Galvanomagnetic Investigation of the Fermi Surface of Magnesium*

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The galvanomagnetic properties of several single-crystal specimens of magnesium have been investigated. The results of this investigation are presented and a Fermi surface topology consistent with the data is discussed. Many of the detailed features of the galvanomagnetic properties are found to result from the effects of magnetic breakdown. The magnetic breakdown associated with the "giant orbit" which Priestley observed in his pulsed-field de Haas-van Alphen study of magnesium is found to be complete for magnetic-field strengths of 5400 G. An open orbit whose net direction is parallel to the hexagonal axis is observed for magnetic-field strengths as large as 70 kG. This orbit probably results from magnetic breakdown across three different energy gaps.

1. INTRODUCTION

DURING the past few years a great deal of experimental and theoretical work has been performed in an attempt to understand the electronic band structure of metals. Various experimental techniques have been used to obtain different types of information about the band structures. The de Haas-van Alphen effect has been used to measure extremal cross-sectional areas of the Fermi surfaces, cyclotron resonance to measure cyclotron masses, magnetoacoustic resonance to determine calipers, the anomalous skin effect to measure total surface area, and the galvanomagnetic effects to determine the general topological properties. A reasonably complete understanding of the electronic band structure of any given metal necessitates a thorough experimental investigation of all of the above properties. The electronic band structure of some metals has been computed by determining the effective potential which acts on the conduction electrons. The results of these band calculations indicate that in many cases the electrons' energy as a function of their k vectors behaves as if they were nearly free. Magnesium is one of the metals for which this is found to be true.

Falicov[1] carried out extensive band calculations for magnesium, the results of which yielded a model for the Fermi surface which was in good qualitative agreement with that constructed by Harrison[2] using the single orthogonalized plane wave (OPW) method for an ideal hexagonal close-packed divalent metal. Although the de Haas-van Alphen data of Gordon *et al.*,[3] and Priestley[4] and the anomalous skin-effect data of Fawcett[5] have been found to be highly compatible with Falicov's model, the limited data available for the galvanomagnetic properties of magnesium[6] suggested a Fermi surface topology which appeared to be incompatible with it. For this reason, we have undertaken a detailed investigation of the galvanomagnetic properties of magnesium. The results of this investigation are presented in this paper and a Fermi surface topology consistent with the data is discussed.[7]

2. THEORY OF THE GALVANOMAGNETIC EFFECTS

Recent papers by Lifshitz, Azbel, and Kaganov,[8] and by Lifshitz and Peschanskii[9] have shown that an investigation of the low-temperature galvanomagnetic properties of a metal single crystal can, in the limit of high magnetic-field strengths and sample purity, yield information about the topology of the Fermi surface of the metal. In particular, such an investigation can reveal the presence of open sections of the Fermi surface which can give rise in the presence of a magnetic field to electron trajectories that are infinitely extended in momentum space. This theory has been worked out in considerable detail for the particular case of transverse magnetoresistance.

The work of Refs. 8 and 9 above and later papers by Alekseevski *et al.*[10] and Fawcett[11] show that there is an important qualitative difference between the high-field transverse magnetoresistance of an odd-valent metal such as Cu, Ag, or Al and that of an even-valent metal such as Mg, Zn, or Sn. For the former group of metals the magnetoresistance tends to saturate in high magnetic fields except for those directions of the magnetic

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[1] L. M. Falicov, Phil. Trans. Roy. Soc. (London) **A255**, 55 (1962).
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[3] W. L. Gordon, A. S. Joseph, and T. G. Eck, *The Fermi Surface*, edited by W. A. Harrison and M. B. Webb (John Wiley & Sons, Inc., New York, 1960), p. 84.
[4] M. G. Priestley, thesis, University of Cambridge, England, 1961; Proc. Roy. Soc. (London) (to be published).
[5] E. Fawcett, J. Phys. Chem. Solids **4**, 320 (1961).
[6] N. E. Alekseevskii and Yu P. Gaidukov, Zh. Eksperim. i Teor. Fiz. **38**, 1720 (1960) [translation: Soviet Phys.—JETP **11**, 1242 (1960)].
[7] For a preliminary report of this work see R. W. Stark, T. G. Eck, W. L. Gordon, and F. Moazed, Phys. Rev. Letters **8**, 360 (1962).
[8] I. M. Lifshitz, M. I. Azbel, and M. I. Kagonov, Zh. Eksperim. i Teor. Fiz. **31**, 63 (1956) [translation: Soviet Phys.—JETP **4**, 41 (1957)].
[9] I. M. Lifshitz and V. G. Peschanskii, Zh. Eksperim. i Teor. Fiz. **35**, 1251 (1958) and **38**, 188 (1960) [translations: Soviet Phys.—JETP **8**, 875 (1959) and **11**, 137 (1960)].
[10] N. E. Alekseevskii, Yu. P. Gaidukov, I. M. Lifshitz, and V. G. Peschanskii, Zh. Eksperim. i Teor. Fiz. **39**, 1201 (1960) [translation: Soviet Phys.—JETP **12**, 837 (1961)].
[11] E. Fawcett, Phys. Rev. Letters **6**, 534 (1961).

field, H, which give rise to electron trajectories on the Fermi surface that are infinitely extended in momentum space. For the latter group of metals, nonsaturation of the magnetoresistance is the general rule even for those directions of H which do not give rise to such extended electron trajectories. It is only in special situations that saturation occurs for even-valent metals. Thus, it is apparent that the important basic difference between an investigation of the transverse magnetoresistance of an odd-valent metal and that of an even-valent metal lies in the fact that the significant magnetic-field directions for the former are those for which nonsaturation of the magnetoresistance is observed, while for the latter the significant directions are those for which there is saturation of the magnetoresistance.

