Topology of the Fermi Surface of Gallium*

W. A. Reed† and J. A. Marcus
Northwestern University,‡ Evanston, Illinois
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High-field magnetoresistance, Hall effect, planar Hall effect, and transverse even effect have been measured on gallium single crystals at 4.2°K with the current along the crystallographic axes and the magnetic field in the major crystallographic planes. The results are interpreted in terms of the Lifshitz, Azbel', and Kaganov theory. The magnetoresistance is quadratic in the magnetic field except when both the current and the field are in the *ab* plane, where it saturates. These results are attributed to a surface which permits open orbits along the k_c axis and to compensation between the number of holes and electrons. In addition, subsidiary minima are observed in the magnetoresistance rotation curves, but the field dependence remains quadratic at these points. The Hall and planar Hall data are highly dependent upon the magnetic field direction and show some features similar to the magnetoresistance. The nearly-free-electron (single-orthogonalized-plane wave) Fermi surface has been constructed for gallium and it is found that, after certain modifications, the sixth band predicted by this model has the basic topological features required by these data. The origin of the transverse even voltage is discussed in terms of the Lifshitz theory.

INTRODUCTION

CONTINUED interest in the high-field galvanomagnetic effects in gallium is due to the success of the theory developed by Lifshitz *et al.*[1,2] in relating these effects in other metals to the topology of the Fermi surface,[3–5] and to the apparent inconsistencies in the published data on gallium.[6] Although the reported magnetoresistance and Hall effects exhibit the complicated anisotropy characteristic of metals with multiply connected Fermi surfaces, no deviations from simple quadratic-field dependence of the magnetoresistance were observed, even in the vicinity of extremely sharp minima. Recognizing that at sharp minima the true character of the field dependence is difficult to determine by the conventional potentiometric method, a dc-amplifier and a quasi-continuous recording system were used in the present investigation and saturation effects have been found for a narrow range of field directions.

For the interpretation of galvanomagnetic data taken in the high field region, the most important results of the Lifshitz theory may be summarized as follows:

A. When only closed orbits exist and the number of holes does not equal the number of electrons ($n_e \neq n_h$), the magnetoresistance saturates for all directions of the magnetic field and current. The Hall coefficient R is related to the Fermi surface by the expression $R=(\Delta nec)^{-1}$, where $\Delta n=n_e-n_h$.

B. When only closed orbits exist and $n_e=n_h$, the magnetoresistance rises quadratically with the magnetic field for all directions of field and current except for $B\|I$, where it saturates. The Hall coefficient is a constant and is not related to the Fermi surface in a simple way.

C. When the Fermi surface is multiply connected and permits open trajectories with a single average direction, the magnetoresistance is quadratic in the magnetic field and depends upon the current direction as

$$\Delta\rho/\rho=a+bB^2\cos^2\alpha,$$

where a and b are constants and α is the angle between the current direction and the direction of open orbits. The Hall coefficient is a constant but cannot be directly related to the shape of the Fermi surface.

D. When the Fermi surface is multiply connected and permits more than one direction of open orbits, the magnetoresistance saturates for all directions of the current as in case A, but now the Hall coefficient is proportional to B^{-2}.

While the above relations between various types of orbits and the expected galvanomagnetic behavior make it possible to determine the topology of the Fermi surface from a complete set of galvanomagnetic measurements, the interpretation is considerably simplified if one starts with a model which has some other physical basis. The single-orthogonalized-plane wave (single-OPW) or nearly-free-electron model was chosen as a starting point in this work since Harrison[7] has shown that the surfaces predicted for the cubic and hexagonal metals are in reasonable agreement with the experimental data and that this model can be expected to give

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† National Science Foundation Cooperative Fellow. Now at the Bell Telephone Laboratories, Murray Hill, New Jersey.

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[1] I. M. Lifshitz, M. I. Azbel', and M. I. Kaganov, J. Exptl. Theoret. Phys. (U.S.S.R.) **31**, 63 (1956) [translation: Soviet Phys.—JETP 4, 41 (1957)].

[2] I. M. Lifshitz and V. G. Peschanskii, J. Exptl. Theoret. Phys. (U.S.S.R.) **35**, 1251 (1958) [translation: Soviet Phys.—JETP **8**, 875 (1959)].

[3] J. Kunzler and J. Klauder, *Proceedings of the Seventh International Conference on Low-Temperature Physics* (University of Toronto Press, Toronto, 1960) p. 213.

