Magnetoresistance in a Multivalley Model with ⟨110⟩-Ellipsoids of General Shape

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(Received April 13, 1959)

Expressions are derived for the three weak-field magnetoresistance coefficients, b, c, and d, using a multivalley model having ellipsoids of general shape along the ⟨110⟩ directions in k space. The results are given in terms of statistical and scattering integrals and of the two mass ratios K and L needed to specify the relative values of the three effective-mass components characterizing the ellipsoids. The properties of b, c, and d as functions of K and L are discussed, including in particular the fact that the symmetry conditions which are appropriate for each of the three ellipsoid-of-revolution models are satisfied along certain lines in the K-L plane.

INTRODUCTION

THE galvanomagnetic properties of the three cubically symmetric multivalley models having constant-energy surfaces which are ellipsoids of revolution along the ⟨100⟩, ⟨110⟩, and ⟨111⟩ directions in k space have been previously investigated.[1-4] However, cubic symmetry does not require ellipsoids of revolution (hereafter abbreviated EOR) for the ⟨110⟩ model, but only that the principal axes of each ellipsoid lie in certain directions which do not violate the restrictions imposed by the reflection planes on which the ellipsoid is centered. For example, the ellipsoid in the first quadrant of the k_x-k_y plane has principal axes (see Fig. 1) in the [00$\bar{1}$], [$\bar{1}$10], and [110] directions. (The particular sense chosen for each axis establishes a specific right-handed coordinate system which will be used later.) The purpose of this paper is to investigate the weak-field magnetoresistance of this generalized ⟨110⟩ model, and to compare the results with the simple band model (spherical energy-surfaces) and with the three EOR models.

In a weak magnetic field we may write

$$\frac{\Delta\rho}{\rho_0}=M_{\alpha\beta\gamma}^{\delta\epsilon\zeta}\frac{\mu_H^2H^2}{c'^2}, \tag{1}$$

where $\Delta\rho/\rho_0$ is the fractional change in the zero-field resistivity ρ_0, μ_H is the Hall mobility ($\mu_H=R/\rho_0$), R is the Hall coefficient, H is the magnetic field strength, $M_{\alpha\beta\gamma}^{\delta\epsilon\zeta}$ is a dimensionless proportionality constant, and c' is a factor having the dimensions $\mu_H H$ and a magnitude which depends upon the system of units used. In emu, Gaussian, and practical units, $c'=1$, 3×10^{10} cm/sec, and 10^8 cm^2-gauss/v-sec, respectively. The subscript and superscript of $M_{\alpha\beta\gamma}^{\delta\epsilon\zeta}$ indicate, respectively, the direction of the sample current and of the magnetic field relative to the cubic axes of the crystal. A weak field implies $(\mu_H H/c')\ll1$. From an expression of Seitz[5] which is valid to second order in magnetic field for any cubically-symmetric crystal model, it may be shown[6] that

$$\mathbf{E}=\rho_0\left[\mathbf{I}+a(\mathbf{I}\times\mathbf{H})+b\frac{\mu_H^2H^2}{c'^2}\mathbf{I}+c\frac{\mu_H^2}{c'^2}\mathbf{I}\cdot\mathbf{HH}+d\frac{\mu_H^2}{c'^2}\mathcal{T}\mathbf{I}\right], \tag{2}$$

and

$$M_{\alpha\beta\gamma}^{\delta\epsilon\zeta}=b+c\left(\textstyle\sum_j \iota_j\eta_j\right)^2+d\left(\textstyle\sum_j \iota_j^2\eta_j^2\right). \tag{3}$$

In Eq. (2), $\mathbf{E}$, $\mathbf{I}$, and $\mathbf{H}$ are the electric field, current density, and magnetic field strength, respectively, and $\mathcal{T}$ is a diagonal tensor in the cubic-axis system of the crystal whose elements are the squares of the magnetic field components. In the same coordinate system the ι_j and η_j of Eq. (3) are the direction cosines of the current and magnetic field vectors. The parameters b, c, and d used here differ from those of Seitz in that the factor $(\mu_H/c')^2$ has been removed, thus making them dimensionless.