Reference 10 treats in considerable detail the qualitative effects of Fermi surface topology on the transverse magnetoresistance and allows us to draw the following conclusions for an even-valent metal:

(1) If, for a specific direction of H, all electron trajectories on the Fermi surface close within one or more cells of the reciprocal lattice in such a manner that there is volume compensation of the "electrons" and "holes" ($V_1=V_2$), the resistivity ρ ($\rho=E\|J/J$, where $E\|J$ is the component of the electric field E parallel to the current density J) is proportional to H^2 in the high-field limit. The definitions of V_1 and V_2 in terms of integrals over the Fermi surface are given in Eq. (25) of Ref. 8. For $V_1=V_2$, the Hall coefficient R is a constant but has no simple physical interpretation.

(2) If, for a specific direction of H, all electron trajectories on the Fermi surface close within one or more cells of the reciprocal lattice in such a fashion as to destroy volume compensation ($V_1\neq V_2$), then the resistivity ρ will reach saturation in the high-field limit. This can result from the geometry of the Fermi surface or it can result from a change in connectivity such as occurs with magnetic breakdown[12–14] across energy gaps which separate the various sheets of the Fermi surface. If magnetic breakdown occurs, the electron trajectories will be essentially those of a free electron in the vicinity of the energy gap. If the energy gap separates two bands of like character, i.e., both hole or both electron, magnetic breakdown will not destroy volume compensation, since the orbits on the combined bands will close with the hole or electron character of the individual bands. However, if the energy gap separates two bands of opposite character, that is, one hole band and one electron band, the electron or hole character of the orbits which pass through the regions of magnetic breakdown can be such as to destroy volume compensation. For $V_1\neq V_2$, the Hall coefficient is constant and is given by

$$R=h^3/[2ec(V_1-V_2)],$$

where h is Planck's constant, e is the charge on the electron, and c is the speed of light.

(3) If, for a given direction of H, there exists a layer of open trajectories with a single average direction, then in the high-field limit, $\rho=A+BH^2\cos^2\gamma$, where A and B are constants and γ is the angle between J and the open orbit direction in reciprocal space. When the thickness of the layer of open trajectories is small, there is an important qualitative difference between the magnitude of A for an odd-valent metal and that for an even-valent metal. For an odd-valent metal A will be of the same order of magnitude as the saturation value of the magnetoresistance when only closed orbits are present on the Fermi surface. For an even-valent metal, as the thickness of the layer of open trajectories goes to zero ρ saturates if H is approaching a direction for which $V_1\neq V_2$, but ρ approaches CH^2 if H is approaching a direction for which $V_1=V_2$. [See Eq. (8) of Ref. 10 and the discussion following it.] Thus, for the latter situation ($V_1=V_2$), with experimentally attainable magnetic-field strengths and sample purities, a very small band of open trajectories will not cause ρ to saturate when $\gamma=\pm\frac{1}{2}\pi$ because the "constant" A will not reach saturation at these field strengths. However, the presence of the small band of open trajectories will produce either a sharp extremum or a sharp kink in the magnetoresistance rotation pattern.[10] For a layer of open trajectories with a single average direction, the Hall coefficient is again constant but has no simple physical interpretation.

(4) If, for a given direction of H, there exist layers of open trajectories with *different* average directions the magnetoresistance will saturate in the high-field limit. The Hall coefficient is not constant in this case but is proportional to $1/H^2$.

For an even-valent metal the magnetoresistance can saturate for cases 2, 3, and 4. While it is necessary to know all of the directions of H which produce saturation of the magnetoresistance it is also necessary to know which case (i.e., 2, 3, or 4) is pertinent for a given direction of H. Case 4 behavior can be distinguished by an investigation of the Hall coefficient, since this is the only case where R is proportional to $1/H^2$. Reference 10 illustrates the use of current "rotation" diagrams to determine whether saturation of the magnetoresistance is associated with lack of volume compensation (case 2) or with open trajectories with a single average direction (case 3). If the saturating magnetoresistance is the result of case-2 behavior, the Hall coefficient will yield the value of the quantity, V_1-V_2.

3. FERMI SURFACE OF MAGNESIUM

Falicov's Fermi surface,[1] as modified by Cohen and Falicov, to take into account the effects of spin-orbit coupling[15,16] and magnetic breakdown,[12] is, in essence,

[12] M. H. Cohen and L. M. Falicov, Phys. Rev. Letters **7**, 231 (1961).
[13] E. I. Blount, Phys. Rev. **126**, 1636 (1962).
[14] A. B. Pippard, Proc. Roy. Soc. (London) **A270**, 1 (1962).
[15] M. H. Cohen and L. M. Falicov, Phys. Rev. Letters **5**, 544 (1960).
[16] L. M. Falicov and M. H. Cohen, Phys. Rev. **130**, 92 (1963).

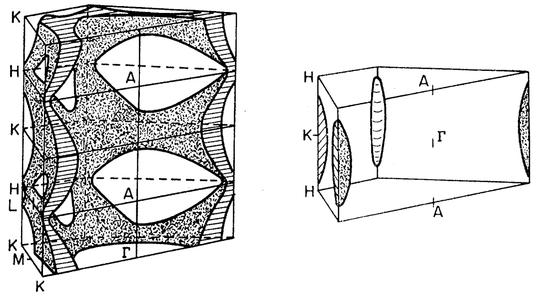


FIG. 1. Portions of Falicov's model for the Fermi surface of magnesium. (a) The second-band hole surface (the "monster"). (b) "cigar" portions of the third-band electron surface.

a single OPW model[2] modified by extensive band calculations. The surface, portions of which are shown in Figs. 1(a) and 1(b), consists of several closed sheets in the first, third, and fourth bands plus a multiply connected hole sheet in the second band [Fig. 1(a)]. Only the second-band hole sheet can give rise to open trajectories in the absence of magnetic breakdown. Its connectivity parallel to the hexagonal axis is the result of a small spin-orbit interaction.[15,16] The neglect of such small terms leads to the more familiar double-zone scheme Fermi surface which does not support open trajectories along the hexagonal axis. The cigar-shaped portions of the Fermi surface in the third band are shown in Fig. 1(b). These portions of the surface are closed and cannot, under normal circumstances, support open trajectories.