[4] Y. P. Gaidukov, J. Exptl. Theoret. Phys. (U.S.S.R.) **37**, 1281 (1959) [translation: Soviet Phys.—JETP **10**, 913 (1960)].

[5] N. E. Alekseevskii, Y. P. Gaidukov, I. M. Lifshitz, and V. G. Peschanskii, J. Exptl. Theoret. Phys. (U.S.S.R.) **39**, 1201 (1960) [translation: Soviet Phys.—JETP **12**, 837 (1961)].

[6] J. Yahia and J. A. Marcus, Phys. Rev. **113**, 137 (1959).

[7] W. A. Harrison, Phys. Rev. **118**, 1190 (1960).

a good first approximation for the other polyvalent metals. The single-OPW surfaces were constructed for gallium and with only minor modifications are found to be consistent with the results of magnetoresistance, Hall effect, planar Hall effect, and transverse even effect at 4.2°K.

EXPERIMENTAL DETAILS

Preparation of Samples

The crystals were prepared from 99.999% pure gallium obtained from the Aluminum Company of America. The molten metal was placed in a modified Schubnikow mold made of Plexiglas and seeded at one end with a crystal of known orientation. The crystals, 1 mm square and 15 cm long, were then cut into 2-cm lengths and mounted.

Crystal orientations were determined from Laue transmission photographs and measurements were confined to those samples for which the crystallographic axes were aligned with the specimen axes to within one degree.

The crystals are labeled in the following way: The first letter indicates the crystallographic axis parallel to the current, and the second letter indicates the axis perpendicular to the mirror face. (One face of the crystal is a mirror since the cover plate of the mold had a polished surface.) The number following the letters indicates the number of such crystals which have been mounted. Thus, crystal *CB*-III has the current along the *c* axis with the *b* axis perpendicular to the mirror face and it is the third *CB* crystal mounted.

The current and potential leads were attached in the manner described by Yahia and Marcus.[6] A total of eight potential leads were spot welded to each crystal so that the potential measured between one pair of leads could be checked against that measured between a similar pair on the same crystal. The placement and numbering of the leads is shown in Fig. 1. The details of the experimental techniques are given elsewhere.[8]

Potential Measurement Technique

The potentials were measured on a Keithley model 150 microvoltmeter. The precision of this instrument was 2% full scale on each range. Two hundredths of a microvolt was the least division on the most sensitive scale and represented the limit of the noise. On all scales the Keithley supplied ±10 v output which was fed into the *y* axis of a Mosely 2S *x-y* recorder. The input to the *x* axis was wired so that this axis would record either the magnitude of the magnet current or the direction of the magnetic field.

Due to the area enclosed by the potential leads, any change in the magnet current or the magnet angle induced a transient potential in the circuit. The data was therefore taken point-wise, but the points were taken close enough together so that no details of the curve were missed and in effect a continuous curve was plotted. The raw data thus appeared as almost continuous curves of voltage vs magnet angle or voltage vs magnet current and were reduced in the standard manner. Since the raw data curves were quasi-continuous, the reduced curves were plotted quasi-continuously. For this reason, most of the curves presented are continuous and show no data points. To obtain the saturation of the magnetoresistance at the bottoms of the extremely sharp minima it was necessary to take a rotation curve at each field strength and then plot the minima of the rotation curves vs magnetic field intensity. These curves for which discrete data were taken do show the experimental points.

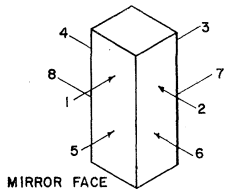

FIG. 1. Placement of potential leads on gallium single crystals.

The standard procedure of reversing both the current and the magnetic field was used to make the potential measurements. The magnetoresistance *voltage* is the longitudinal potential which reverses with current but not with field; the Hall voltage is the transverse potential which reverses with both current and field; and the transverse even voltage is the transverse potential which reverses with current but not with field. The magnetoresistance has the usual definition of

$$[\rho_T(B)-\rho_T(0)]/\rho_T(0).$$

EXPERIMENTAL RESULTS

Since these data are interpreted in terms of the Lifshitz theory, the requirement that the measurements be taken in the high-field region ($B_0/B \ll 1$) must be satisfied. One can form a rough idea of the meaning of "high fields" at a given temperature from the equation $B_0=\rho_0 nec$, where ρ_0 is the resistivity in zero magnetic field, n is the number of electrons per cc, e is the charge of the electron, and c is the speed of light. Gallium has three electrons per atom and the value of the resistivity at 4.2°K is approximately 4×10^{-22} esu, so that $B_0=900$ gauss. If, however, the effective number of electrons per atom[9] is 0.3, then $B_0=90$ gauss. Since the measurements were made in fields up to 19 kgauss, there is little doubt that they were made well into the high field region.