The aim of the calculation presented here is to obtain expressions for b, c, and d. It seems particularly desirable to express the results in terms of these three quantities, since then any magnetoresistance coefficient is immediately obtainable by using Eq. (3). Expressions for b, c, and d for the three EOR models have been summarized elsewhere.[7]

THE MODEL

The model is based on the following assumptions:

1. Only one type of carrier is present.
2. The band edge occurs at 12 equivalent points along the ⟨110⟩ directions in k space.

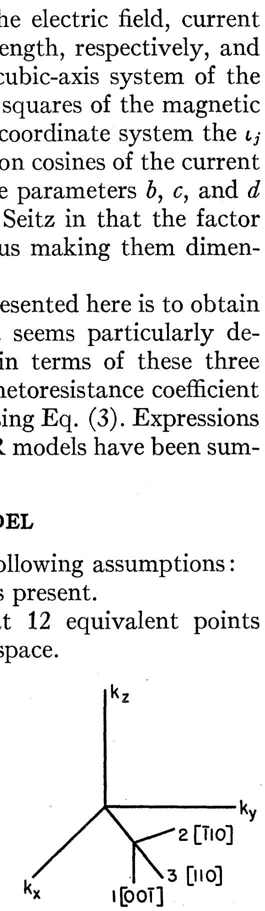

FIG. 1. The principal axes 1, 2, and 3 for the ellipsoid in the first quadrant of the k_x-k_y plane, where k_x, k_y, and k_z are the axes of cubic symmetry of the crystal.

[1] B. Abeles and S. Meiboom, Phys. Rev. **95**, 31 (1954).
[2] M. Shibuya, Phys. Rev. **95**, 1385 (1954).
[3] C. Herring, Bell System Tech. J. **34**, 237 (1955).
[4] C. Herring and E. Vogt, Phys. Rev. **101**, 944 (1956).
[5] F. Seitz, Phys. Rev. **79**, 372 (1950).
[6] G. L. Pearson and H. Suhl, Phys. Rev. **83**, 768 (1951).
[7] R. S. Allgaier, Phys. Rev. **112**, 828 (1958).

3. Near a band edge, the energy $\mathcal{E}$ can be approximated by an ellipsoidal function of $\mathbf{k}$ (the wave vector of the charge carrier relative to its value at the band edge) which in the principal-axis system is

$$\mathcal{E}=\pm\frac{\hbar^2}{2}\left(\frac{k_1^2}{m_1}+\frac{k_2^2}{m_2}+\frac{k_3^2}{m_3}\right), \tag{4}$$

where the m's are the effective masses along the coordinate axes 1, 2, and 3 of the ellipsoid.

4. At a fixed temperature, the scalar scattering time τ depends on the energy only. This condition may be generalized to a τ which is a diagonal tensor in the principal-axis system, so long as all components have the same energy dependence, merely by replacing each m_i in the result by m_i/τ_i, where τ_i is the corresponding tensor component of τ.[4]

THE CALCULATION

We consider first the effects from a single ellipsoid. The jth component of the current density from one ellipsoid may be written

$$i_j=\sigma_{jk}E_k+\sigma_{jkl}E_kH_l+\sigma_{jklm}E_kH_lH_m, \tag{5}$$

if terms of higher power than E and H^2 are neglected. (Summation over a repeated index is implied in this and all subsequent equations.) By solving Boltzmann's equation, the current density may also be expressed as an integral over k space of a function of $\mathcal{E}$, τ, $\mathbf{E}$, $\mathbf{H}$, the carrier charge q, the unperturbed carrier energy distribution f_0, and the effective mass components m_i.[1] Comparison of this expression with Eq. (5) yields (in the principal-axis coordinate system of the ellipsoid)