The giant orbit which Priestley[4,17] observed during his high-field de Haas-van Alphen study of magnesium has been attributed by Cohen and Falicov[12,17] to the presence of magnetic breakdown between the second-band hole sheet (the "monster") and the cigar portions of the third-band electron sheets. This breakdown occurs in and near the basal plane and as is shown later has a decisive effect on the galvanomagnetic properties of magnesium.

4. EXPERIMENTAL PROCEDURE

The bulk of the experimental data compiled during this investigation was obtained from specimens cut with an acid string saw from a large single crystal of magnesium which had a residual resistance ratio ($R_{300°K}/R_{4.2°K}$) of 450. The specimens had typical dimensions of $0.060\times0.040\times0.500$ in. and were oriented to within $\frac{1}{2}°$ of a desired crystallographic direction using standard x-ray techniques. Current was introduced into the ends of a specimen by means of phosphor-bronze spring clips and three orthogonal pairs of point contact potential probes were mounted as shown in Fig. 2. The specimen was then suspended vertically in a liquid helium bath between the pole faces of a dc electromagnet that could be rotated in the horizontal plane. A constant current of approximately 0.2 A was passed through the specimen and the potential between a given pair of probes was continuously recorded as the magnetic field of constant strength was rotated by a small friction drive at a rate of 20°/min. The transverse magnetoresistance voltage (measured between the 1-2 probes of Fig. 2) was typically 10^{-5} V compared with a noise background of about 4×10^{-9} V.

[17] M. G. Priestley, L. M. Falicov, and Gideon Weisz, Phys. Rev. **131**, 617 (1963).

5. TRANSVERSE MAGNETORESISTANCE

Four different types of behavior for the transverse magnetoresistance were discussed in the theory section of this paper. The data obtained in this investigation showed regions of type-1, 2, and 3 behavior, but no evidence was found for the presence of a type 4 region in magnesium. As expected, regions of type 1 (all closed orbits and $V_1=V_2$) were found to predominate. Type-2 behavior was only found for the one isolated direction of H parallel to the hexagonal axis.

Figure 3 is a stereographic projection of those directions of H in *reciprocal space* for which the transverse magnetoresistance exhibits type 3 behavior. Directions of H will be given by the coordinates θ, the angle between H and the polar axis b_3, and ϕ, the angle between the plane of H and b_3 and the plane of b_1 and b_3. Current directions will be designated by θ' and ϕ' defined in the same manner. The crosses in Fig. 3 show the current directions for the specimens investigated.

The circular region about the pole of the stereogram ($\theta\lesssim5°$) is a two-dimensional type-3 region with open trajectories having a net direction parallel to the basal plane. The radial lines are one-dimensional type-3 regions with open trajectories whose net direction is perpendicular to the plane represented by the radial line. The periphery of the stereogram (H parallel to the basal plane) is a one-dimensional region with open orbits parallel to b_3.

For H along the radial lines of Fig. 3, the transverse magnetoresistance was only observed to saturate when J was in the plane of H and b_3. Figure 4 shows a series of transverse magnetoresistance versus magnetic-field

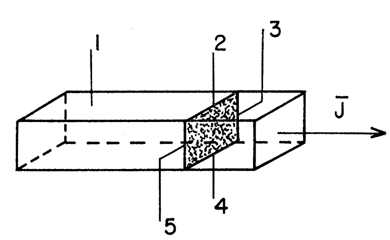


FIG. 2. Specimen geometry showing placement of potential probes. The magnetic field was rotated in the 2435 plane which was perpendicular to J. The transverse magnetoresistance was measured between the 1–2 probes. The electric field in the 2435 plane consists of a part which is an even function of H (the transverse even field) and a part which is an odd function of H (the Hall field). The vector components of these fields were measured using probes 2-4 and 3-5.

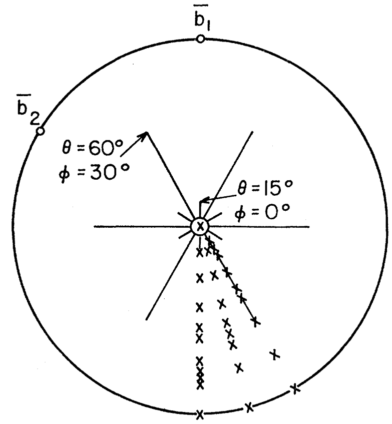


FIG. 3. Stereogram of the magnetic-field directions which give rise to type-3 behavior of the transverse magnetoresistance of magnesium. b_1, b_2, and b_3 are the basis vectors of the hexagonal reciprocal lattice. The pole of the stereogram is along the sixfold b_3 axis. The crosses show the current directions for the specimens investigated.

strength curves for H in the $\phi=0°$ plane and J in the $\phi'=180°$ plane (the same plane but on opposite sides of b_3.) The transverse magnetoresistance tends to saturate for directions of H in this plane as far as $\theta=13°$ from b_3. At $\theta=15°$ the transverse magnetoresistance has an apparent linear dependence with magnetic-field strength while for $\theta>15°$ it tends to vary as H^2 and there is no evidence of a sharp minimum in the magnetoresistance rotation pattern as H passes through the $\phi=0°$ plane. The linear variation of the magnetoresistance for H in the $\theta=15°$, $\phi=0°$ direction thus marks the transition between the two different regions and the maximum value of θ in the $\phi=0°$ plane for which open trajectories are present on the Fermi surface is $\theta=15°$.

