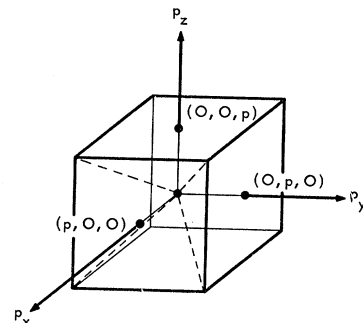


FIG. 1. The cubic energy surface at the Fermi energy in momentum space. Dashed lines show the pyramidal region, with apex at the origin and base $p_x = +p$, discussed in the text.

¹ C. Goldberg, E. Adams, and R. Davis, *Phys. Rev.* **105**, 865 (1957).

² H. Miyazawa, in *Proceedings of the Conference on the Physics of Semiconductors, Exeter* (The Institute of Physics and The Physical Society, London, 1962), p. 636.

³ W. Shockley, *Phys. Rev.* **79**, 191 (1950).

⁴ J. W. McClure, *Phys. Rev.* **101**, 1642 (1956).

⁵ R. G. Chambers, *Proc. Roy. Soc. (London)* **A238**, 344 (1957).

⁶ A. C. Beer, *Galvanomagnetic Effects in Semiconductors* (Academic Press Inc., New York, 1963), pp. 29-32 and 189-195.

⁷ H. Jones and C. Zener, *Proc. Roy. Soc. (London)* **A145**, 268 (1934).

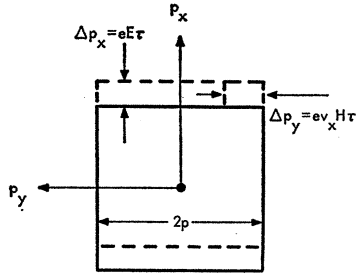


FIG. 2. Displacement of the cubic Fermi surface under the applied forces. The central sections, at $p_z=0$, of the undisplaced (solid lines) and displaced (dashed lines) surfaces are shown, as viewed from the positive z direction.

the x axis, creating a current component i_x . The distribution will also rotate under the action of H ; some of the displaced carriers will drift across the edge parallel to the z axis, thereby producing a y component of current i_y .

The total current is $i = (i_x^2 + i_y^2)^{1/2}$. Its direction with respect to the x axis is the Hall angle θ , where $\tan\theta = i_y/i_x$. Hence, as shown in Fig. 3, the Hall field E_H is $E \sin\theta$. The Hall coefficient at any H is therefore

$$R_H = \frac{E_H}{iH} = \frac{E \sin\theta}{(i_x^2 + i_y^2)^{1/2} H}. \quad (2)$$

For small θ , $\sin\theta \approx \tan\theta$ and $i \approx i_x$. Then

$$R_0 = \frac{E i_y}{i_x^2 H}. \quad (3)$$

Equation (3) is a conventional weak-field approximation, corresponding to a small *average* Hall angle, and neglecting any contribution from magnetoresistance. In the present cases, a small average value for θ means that the *number* of displaced carriers which have drifted across an edge of the constant-energy surface (thus acquiring a large Hall angle) is small compared to those displaced carriers which have not. But in what follows, we do not compute the behavior of this smaller group of carriers by using any weak-field approximation, and hence we avoid the troubles which occur when attempts are made to compute *weak-field* terms in the Jones-Zener expansion.

Next, in the usual fashion, we compute the current components from the displaced and rotated portions of the distribution, since the undisplaced distribution

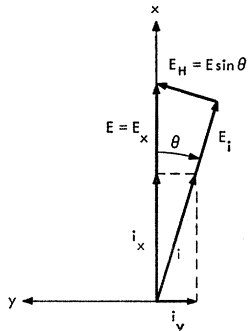


FIG. 3. Orientation of the electric field (E) and current (i) vectors in the presence of the magnetic field. The magnetic field vector, not shown, is normal to the plane of the figure, pointing toward the viewer. The components of E parallel and perpendicular to i are labeled E_i and E_H (the Hall field). The Hall angle is θ .

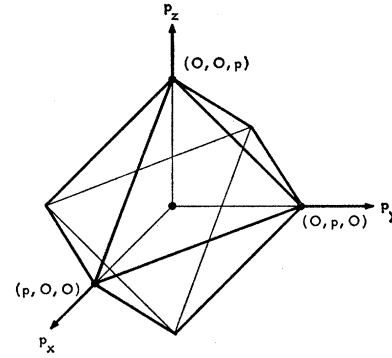


FIG. 4. The octahedral energy surface at the Fermi energy in momentum space.

corresponds to zero current. The volume V_x of the displacement in the x direction (Fig. 2) is

$$V_x = 2(2p)^2 \Delta p_x = 2(2p)^2 (eE\tau). \quad (4)$$

The first factor 2 takes care of the contributions from the volumes at $p_x = +p$ and $-p$. The portion of this displaced distribution which drifts across the edge of the surface, thus producing a current in the y direction, is

$$V_y = 2(2p) \Delta p_x \Delta p_y = 2(2p) (eE\tau) (ev_x H\tau) = 2(2p) (eE\tau) (epH\tau/m). \quad (5)$$