$$\sigma_{jj}=\frac{-a}{m_j^2}\int_0^\infty J_j\tau\frac{\partial f_0}{\partial\mathcal{E}}d\mathcal{E}, \tag{6}$$

$$\sigma_{jkl}=\frac{-ab\epsilon_{ljk}}{m_j^2m_k}\int_0^\infty J_j\tau^2\frac{\partial f_0}{\partial\mathcal{E}}d\mathcal{E}, \tag{7}$$

and

$$\sigma_{jklm}=\frac{-ab^2\epsilon_{mjs}\epsilon_{lsk}}{m_j^2m_km_s}\int_0^\infty J_j\tau^3\frac{\partial f_0}{\partial\mathcal{E}}d\mathcal{E}, \tag{8}$$

where J_j is the integral over a constant-energy surface in k space

$$J_j=\int_S\frac{\hbar^3k_j^2dS}{[(k_1/m_1)^2+(k_2/m_2)^2+(k_3/m_3)^2]^{\frac{1}{2}}}, \tag{9}$$

and $a=q^2/4\pi^3\hbar^3$, $b=q/c'$ (q may be positive or negative), and the ϵ_{jkl} are zero except for

$$\begin{gathered}\epsilon_{123}=\epsilon_{231}=\epsilon_{312}=1,\\ \epsilon_{213}=\epsilon_{132}=\epsilon_{321}=-1.\end{gathered} \tag{10}$$

The choice of the principal-axis coordinate system reduces the 9 possible nonzero σ_{jk} to 3 ($j=k$), the 27 σ_{jkl} to 6 ($j\neq k\neq l\neq j$), and the 81 σ_{jklm} to 12 (6 σ_{jjkk} and 6 σ_{jkjk}). The surface integral is

$$J_j=2^{7/2}3^{-1}\pi(m_1m_2m_3)^{1/2}m_j\mathcal{E}^{3/2}=Fm_j\mathcal{E}^{3/2}. \tag{11}$$

Then Eqs. (7), (8), and (9) become

$$\sigma_{jj}=-\frac{aF}{m_j}G_1, \tag{12}$$

$$\sigma_{jkl}=-\frac{abF\epsilon_{ljk}}{m_jm_k}G_2, \tag{13}$$

and

$$\sigma_{jklm}=-\frac{ab^2F\epsilon_{mjs}\epsilon_{lsk}}{m_jm_km_s}G_3, \tag{14}$$

where

$$G_n=\int_0^\infty\tau^n\mathcal{E}^{\frac{3}{2}}\frac{\partial f_0}{\partial\mathcal{E}}d\mathcal{E}. \tag{15}$$

All of the nonzero conductivity tensor components from a single ellipsoid are listed in Appendix A. The components of the tensors of each rank differ from one another by factors which are combinations of the mass ratios

$$K=m_3/m_1 \quad\text{and}\quad L=m_2/m_1. \tag{16}$$

The mass component m_i lies along the ith principal axis of the ellipsoid, and the principal axes 1, 2, and 3 of the ellipsoid in the first quadrant of the k_x-k_y plane of the crystal are in the $[00\bar{1}]$, $[\bar{1}10]$, and $[110]$ directions, respectively (see Fig. 1). Thus $L=1$ corresponds to equal transverse masses, and K is the ratio of a longitudinal to a transverse mass, a quantity which has generally been used in the past as a parameter to describe the EOR models.