The length of the longer set of radial lines shown in Fig. 3 was determined in a different manner. The transverse magnetoresistance tended to saturate for $\theta\leq 30°$ for H in the $\phi=30°$ plane and J in the $\phi'=210°$ plane. It did not tend to saturate for $\theta>30°$ due to the relatively low purity of the specimens used and to the relatively small band of open trajectories that existed for large θ. However, the characteristic sharp minimum in the rotation diagrams which was associated with saturating magnetoresistance for $\theta\leq 30°$ persisted for angles of θ as large as 60°. Figure 5 shows transverse magnetoresistance rotation diagrams at various magnetic-field strengths for J in the $\theta'=30°$; $\phi'=210°$ direction. The dip in the center of the rotation diagrams occurs as H passes through the plane of J and b_3. The upper curve, which is plotted on a different vertical scale, is for a specimen of about twice the purity of the one from which the lower set of curves was taken. Here the minimum has become a sharp spike downward. The transverse magnetoresistance varies as $H^{1.4}$ in the bottom of the spike whereas when θ is only a few degrees larger than 60° the minimum has completely disappeared and the magnetoresistance varies as H^2. This corresponds to the type-3 behavior discussed above and allows us to fix the length of the longer set of radial lines at $\theta=60°$ even though the transverse magnetoresistance does not seem to saturate beyond $\theta=30°$.

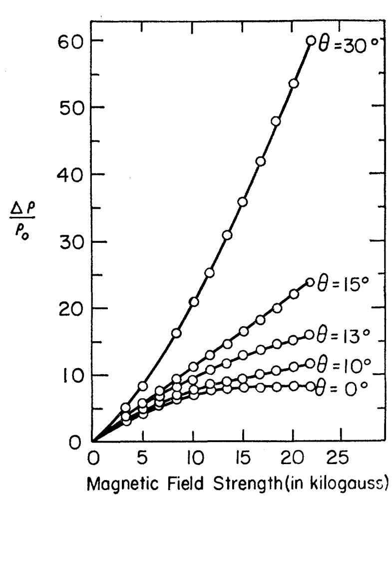


FIG. 4. Transverse magnetoresistance as a function of magnetic-field strength for H in the $\phi=0°$ plane and J in the $\phi'=180°$ plane for several values of θ. $\Delta\rho=\rho(H)-\rho_0$, where ρ_0 is the resistivity for $H=0$ at 4.2°K.

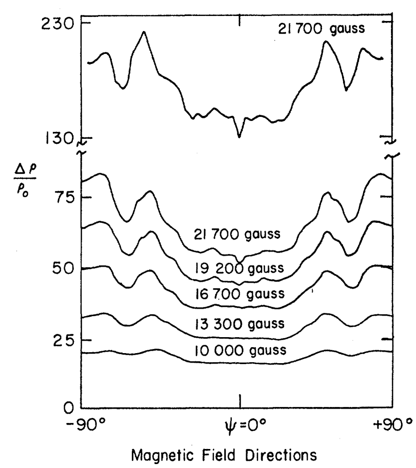


FIG. 5. Transverse magnetoresistance rotation diagram for J in the $\theta'=30°$, $\phi'=210°$ direction. The lower set of curves was taken from a sample with a residual resistance ratio (rrr) of 450 and the upper curve from a sample with an rrr of 900. ψ is the angle between H and the $\phi=30°$ plane. The sharp minimum at $\psi=0°$ occurs as H passes through the tip of one of the longer radial lines of Fig. 3.

Supporting evidence for the existence of the band of open trajectories for H in the $\phi=30°$ plane and θ as large as 60° was obtained from current "rotation" diagrams. When the direction of H is such as to produce a band of open trajectories, the transverse magnetoresistance is given, in the high-field limit, by $\rho=A+BH^2\cos^2\gamma$. We have interpreted the lack of saturation for $\gamma=\pm\frac{1}{2}\pi$ and $\theta>30°$ as the result of our inability to reach the high limit with the specimen purities and magnetic-field strengths available to us. However, if we hold H fixed in magnitude and direction at some point along the $\phi=30°$ line and "rotate" J with respect to the open orbit direction we should find that $\rho(\gamma)$

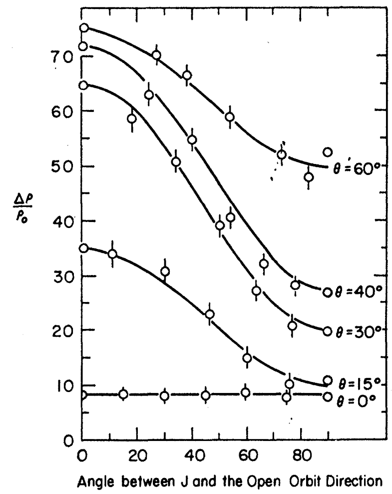


FIG. 6. Current "rotation" diagrams for various values of θ for H in the $\phi=30°$ plane. 90° corresponds to J parallel to the $\phi=30°$ plane.

contains a component which varies as $\cos^2\gamma$ if that direction of H does indeed give rise to open trajectories. Such current "rotation" diagrams have been plotted by selecting data for the appropriate directions of H and J from the transverse magnetoresistance rotation diagrams. Figure 6 shows plots of $\rho(\gamma)$ for several directions of H in the $\phi=30°$ plane. The solid lines, which are $\cos^2\gamma$ curves, fit the data quite well for values of θ as large as 60°. There was no apparent $\cos^2\gamma$ dependence when θ was greater than 60°.[18] Thus, these plots support the previous conclusion that open orbits exist for H in the $\phi=30°$ plane for angles of θ as large as 60°.

The periphery of the stereogram corresponds to magnetic-field directions parallel to the basal plane. At the time of our preliminary report[7] no evidence had been found for open trajectories for these directions of H. However, recent measurements using specimens of higher purity and additional measurements by Brown[19] to 80 kG using the facilities of the NASA Lewis Research Center[20] have revealed the presence of open orbits parallel to b_3 for H parallel to the basal plane. Figure 7 shows transverse magnetoresistance rotation diagrams with J in the $\theta'=90°$, $\phi'=210°$ direction at magnetic-field strengths of 18 and 61.5 kG. The sharp minimum at $\psi=0°$ occurs as H passes through the basal plane and the magnetoresistance at the minimum tends to saturate. That this saturation is due to open orbits parallel to b_3 has been verified by observations on a specimen with J parallel to b_3.[19] For this specimen the magnetoresistance varied as H^2 for all orientations of H parallel to the basal plane.