The residual resistance ratios ($R_{290°K}/R_{4.2°K}$) of the crystals used were between 20×10^3 and 25×10^3. From these values the mean free path of an electron at 4.2°K is estimated to be about one-half of the smallest crystal

[8] W. A. Reed, Ph.D. thesis, Northwestern University, Evanston, Illinois, 1962 (unpublished).

[9] L. Weisberg and R. Josephs, Bull. Am. Phys. Soc. 5, 430 (1960).

dimension. Even if a considerable amount of surface scattering were to exist, it would not affect the validity of the conclusions, since surface scattering changes only the absolute values and not the relative values of the potentials measured. The Lifshitz theory uses only the field dependence and relative magnitudes of the potentials to determine the topology of the Fermi surface and does not use the absolute values of these potentials. The preceding argument was checked experimentally by making transverse measurements on a crystal 3-mm square and 2-cm long. The relative values of the voltages measured on this crystal were the same as those measured on the 1 mm square crystals.

The data consist of rotation and field dependence measurements of the magnetoresistance, Hall voltage, planar Hall voltage, and transverse even voltage for currents along the three crystallographic axes. The magnetic field was rotated in the plane perpendicular to the current (transverse), planes containing the current and one other axis (longitudinal), and several other arbitrary planes which did not contain the current but did contain one of the axes.

An approximately-quadratic field dependence characterizes the magnetoresistance for almost all directions of the magnetic field. Since, in the case of equal number of holes and electrons and in the case of open orbits, the Lifshitz theory predicts a strict B^2 dependence, this was checked experimentally by fitting the field dependence curves to the equation $\Delta\rho/\rho=aB^n$. It was found, in the cases checked, that the value of n was between 1.75 and 2.00, with most of the values lying near 1.90. The deviation from a true quadratic dependence has also been observed in copper[3] and gold.[4] A tentative explanation is that the imperfections in the crystal cause the low-value of n either by disrupting the open orbits or by changing the compensation of the number of holes and electrons. This deviation from strict quadratic dependence is ignored for the purpose of interpreting the data in terms of the theory, and the type of field dependence just described is idealized and called "quadratic."

The transverse and longitudinal magnetoresistance rotation curves for the magnetic field in the bc plane are shown in Fig. 2. For $I\|a$ [Fig. 2(a)] the transverse magnetoresistance is quadratic in the magnetic field for all directions of B except at $\theta_c=90°$, where $\Delta\rho/\rho$ saturates. ("θ_c" is the angle the magnetic field makes with the c axis in the plane indicated.) There are subsidiary minima at $\theta_c=0°$ and 60°, but they show a quadratic dependence. Field dependence curves for $\theta_c=0°$ ($B\|c$) and $\theta_c=90°$ ($B\|b$) are shown in Fig. 3. These curves are typical of the field dependence observed for quadratic rise and saturation in the magnetoresistance. The extreme anisotropy between these two curves should be noted. At a field of 19 kgauss the magnetoresistance has a value of 24.6×10^4 for $B\|c$ but a value of only 5.7 for $B\|b$.

When $I\|b$ [Fig. 2(b)] the curve is more complicated but still has a quadratic dependence on B for all directions of the magnetic field except for $B\|I$ (longitudinal magnetoresistance). The same is true when $I\|c$ [Fig. 2(c)]. In both of these curves, subsidiary minima occur when the magnetic field is parallel to certain directions which correspond in most cases to well-defined crystallographic directions. These directions and their ideal angles (θ_b) are given in Table I. Although it does not seem necessary theoretically that the minima occur exactly at crystallographic directions, the deviations between the ideal angles and the measured angles (except for one case) are within the experimental error.