The jth component of the current density due to all the ellipsoids may be written

$$I_j=\Sigma_{jk}E_k+\Sigma_{jkl}E_kH_l+\Sigma_{jklm}E_kH_lH_m. \tag{17}$$

In order to seek the minimum number of distinct terms, Eq. (17) is referred to the cubic axes of the crystal. The quantity I_j is obtained by adding the i_j from each ellipsoid, after having transformed each i_j to the cubic axis coordinate system of Eq. (17). The necessary transformation matrices are described in Appendix B. The results are

$$\Sigma_{jj}=-\frac{2aFG_1}{m_1}\left(1+\frac{1}{K}+\frac{1}{L}\right), \tag{18}$$

$$\Sigma_{jkl}=-\frac{2abFG_2}{m_1^2}\left(\frac{1}{K}+\frac{1}{KL}+\frac{1}{L}\right)\epsilon_{jkl}, \tag{19}$$

$$\Sigma_{jjjj}=\frac{ab^2FG_3}{m_1^3}\left(\frac{1}{K^2}-\frac{2}{KL}+\frac{1}{L^2}\right), \tag{20}$$

$$\Sigma_{jjkk}=\frac{ab^2FG_3}{m_1^3}\left[\frac{1}{KL^2}+\frac{1}{LK^2}+\frac{1}{K}+\frac{1}{L}+\frac{1}{KL}+\frac{1}{2}\left(\frac{1}{K^2}+\frac{1}{L^2}\right)\right], \tag{21}$$

and

$$\Sigma_{jkjk}+\Sigma_{jkkj}=-\frac{ab^2FG_3}{m_1{}^3}\left(\frac{1}{K^2}+\frac{4}{KL}+\frac{1}{L^2}\right). \tag{22}$$

The terms Σ_{jkjk} and Σ_{jkkj} are written together because they are the coefficients of the same combination of components of **E** and **H** and have no separate physical significance.

We next express the conductivity components in terms of the resistivity components defined by

$$E_j=\Lambda_{jk}I_k+\Lambda_{jkl}I_kH_l+\Lambda_{jklm}I_kH_lH_m. \tag{23}$$

The Λ's may be expressed in terms of the Σ's (see Eq. 3.29, reference 1). When this is done, and the result is compared with Eq. (2), we obtain b, c, and d in terms of a statistical and scattering factor and the mass ratios K and L. The relationships are

$$b=\left\{\frac{G_1G_3}{2G_2{}^2}\frac{(KL+K+L)}{(K+L+1)^2}\left[6+\frac{(K-1)^2}{K}+\frac{(L-1)^2}{L}+\frac{1}{2}\frac{(K-L)^2}{KL}\right]-1\right\}, \tag{24}$$

$$c=\left\{\frac{G_1G_3}{2G_2{}^2}\frac{(KL+K+L)}{(K+L+1)^2}\left[-6-\frac{(K-L)^2}{KL}\right]+1\right\}, \tag{25}$$

$$d=\left\{\frac{G_1G_3}{2G_2{}^2}\frac{(KL+K+L)}{(K+L+1)^2}\left[-\frac{(K-1)^2}{K}-\frac{(L-1)^2}{L}+\frac{3}{2}\frac{(K-L)^2}{KL}\right]\right\}. \tag{26}$$

DISCUSSION

Before discussing the expressions for b, c, and d, we will quote briefly some pertinent results for the simple band model and for the three EOR models. For each EOR model there is a symmetry condition which relates b, c, and d, regardless of the scattering law, the statistics, or K, the ratio of longitudinal to transverse mass. There are also restrictions on the signs of $b+c$ and d. These features are summarized in Table I. When $K=1$, all three EOR models reduce to the simple band model with spherical energy-surfaces. The properties of the simple band model are also listed in Table I.

An inspection of Eqs. (24)–(26) shows that they are not affected by exchanging K and L. This may be explained by considering the effect on the ellipsoid whose principal axes are shown in Fig. 1. Interchanging K and L interchanges the axes 2 and 3; i.e., the ellipsoid is rotated 90° about its 1-axis. However, the other three ellipsoids in the k_x-k_y plane are each rotated 90° about parallel axes, and the net effect is to exchange their orientations, pair by pair. The calculation presented here recognizes ellipsoid orientation, but not position. The position of an ellipsoid would appear in the mean free time τ if intervalley scattering were considered. Then τ would be influenced by the magnitude of the wave number of the intervalley phonon, which would depend on the separation of the valleys in k space. We have assumed a τ which depends most generally on the energy and wave number of the charge carrier relative to an individual ellipsoid. Thus no effect at all can result from exchanging ellipsoid orientations, and this model therefore reduces to the ⟨110⟩-EOR model not only when $L=1$, but also when $K=1$, and the symmetry condition $b+c-d=0$ holds along these two lines in the K-L plane.