When H is parallel to b_3 ($\psi=\pm 90°$ in Fig. 7) all of the orbits on the Fermi surface must be closed because of the sixfold symmetry about b_3. Thus, the magnetoresistance saturation for this orientation must result from type-2 behavior (all closed orbits and $V_1\neq V_2$). This is the only direction of H for which type-2 behavior was observed. Later we will discuss the use of the Hall coefficient to determine V_1-V_2 for this particular direction of H.

Falicov[1] predicted another set of open trajectories for magnesium for magnetic-field directions in planes of the type $\phi=30°$ and for $70°\leq\theta\leq 81°$. We did not find any evidence for these open trajectories. This is not surprising, however, since their existence depends very sensitively on the dimensions of the Fermi surface and they would not be expected to be present if Falicov's model for the Fermi surface were only slightly modified.

6. INTERPRETATION OF THE TRANSVERSE MAGNETORESISTANCE

The transverse magnetoresistance results can be interpreted with Falicov's model for the Fermi surface of magnesium if the model is suitably modified to include the effects of spin-orbit coupling[16] and magnetic breakdown.[17] First, we will consider the open orbits parallel to b_3, present for magnetic-field directions parallel to the basal plane. These open orbits must be carried, at least in part, by the vertical "tentacles" of the monster [Fig. 1(a)]. The simplest explanation for this open orbit would be to assume that the energy gap around point H in the AHL plane is sufficiently large so that the electron trajectories are those predicted by the single-zone scheme for magnetic-field strengths as large as 70 kG. If this were the case, the monster would

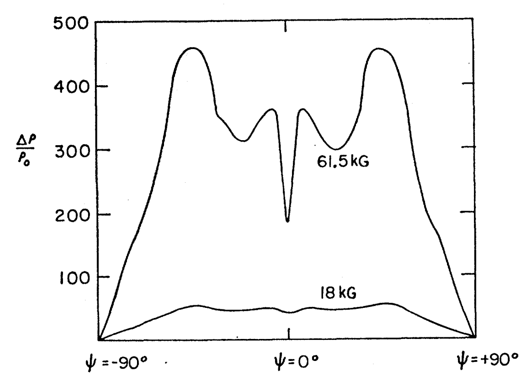


FIG. 7. Transverse magnetoresistance rotation diagram for J in the $\theta'=90°$, $\phi'=210°$ direction. H is parallel to b_3 for $\psi=\pm 90°$ and to the basal plane for $\psi=0°$. For $\psi=\pm 90°$ the transverse magnetoresistance has reached complete saturation for $H=15$ kG.

[18] The open orbit equation $\Delta\rho/\rho_0=A+BH^2\cos^2\gamma$ is a special case of the more general transverse magnetoresistance expression for H parallel to a crystallographic mirror plane given by

$$\Delta\rho/\rho_0=\rho_{xx}+(\rho_{yy}-\rho_{xx})\cos^2\gamma,$$

where ρ_{xx} and ρ_{yy} are the normalized resistivity components measured, respectively, parallel to and perpendicular to the mirror plane and γ is measured from the perpendicular to the plane. For case-3 behavior $\rho_{xx}=A$ and $\rho_{yy}=BH^2$. For case-1 behavior $\rho_{xx}=CH^2$ and $\rho_{yy}=C'H^2$ so that $\Delta\rho/\rho_0=[C+(C'-C)\cos^2\gamma]H^2$. Our measurements have shown that $C\simeq C'$ for case-1 behavior in magnesium.

[19] G. V. Brown, MS thesis, Case Institute of Technology, Cleveland, 1963 (unpublished).

[20] J. C. Fakan, *High Magnetic Fields*, edited by H. Kolm, B. Lax, F. Bitter, and R. Mills (John Wiley & Sons, Inc., New York, 1962), p. 211.

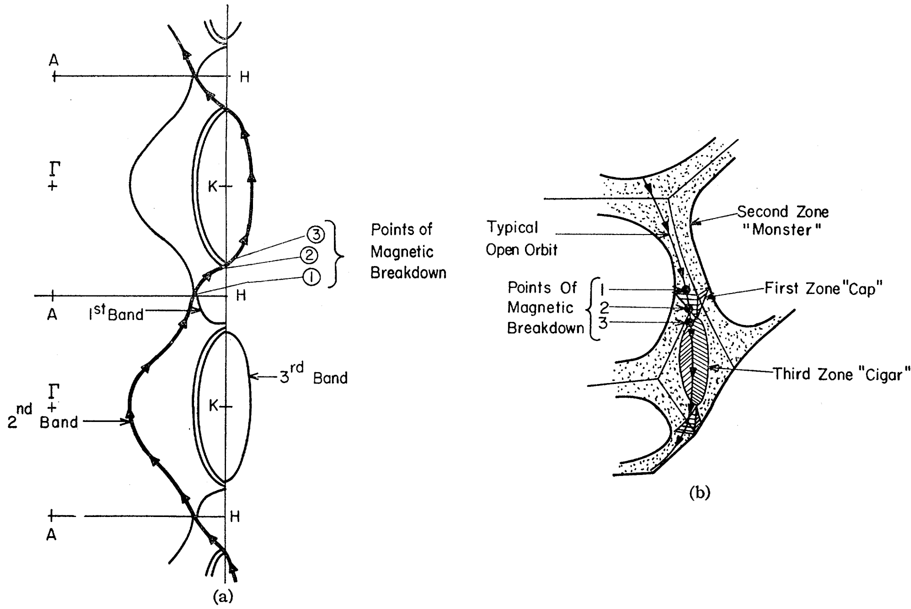


FIG. 8. (a) The Fermi surface of magnesium in the reduced zone scheme. The arrow shows the open orbit associated with magnetic breakdown across three different energy gaps. (b) The surface in the extended zone scheme showing a typical open orbit whose net direction is parallel to b_3. This open orbit is caused by magnetic breakdown of the three small energy gaps indicated.

appear as shown in Fig. 1(a). However, this would require an energy gap around H in the AHL plane that is at least an order of magnitude larger than the maximum possible spin-orbit energy gap.[16] Furthermore, all of the energy gaps are small in the vicinity of the HK line[17] of the Brillouin zone. Thus, it appears that we should reject the simple interpretation requiring an inordinately large spin-orbit energy gap around H and instead interpret the openness parallel to b_3 using the small energy gaps along the HK line.