For the magnetic field in the ac plane, the rotation curves are shown in Fig. 4. The transverse magneto-

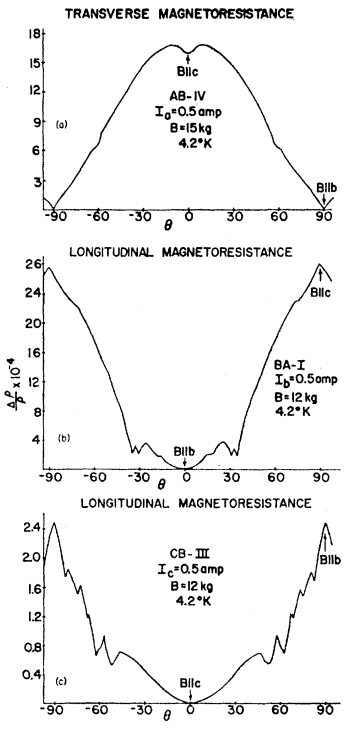

FIG. 2. Magnetoresistance rotation curves for gallium single crystals for B in the bc plane. (a) $I\|a$, (b) $I\|b$, (c) $I\|c$.

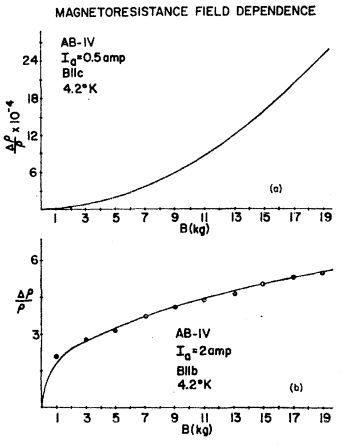

FIG. 3. Magnetoresistance field dependence curves for gallium single crystals for $I\|a$. (a) $B\|c$, (b) $B\|b$.

resistance ($I\|b$, Fig. 4a) has a strong dependence upon the direction of the magnetic field. When $B\|a$ there is a very sharp minimum where in one degree of rotation $\Delta\rho/\rho$ changes from 9×10^4 to 0.1×10^4 and back to 9×10^4. At the bottom of this minimum, saturation is observed. For all other directions of the field, the magnetoresistance has a quadratic dependence, even at the subsidiary minima which occur at angles which approximately correspond to the crystallographic directions. These directions and their ideal angles (θ_a) are given in Table II. The one case where the difference between the measured and ideal angle is greater than the experimental error is for $\theta_a=37°$. The measurements on several crystals show a sharp minima at 37° and not at 40.2°, the predicted angle for the [201] direction.

When $I\|a$ and $I\|c$ [Figs. 4(b) and 4(c)] the longitudinal-rotation curves are perfectly smooth functions of angle, and the field dependence is quadratic for all magnetic-field directions except for $B\|I$. While these rotation curves were carefully checked for subsidiary minima, particularly at θ_a near 60°, 40°, and 16°, none was found. This lack of subsidiary minima is not understood and will be discussed later.

For the magnetic field in the *ab* plane, the only rotation curve which could be obtained is for $I\|c$ (Fig. 5). The magnetoresistance saturates when $I\|a$ and $B\|b$ [Fig. 2(a)] or $I\|b$ and $B\|a$ [Fig. 4(a)] but the saturation is so critically dependent upon the magnetic field direction it is necessary to construct field dependence curves from a series of rotation curves in which the field is rotated across the *ab* plane. Because the crystals could not be aligned with sufficient accuracy in the magnetic field, the longitudinal rotation curves could not be obtained. However, it was possible to tip the crystals so that the magnetic field crossed the *ab* plane at several different angles to the axes. Each time the field crossed this plane and $I\|a$ or $I\|b$ the magnetoresistance showed a deep minimum, and saturation was observed for the eight angles measured (Fig. 6). From this result it is inferred that saturation would be observed for all directions of B in the *ab* plane if the crystal could be aligned well enough in the magnetic field.

When $I\|c$ (Fig. 5) the magnetoresistance is quadratic in the magnetic field for all directions of B. At $\theta_a=0°$,

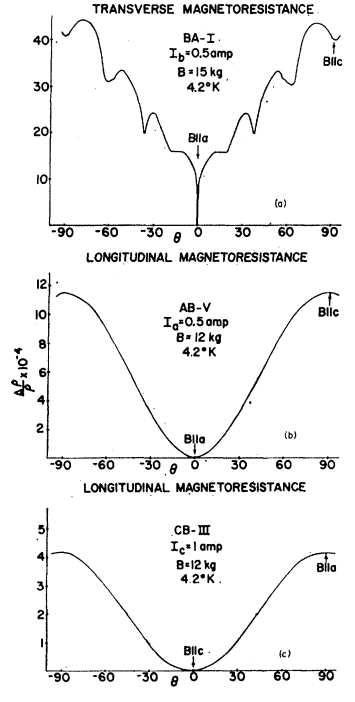

FIG. 4. Magnetoresistance rotation curves for gallium single crystals for B in the *ac* plane. (a) $I\|b$ (b) $I\|a$, (c) $I\|c$.