TABLE I. Behavior of the weak-field magnetoresistance coefficients b, c, and d for the simple band model and for the three ellipsoid-of-revolution models.

Model	Symmetry relation	$b+c$	d
Simple band model	$\cdots$	0	0
⟨100⟩ EOR	$b+c+d=0$	>0	<0
⟨110⟩ EOR	$b+c-d=0$	>0	>0
⟨111⟩ EOR	$b+c=0$	0	>0

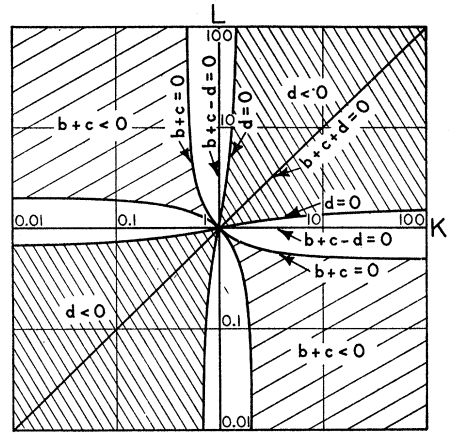

FIG. 2. Relations among the weak-field coefficients as a function of the mass ratios $K=m_3/m_1$ and $L=m_2/m_1$. The quantity $b+c$ is negative only in the lightly shaded regions and d is negative only in the more darkly shaded regions.

We consider next the line $K=L$. Inspection of Eqs. (24), (25), and (26) reveals that in this case $b+c+d=0$; this is the symmetry condition appropriate for the ⟨100⟩-EOR model. This result may also be explained with the aid of Fig. 1. The condition $K=L$ implies that $m_2=m_3$; i.e., the ellipsoid has become an EOR with its symmetry axis parallel to a cubic axis of the crystal. Again, since only the orientation of the ellipsoids is significant, this situation is indistinguishable from the ⟨100⟩-EOR model. We wish to emphasize at this point that in the cases discussed thus far, not only are the symmetry conditions for the appropriate EOR models satisfied, but the expressions for b, c, and d individually reduce to those for the simpler models.

Figure 2 plots the K-L plane on a log-log scale, and illustrates the special situations just described, as well as some additional features which are perhaps more surprising. It shows, first of all, that there are also lines in the K-L plane along which $b+c=0$, the condition appropriate for the $\langle 111\rangle$-EOR model. These lines are

$$K=2-L \quad \text{and} \quad (1/K)=2-(1/L). \tag{27}$$

It is clear that no $\langle 110\rangle$ ellipsoid can reduce to a $\langle 111\rangle$ EOR (except for the trivial case $K=L=1$). The expressions for b, c, and d do not reduce to the simpler model in this case. Note from Fig. 2 that the lines $b+c=0$ are actually boundaries between regions where $b+c$ is positive and negative. A negative $b+c$ does not occur for any of the EOR models.

What other conditions of the type $b+c+nd=0$ may be satisfied in the K-L plane? It is easily shown that n is of the form

$$n=(1-x)/(1-3x), \tag{28}$$

where x is a function of K and L and may take on any non-negative value. Therefore, any value of n, positive or negative, may occur except $\frac{1}{3}<n<1$. This exclusion may be linked to the requirement that no longitudinal magnetoresistance coefficient be negative.