Figure 8(a) shows a cross section of the Fermi surface of magnesium in the first, second, and third zones in the reduced zone scheme and shows a typical open trajectory. Figure 8(b) shows a detail of the surface in the extended zone scheme in the vicinity of the HK line. The energy gap at point 1 of Figs. 8(a) and (b) is the spin-orbit gap which Falicov and Cohen[16] estimate should be broken down for magnetic-field strengths as small as 200 G. Priestley *et al.*'s[17] calculations indicate that the gaps at points 2 and 3 of Figs. 8(a) and (b) should be broken down by fields of the order of a few kilogauss. With magnetic breakdown of these energy gaps the Fermi surface will support a narrow band of open trajectories parallel to b_3. A typical open trajectory is shown in Fig. 8(b). The electron starts on the inner surface of the monster in the second zone, breaks through the spin-orbit induced energy gap at point 1 to the first zone hole surface (the "cap"), breaks through the gap at point 2 back to the second zone hole surface, breaks through from the second zone to the third zone electron surface (the "cigars") at point 3, traverses the length of the cigar, and then repeats the process in reverse order.

The two types of open trajectories discussed above are the only two which can be supported parallel to b_3 by the Fermi surface of magnesium in its presently accepted form. The first of these is unlikely since it requires the spin-orbit energy gap near H in the AHL plane to be at least an order of magnitude larger than the calculated value. The second type of open trajectory is compatible with both Falicov's band calculations and a small spin-orbit gap near H. Priestley's[4,17] high-field de Haas-van Alphen measurements in magnesium have experimentally verified the existence of small energy gaps up from K along HK. The existence of the band of open trajectories parallel to b_3 is further experimental evidence for small band gaps in the vicinity of the HK line.

All of the remaining sets of open orbits, as well as the type-2 region for H parallel to b_3, can also be explained by magnetic breakdown across the small energy gaps near HK. However, for these, the magnetic breakdown occurs near K between the monster and the cigars. Cohen and Falicov[12] invoked this particular magnetic breakdown to explain the presence of the "giant orbit" which Priestley[4,17] observed during his high-field de Haas-van Alphen investigation of magnesium. Figure 9 shows a basal-plane cross section of the monster and the cigars together with the orbits obtained for H parallel to b_3. Orbits of the kind labeled 1 and 2 exist for magnetic-field strengths sufficiently small that the energy gaps at points "a" are not broken down. With the onset of magnetic breakdown the 1 and 2 orbits disappear and are replaced by 3, the giant orbit. Magnetic breakdown across the energy gaps at points "a" changes the character of the closed orbits on the Fermi surface with the result that volume compensation is destroyed. This, then, is the cause of the region of type-2 behavior for the transverse magnetoresistance when H is parallel to b_3.

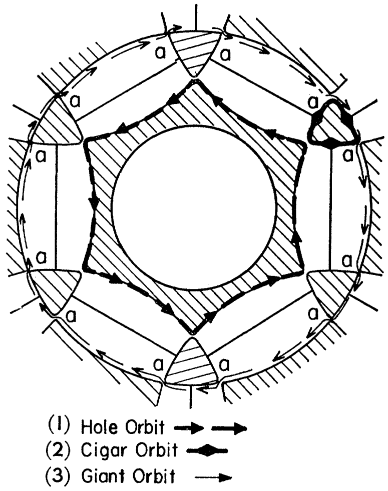


FIG. 9. Basal-plane cross section of the monster and cigar sheets of the Fermi surface of magnesium showing the orbits which exist before and after magnetic breakdown of the energy gaps at points "*a*."

This same magnetic breakdown is also responsible for the existence of the open trajectories associated with the radial lines on the stereogram. As H is tilted away from b_3 in planes of the type $\phi=30°$, one obtains a layer of open trajectories that pass through two regions of breakdown, above a region of breakdown, through two regions of breakdown, etc. (*ee* orbits) and have a net direction perpendicular to the plane containing H and b_3. Figure 10(a) shows the projection on the basal plane of this general type of trajectory which accounts for the longer of the radial lines of Fig. 3. When H is tilted from b_3 in planes of the $\phi=0°$ type, open trajectories are obtained which pass alternately through and above two regions of magnetic breakdown. These trajectories, labeled *ff* in 10(b), vanish for $\theta>15°$. The two-dimensional type-3 region within a cone of $\theta\lesssim5°$ about b_3 is also caused by this kind of magnetic breakdown. While the open trajectories associated with the radial lines are periodic in passing through and above regions of breakdown, the ones generated within the two-dimensional region are in general aperiodic.

Figure 11 is a perspective drawing of the monster in an extended zone scheme. Also shown are those portions of the cigars which were found to be in contact with the monster via magnetic breakdown near point K for magnetic-field strengths of 23 000 G. The upper and lower portions of the cigars are not shown for the sake of clarity. A band of the *ee* open trajectories is shown on the surface for H tilted approximately 50° from b_3 in the $\phi=30°$ plane. Note that there are two points on the combined surface which limit the thickness of the band of open trajectories as H is tilted from b_3; point 1 is the lowest point of the region where magnetic breakdown occurs, point 2 is the minimum height of the monster waist. When H is tilted further away from b_3 the thickness of the band of open trajectories diminishes until it finally vanishes for $\theta=60°$. The range in θ of magnetic-field directions which produce this open trajectory will increase if the vertical extent of the magnetic breakdown is increased (i.e., point 1 is lowered) or if the minimum height of the monster waist is increased (i.e., point 2 is raised) and the range in θ will correspondingly decrease if either of these two limiting heights are decreased.