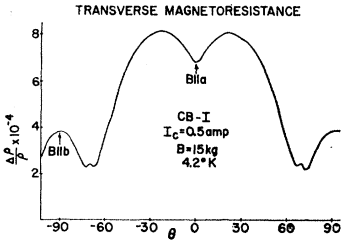

FIG. 5. Magnetoresistance rotation curve for gallium single crystals for B in the *ab* plane and $I\|c$.

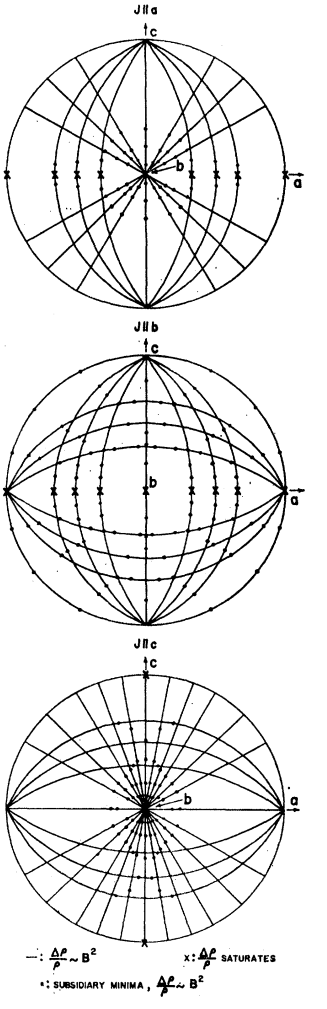

FIG. 6. Stereograms of the magnetoresistance of gallium single crystals. Lines indicate the planes in which B was rotated and where $\Delta\rho/\rho\sim B^2$; crosses indicate where $\Delta\rho/\rho$ saturates; dots indicate where subsidiary minima were observed, $\Delta\rho/\rho\sim B^2$.

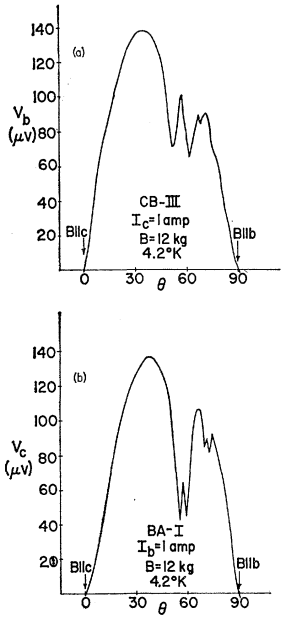

FIG. 7. Planar Hall rotation curves for gallium single crystals for B in the bc plane. (a) $I\|c$, (b) $I\|b$.

67°, and 72°, there are subsidiary minima which approximately correspond to the [100], [250], and [130] directions, respectively (the ideal angles are 0°, 68.1°, and 71.5°), but these minima show quadratic rise and do not saturate.

Rotation curves were taken on all of the crystals in a number of planes which contained only one crystallographic axis. These measurements show it is likely that the magnetoresistance is at all times quadratic in the magnetic field *except when the current and field are in the ab plane*. These rotation curves show subsidiary minima

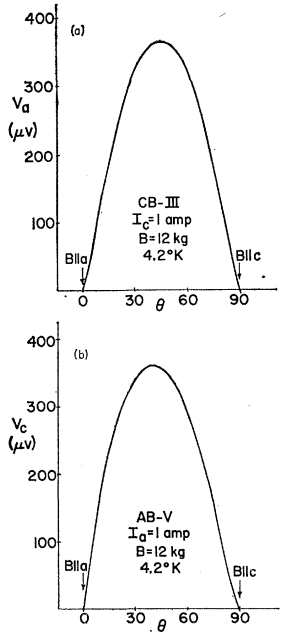

FIG. 8. Planar Hall rotation curves for gallium single crystals for B in the ac plane. (a) $I\|c$, (b) $I\|a$.

similar to those described above. Stereograms indicating the planes in which the magnetic field was rotated and the locations of subsidiary minima are shown in Fig. 6.