The corresponding current components are

$$i_j = (2/h^3) V_j ev_j, \quad j = x, y. \quad (6)$$

Thus

$$i_x = 16p^3 e^2 \tau E / h^3 m \quad (7)$$

and

$$i_y = 8p^3 e^3 \tau^2 EH / h^3 m^2. \quad (8)$$

Substituting Eqs. (7) and (8) into Eq. (3) for the weak-field Hall coefficient gives

$$R_0 = h^3 / 32ep^3. \quad (9)$$

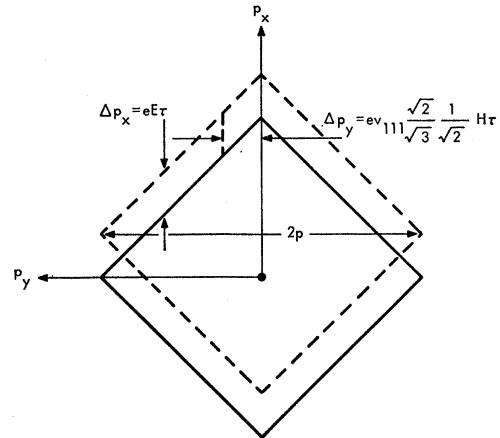


FIG. 5. Displacement of the octahedral Fermi surface under the applied forces. The central sections, at $p_z=0$, of the undisplaced (solid lines) and displaced (dashed lines) surfaces are shown, as viewed from the positive z direction.

But the carrier density n is related to the volume of occupied momentum space:

$$n = (2/h^3)(2\phi)^3; \quad (10)$$

using this relation to eliminate ϕ from Eq. (9) leads finally to

$$R_0 = 1/2ne. \quad (11)$$

Thus $r = \frac{1}{2}$ for a cubic energy surface.

THE OCTAHEDRAL SURFACE

An octahedral energy surface is sketched in Fig. 4, and the effect of the applied forces on the distribution is shown in Fig. 5. The vertices of the octahedron are located at $(\pm\phi, 0, 0)$, $(0, \pm\phi, 0)$, and $(0, 0, \pm\phi)$. Because the rectangular geometry is absent in this case, more care must be exercised, but the procedure remains straightforward. Again we put E and H in the x and z directions, respectively.

The faces of the octahedron are perpendicular to $\langle 111 \rangle$ directions. Hence the velocity parallel to any coordinate axis is $1/\sqrt{3}$ of the total velocity v_{111} on any face. The change in transverse velocity when a carrier drifts across the edges lying in the x - z plane will be $2/\sqrt{3}$ times the total velocity. There is no change in transverse velocity when carriers cross the edges lying in the y - z plane, and carriers do not drift across the edges lying in the x - y plane.

The velocity v_{111} is given by $v_{111} = \phi_{111}/m$, where ϕ_{111} is the distance of a $\{111\}$ face from the origin. This coordinate is related to the cubic axis coordinates by $\phi_{111} = (1/\sqrt{3})\phi_x$ or ϕ_y or ϕ_z . To compute the magnetic force, we need the projection of v_{111} onto the x - y plane. This projection lies in a $\langle 110 \rangle$ direction, and is given by $(\sqrt{2}/\sqrt{3})v_{111}$. The volumes V_x and V_y are conveniently computed in terms of the area of the appropriate face of the octahedron, projected onto the y - z plane, times an element of length in the x direction, rather than in terms of the area of the constant-energy surface, times an element of length normal to it.

Proceeding as in the cubic case,

$$V_x = 2(\sqrt{2}\phi)^2(eE\tau), \quad (12)$$

$$\begin{aligned} V_y &= 2(2\phi)(eE\tau) \left(e v_{111} \frac{\sqrt{2}}{\sqrt{3}} \frac{1}{\sqrt{2}} H\tau \right) \\ &= 2(2\phi)(eE\tau)(e\phi H\tau/3m). \end{aligned} \quad (13)$$

The current components are

$$\begin{aligned} i_x &= (2/h^3)(4\phi^2)(eE\tau)(e)(v_{111}/\sqrt{3}) \\ &= 8\phi^3 e^2 \tau E / 3h^3 m, \end{aligned} \quad (14)$$

$$\begin{aligned} i_y &= (2/h^3)(4\phi)(eE\tau)(e\phi H\tau/3m)(e)(2v_{111}/\sqrt{3}) \\ &= 16\phi^3 e^3 \tau^2 EH / 9h^3 m^2. \end{aligned} \quad (15)$$

Again substituting the current components into Eq. (3) for the weak-field Hall coefficient,

$$R_0 = (h^3/4e\phi^3). \quad (16)$$

Since half the volume of the octahedron is $\frac{1}{3}$ of the product of the area of a central cross section and the perpendicular distance to the appropriate vertex,

$$n = (2/h^3)(\frac{2}{3})\phi(2\phi^2); \quad (17)$$

using this, as before, to eliminate ϕ from Eq. (16) gives

$$R_0 = 2/3ne. \quad (18)$$

Thus for an octahedral surface, $r = \frac{2}{3}$.

CONCLUSIONS

We have derived in an elementary fashion the weak-field Hall anisotropy factor for two cases of constant-energy surfaces bounded by plane surfaces, a cube and an octahedron. These were chosen because they had been derived previously by a much more complicated method, and because they are surfaces which approximate those in actual materials. The cube is not very different from the heavy-mass valence band in Ge,¹ and the octahedron resembles the hole band in W which is centered on the point H in the bcc Brillouin zone.⁸

We intend to extend this simple technique to other cases of interest in a later publication. So far as we know, the value $r = \frac{1}{2}$ for a cube is the largest deviation from $r = 1$ (for a sphere) for any single, cubically symmetric surface. We would like to find out what general shapes of surfaces might lead to larger deviations. We also intend to investigate examples of multi-valley models, and models in which the Fermi surface has necks extending to the boundaries of the Brillouin zone.

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⁸ L. F. Mattheiss, Phys. Rev. **139**, A1893 (1965).