An analysis of the geometry of the *ee* and *ff* open orbits allows one to determine the vertical separation between points 1 and 2 of Fig. 11 and the horizontal distance of point 2 from the center of the Brillouin zone. These two lengths are $\frac{1}{2}(h_b+h_w)$ and L. h_b is the length measured parallel to b_3 of the region of magnetic breakdown, h_w is the minimum thickness measured parallel to b_3 of the monster waist, and L is the distance from Γ to the projection of point 2 on the basal plane. The results which are quite insensitive to the exact shape of the cigar cross section are:

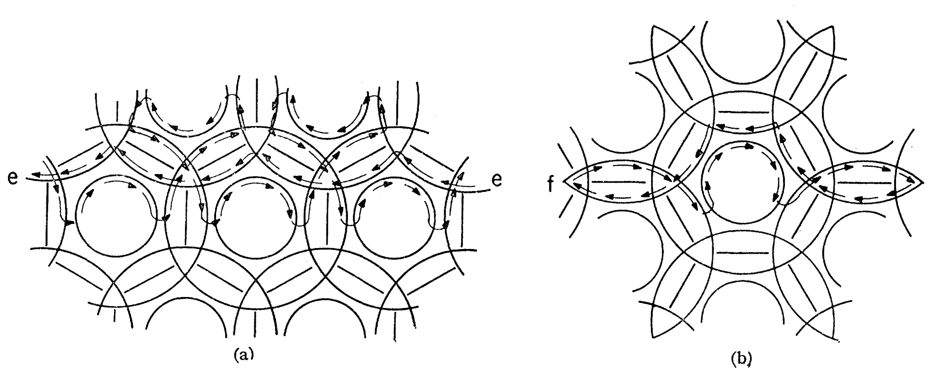
$$\tfrac{1}{2}(h_b+h_w)=0.23\ \text{Å}^{-1},$$
$$L=0.85\ \text{Å}^{-1}.$$

This value of L is quite consistent with Falicov's[1] dimensions for the waist of the monster.

7. HALL FIELD

The hall coefficient, R, has a simple physical interpretation only when all of the electron trajectories are closed and $V_1\neq V_2$ (case 2).[21,22] In the expression given previously for R (case 2 of the theory section) the

FIG. 10. (a) Projection on basal plane of the types of open orbits (*ee*) associated with the longer radial lines of Fig. 3. (b) Projection on the basal plane of the types of open orbits (*ff*) associated with the shorter radial lines of Fig. 3.



[21] J. E. Kunzler and J. R. Klauder, Phil. Mag. 5, 1045 (1961).
[22] J. R. Klauder, Bell System Tech. J. 40, 1349 (1961).

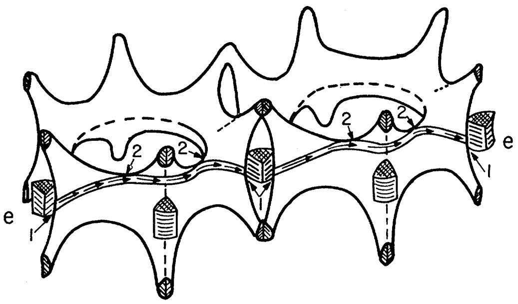


FIG. 11. A perspective drawing of the monster and cigar sheets of the Fermi surface of magnesium showing a band of the *ee* open trajectories.

volumes V_1 and V_2 are volumes in momentum space. Transforming to reciprocal space we have:

$$R=8\pi^3/[2ec(V_1-V_2)].$$

The results of the investigation of the transverse magnetoresistance in magnesium indicate that case-2 behavior is found only for the one isolated direction of H parallel to the hexagonal axis. Thus, this is the only magnetic-field direction in magnesium for which the Hall coefficient can be used to obtain the volume difference V_1-V_2.

The fact that $V_1\neq V_2$ when H is parallel to b_3 is the result of the presence of the giant orbits caused by magnetic breakdown. An exact expression can be obtained for the value of V_1-V_2 associated with the giant orbits which is independent of the detailed shape and dimensions of the Fermi surface. The symmetry of the electron trajectories before and after magnetic breakdown takes place (giving rise to the giant orbits of Fig. 9) is such that $V_1-V_2=2A_{\mathrm{BZ}}l$, where A_{BZ} is the cross-sectional area of the hexagonal face of the Brillouin zone and l is the thickness of the band of giant orbits measured parallel to b_3.[23] The value of l will be determined by and will be equal to the smaller of the two heights h_b and h_w.

Figure 12 shows the magnitude of the Hall coefficient as a function of magnetic-field direction for J in the ($\theta'=90°$; $\varphi'=180°$) direction. A sharp peak occurs when H passes through b_3. Figure 13(a) shows the Hall field as a function of magnetic-field strength for this same current direction and H parallel to b_3. The Hall field is linear above $H\simeq 5400$ G and yields a value for the Hall coefficient of $R=42.7\times 10^{-13}$ Ω cm/G $=4.74\times 10^{-24}$ Gaussian units. A comparison of this with the expression $R=8\pi^3/4ecA_{\mathrm{BZ}}l$ yields a value of $l=0.204$ Å^{-1}.

The detailed behavior of the Hall field as a function of magnetic-field strength for $H\lesssim 2000$ G is shown in Fig. 13(b). The Hall field is linear with the sign of the Hall coefficient indicating hole-type behavior for 250 G$\leq H\leq$1000 G. As the magnitude of H is increased above 1000 G the Hall field goes through a rapid transition until it again becomes linear at $H\simeq 5400$ G. This transition results from the onset of the magnetic breakdown which produces the giant orbit. Thus, the breakdown evidently begins when $H\simeq 1000$ G and is apparently completed when $H\simeq 5400$ G.

Priestley's pulsed field de Haas-van Alphen experiments on magnesium showed that the angular range of the giant orbit about b_3 is constant at $4.2\pm 0.1°$ for magnetic-field strengths above 100 kG.[17] This range gives a value of 0.200 Å^{-1} for the thickness of the band of giant orbits seen in his experiments with magnetic-field strengths as large as 177 kG. This agrees within experimental error with the value obtained from the Hall coefficient. Thus, we can conclude that the thickness of the band of orbits remains constant for magnetic-field strengths above 5400 G and that this thickness is limited geometrically by the minimum height of the monster waist and not by the height of the region of magnetic breakdown.