The planar Hall data for the magnetic field in the bc and ac planes are shown in Figs. 7 and 8. These curves show subsidiary minima for the same directions of the magnetic field as do the corresponding magnetoresistance curves. A quadratic field dependence of the planar Hall voltage is always observed. Planar Hall data for the field in the ab plane could not be measured for the same reasons the magnetoresistance could not be measured in this plane.

TABLE I. Directions of the magnetic field in the bc plane at which subsidiary minima occur in the magnetoresistance.

Crystal direction	[012]	[021]	[031]	[041]	[051]
Ideal angle (θ_b)	73.6°	40.4°	29.6°	23.0°	18.7°
Exp. angle $I\|a$	···	···	30°	···	···
Exp. angle $I\|b$	74°	35°	31°	21°	18°
Exp. angle $I\|c$	···	39°	28°	22°	15°

The Hall measurements were made by measuring the components of the voltage generated transverse to the current when a transverse magnetic field was applied. The voltages measured on the two pairs of mutually perpendicular probes were then combined to form the vector which represents the Hall field. Figures 9(a), 10(a), and 11(a) show the angle between the Hall field and the magnetic field (ϕ) vs the angle between the magnetic field and the crystal axes (θ).

Three types of field dependence are observed for the Hall voltage. At the minima in Figs. 10(a) and 11(a), and for all field directions in Fig. 9(a), the Hall voltage

TABLE II. Directions of the magnetic field in the ac plane at which subsidiary minima occur in the magnetoresistance.

Crystal direction	[101]	[201]	[601]
Ideal angle (θ_a)	59.5°	40.2°	15.8°
Exp. angle $I\|b$	62°	37°	15°

is linear with the exception of $B\|a$ in Fig. 9(a) and $B\|b$ in Fig. 11(a). At these two points the Hall voltage *may* be proportional to B^{-1} but it is difficult to obtain the field dependence of V_H at these points due to the acute dependence of this voltage upon the direction of the magnetic field.[10] At points other than the minima in Figs. 10(a) and 11(a), the Hall voltage increases faster than linear. Kaganov and Peschanskii[11] show that when

[10] It should be remembered that V_H is the result of adding and subtracting four curves. When the raw data curves are highly dependent upon the field direction, the uncertainty in V_H increases.

[11] M. I. Kaganov and V. G. Peschanskii, J. Exptl. Theoret. Phys. (U.S.S.R.) **35**, 1052 (1958) [translation: Soviet Phys.—JETP **8**, 734 (1959)].

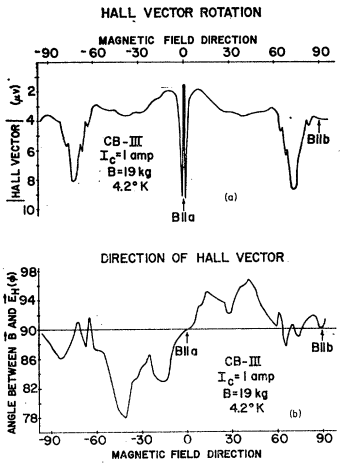

FIG. 9. Hall vector rotation curves for gallium single crystals for B in the ab plane and $I\|c$. (a) Magnitude of Hall vector vs B direction, (b) angle between Hall vector and B vs B direction.

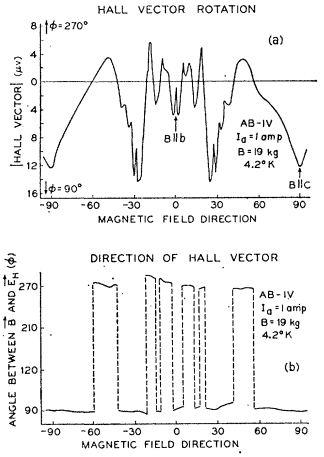

FIG. 11. Hall vector rotation curves for gallium single crystals for B in the bc plane and $I\|a$. (a) Magnitude of Hall vector vs B direction, (b) angle between Hall vector and B vs B direction.

the number of electrons does not exactly compensate the number of holes, the Hall voltage is given by the expression

$$V_H=(aB/nec)-(b\Delta n/n^2ec)(B^3/B_0^2),$$
$$B_0\ll B\ll B_0|n/\Delta n|,$$

where $n=(n_e+n_h)/2$, $\Delta n=n_e-n_h$, and a and b are constants. Thus, when $\Delta n\neq 0$, there is a cubic term in the field dependence. This nonlinearity of the Hall voltage therefore suggests that in gallium the number of holes does not exactly compensate the number of electrons.