Another feature shown in Fig. 2 is the existence of $d=0$ lines in the K-L plane. These are

$$K=[-(L^2-L+1)\pm(L-1)(L^2+6L+1)^{\frac{1}{2}}]/(2L-3). \tag{29}$$

Along these lines, the magnetoresistance becomes isotropic in the sense that the magnetoresistance depends only on the angle between the directions of current and magnetic field, but does not depend on the orientation of the current and magnetic field relative to the cubic axes of the crystal. This is never true for the three EOR models except when they all degenerate to the simple band model with spherical energy-surfaces.

CONCLUSION

We have derived expressions for the weak-field magnetoresistance coefficients b, c, and d for a $\langle 110\rangle$ multivalley-model with ellipsoids of general shape. We find that the condition $b+c+nd=0$ is satisfied along some line in the K-L plane so long as n lies outside the range $\frac{1}{3}<n<1$. This therefore includes the conditions $b+c+d=0$, $b+c-d=0$, and $b+c=0$ which are appropriate for the $\langle 100\rangle$, $\langle 110\rangle$, and $\langle 111\rangle$ ellipsoid-of-revolution models, respectively. We also find that along certain lines in the K-L plane, magnetoresistance depends only on the angle between the current and magnetic field.

The fact that the symmetry conditions for any of the ellipsoid-of-revolution models may be satisfied by a general $\langle 110\rangle$-model does not necessarily mean that the occurrence of these special symmetry conditions may no longer be interpreted as suggesting a particular ellipsoid-of-revolution model. Any material having the band structure described in this paper may satisfy an infinite variety of symmetry conditions, and it is therefore very improbable that it will satisfy one of the two which are appropriate for the $\langle 100\rangle$ and $\langle 111\rangle$ ellipsoid-of-revolution models.

ACKNOWLEDGMENT

I am indebted to Dr. Frank Stern for many valuable discussions of this problem.

APPENDIX A

Evaluation of Eqs. (12), (13), and (14) leads to the following nonzero conductivity tensor components:

$$\begin{aligned}\sigma_{11}&=-(aF/m_1)G_1,\\ \sigma_{22}&=(1/L)\sigma_{11},\\ \sigma_{33}&=(1/K)\sigma_{11},\end{aligned} \tag{A1}$$

$$\begin{aligned}\sigma_{123}&=-\sigma_{213}=-(abF/m_1m_2)G_2,\\ \sigma_{231}&=-\sigma_{321}=(1/K)\sigma_{123},\\ \sigma_{312}&=-\sigma_{132}=(L/K)\sigma_{123},\end{aligned} \tag{A2}$$

and

$$\begin{aligned}&\sigma_{1122}=(ab^2F/m_1^2m_3)G_3,\\ &\sigma_{1133}=(K/L)\sigma_{1122},\\ &\sigma_{2233}=(K/L^2)\sigma_{1122},\\ &\sigma_{2211}=(1/L^2)\sigma_{1122},\\ &\sigma_{3311}=(1/KL)\sigma_{1122},\\ &\sigma_{3322}=(1/K)\sigma_{1122},\\ &\sigma_{1212}=\sigma_{2121}=\sigma_{1313}=\sigma_{3131}=\sigma_{2323}=\sigma_{3232}=-(1/L)\sigma_{1122}.\end{aligned} \tag{A3}$$

APPENDIX B

The transformation matrix of the transformation from the ellipsoid axes of Fig. 1 to the crystal axes is

$$\begin{array}{c|ccc} & 1 & 2 & 3\\ \hline k_x & 0 & -1/\sqrt{2} & 1/\sqrt{2}\\ k_y & 0 & 1/\sqrt{2} & 1/\sqrt{2}.\\ k_z & -1 & 0 & 0\end{array} \tag{B1}$$

The other five matrices may be obtained by writing down the rows k_x, k_y, and k_z of the matrix (B1) in the following arrangements, with changes of sign as indicated:

$$\begin{array}{ccccc} k_z & k_y & -k_y & k_z & k_x\\ k_x & k_z & k_x & -k_y & k_z.\\ k_y & k_x & k_z & k_x & -k_y\end{array} \tag{B2}$$