Combining $h_w=0.20$ Å^{-1} with our previous value for $\frac{1}{2}(h_b+h_w)$, we find $h_b=0.26$ Å^{-1} for a field of 23 000 G. To understand why the Hall coefficient for H parallel to b_3 is unchanged by the increasing value of h_b once h_b is greater than h_w, we must consider the nature of the orbits associated with the breakdown region which are not giant orbits, i.e., which pass through the region of breakdown above and below the limiting points of the monster waist. These are self-intersecting orbits which pass around the cigar and three of the tentacles of the monster. Pippard[14] has shown that the net area of such an orbit would be the difference between the hole area enclosed and the electron area enclosed. Thus, we would expect their contributions to V_1 and V_2 to be equal to those of the corresponding orbits which occur in the absence of breakdown. This type of orbit has, in fact, been observed by Priestley.[4]

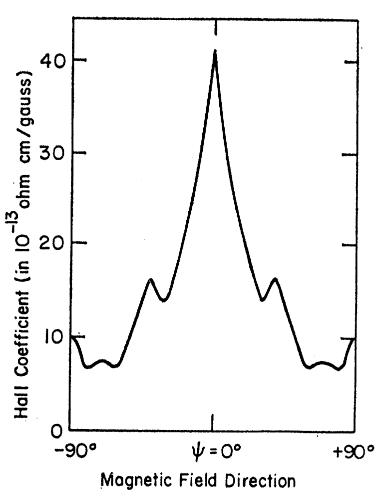


FIG. 12. Magnitude of the Hall coefficient for J in the $\phi'=180°, \theta'=90°$ direction and H in $\phi=90°$ plane. $\psi=0°$ corresponds to H parallel to b_3.

[23] R. W. Stark, thesis, Case Institute of Technology, Cleveland, 1962 (unpublished).

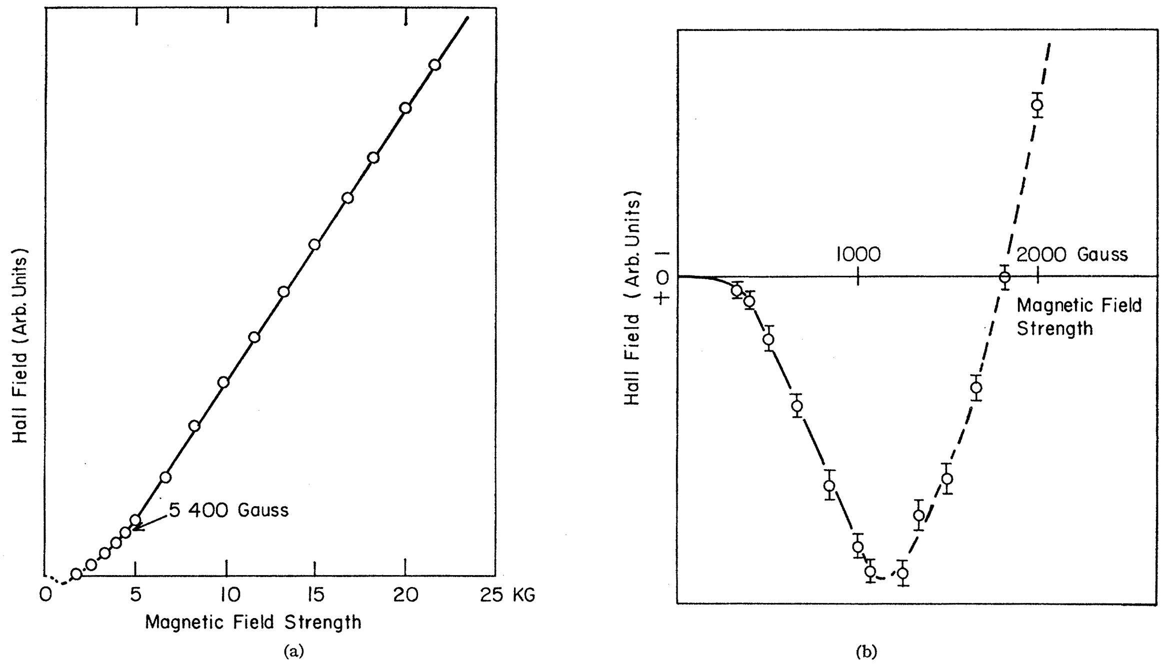


FIG. 13. (a) Hall field versus magnetic-field strength for H parallel to b_3. (b) Detail of the low-field region of Fig. 13 (a).

8. CONCLUSIONS

Many of the striking features of the galvanomagnetic properties of magnesium result from the effects of magnetic breakdown. The previous discussion has shown that these features yield further evidence for the existence of very small band gaps in the vicinity of the KH line of the Brillouin zone. The magnetic breakdown associated with the giant orbit appears to be complete for magnetic-field strengths as small as 5400 G. From this we estimate that the band gap between the monster and the cigars near the ΓKM plane is about 5×10^{-3} eV. The open orbit parallel to b_3 most likely results from the breakdown across three different energy gaps near the KH line. We were not able to observe the transition field for this orbit but its effects were clearly evident for magnetic-field strengths of 25 kG. Thus, we can place a value of 2×10^{-2} eV as an upper limit on the magnitude of each of these three gaps. Recent calculations by Weisz[24] have shown that this orbit should become established in the field range from 17 to 35 kG.

The analysis of the transverse magnetoresistance and the Hall effect data allows us to determine some of the dimensions of the Fermi surface of magnesium. The maximum height of the monster's waist measured parallel to b_3 in the ΓMLA plane of the Brillouin zone occurs along the ΓM line at 0.85 Å^{-1} from Γ with a height at that point of 0.20 Å^{-1}. The height of the region of magnetic breakdown associated with the giant orbit is 0.26 Å^{-1} for magnetic-field strengths of 23 000 G.

[24] G. Weisz (private communication).

ACKNOWLEDGMENTS

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