An interesting feature of the Hall and planar Hall measurements is that they serve as a check on the Onsager relations. A consequence of the relations is that the interchange of the current and potential probes should not change the shape or magnitude of the rotation curves as long as the magnetic field remains in the same plane. The relations for the planar Hall voltage are seen to be valid by comparing part a to part b in Figs. 7 and 8. There are six possible pairs of curves for the Hall voltage, two of which are shown in Fig. 12 (compare a with b and c with d). The magnitude of the voltages agrees in all cases and the shapes are almost identical. In the case of poorest agreement the general shape is similar but the details are not. This disagreement in the details is believed to be due to some experimental difficulty rather than to a failure of the Onsager relations. The experimental verification of these relations is not trivial since for other metals the above agreement is the result of crystal symmetry and not of the Onsager relations. Gallium is one of the few

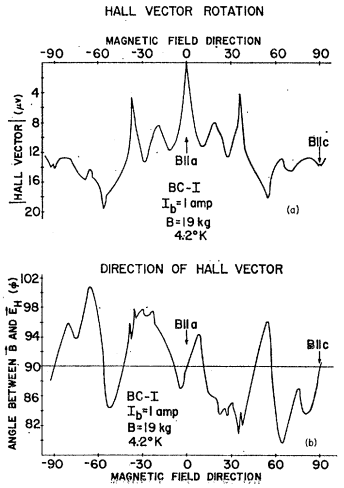

FIG. 10. Hall vector rotation curves for gallium single crystals for B in the ac plane and $I\|b$. (a) Magnitude of Hall vector vs B direction, (b) angle between Hall vector and B vs B direction.

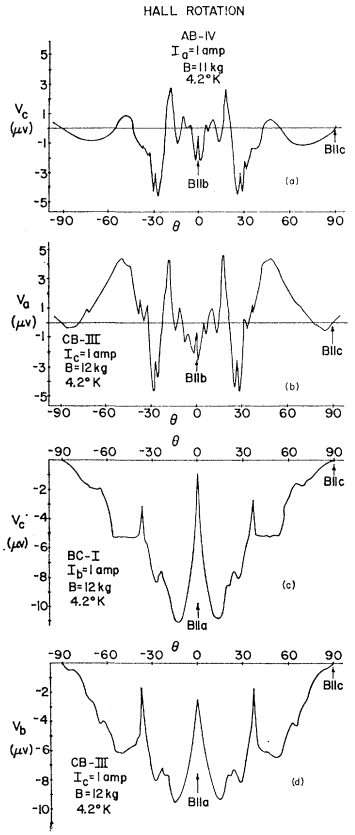

FIG. 12. Hall rotation curves for gallium single crystals, showing validity of the Onsager relations. (a) $I\|a$, $V\|c$; (b) $I\|c$, $V\|a$; (c) $I\|b$, $V\|c$; (d) $I\|c$, $V\|b$.

metals which has low enough symmetry to effectively test these relations.

DISCUSSION OF RESULTS

The outstanding feature of the magnetoresistance is that saturation is observed when both the current and the magnetic field are in the *ab* plane, but quadratic rise is observed for all directions of the magnetic field in the *ab* plane when $I \| c$. This result indicates a Fermi surface having the topology of a cylinder whose axis is parallel to the k_c direction.

The other major feature is that when the magnetic field is not in the *ab* plane, the magnetoresistance is quadratic in the field for all directions of the current (except for $B \| I$ where the magnetoresistance saturates in all cases). This indicates that there is compensation between the number of holes and electrons and the Fermi surface is composed of at least two sheets. This simple surface does not, however, explain the subsidiary minima in the magnetoresistance and Hall effect. Several other *a priori* surfaces have been considered, but without success. Therefore, the Fermi surface predicted by the single OPW model is compared with the data and in the following discussion this surface is considered to be basically correct and it is only modified to satisfy the specific details of the measurements.

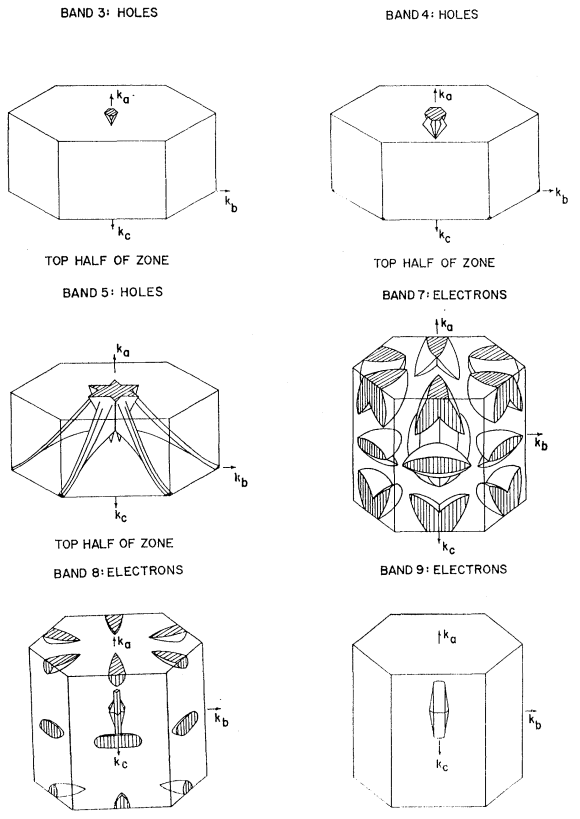

FIG. 13. Fermi surface for gallium constructed from the single-OPW approximation. (See Fig. 14a for band six).

The several bands predicted by the OPW model are shown in Figs. 13 and 14(a) and it can be seen that only the fifth and sixth bands of holes have any possibility of supporting open orbits. Upon closer examination it can be seen that the fifth band will only support open orbits when B is in the *bc* plane and θ_c is approximately 0° and ±60°. However the arms of this surface will probably shrink back in the transition from the OPW model to the real metal since the electrons from the higher bands will fill the holes in the lower bands. Thus, it is assumed that the fifth-band surface supports only closed orbits and open orbits are possible only on the sixth-band surface. The closed surfaces of the other

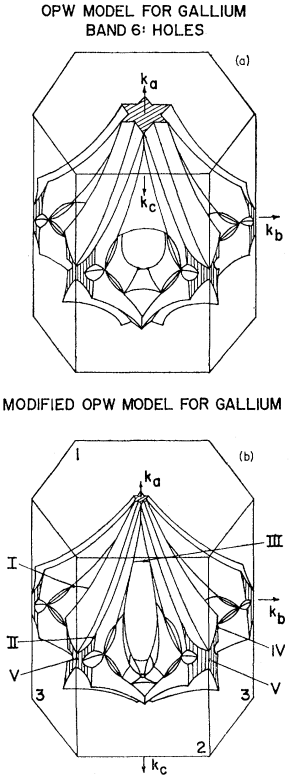

FIG. 14. (a) Sixth band of Fermi surface for gallium constructed from the single-OPW approximation. (b) Sixth band of OPW Fermi surface with modifications indicated from galvanomagnetic data.

bands are not considered here since specific information about them cannot be obtained from the galvanomagnetic measurements. Because of the even number of electrons in the primitive unit cell (Appendix B) all of the bands combine to give compensation of the number of holes and electrons for magnetic field directions for which there are no open orbits, but the magnetoresistance in this case is only weakly dependent upon the field direction. Any strong dependence of the magnetoresistance upon the field direction is associated with open orbits. Therefore, only the sixth band of holes will be considered.

As stated above, the measurements for the field in the *ab* plane indicate that the surface has the properties of a cylinder parallel to the k_c direction. The sixth band

permits such open orbits for all directions of the magnetic field in the ab plane except when $B\|a$. If, however, the surface is modified by lowering the "roof" at point I in Fig. 14(b), open orbits are permitted parallel to k_c for this direction of field. The holes may now enter the cell at point II, travel across the zone on the inside of the surface, and leave by the back face. Without this modification, the orbit which is formed by a plane perpendicular to k_a permits holes to enter the zone at II but does not permit them to travel across the zone (see Fig. 15).

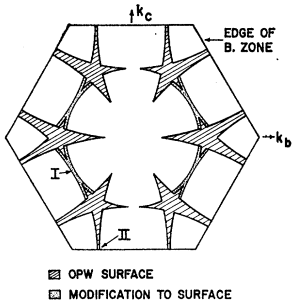

FIG. 15. Cross section of sixth band of OPW Fermi surface for gallium showing necessary modification. Plane of cross section is perpendicular to k_a at an elevation II in Fig. 14(b).

While the OPW surface predicts that the data will show pseudo hexagonal symmetry[12] when the field is rotated in the bc plane and the current is parallel to the a-axis, the actual measurements do not show this symmetry [Figs. 2(a) and 14(a)]. The model predicts saturation of the transverse magnetoresistance when $I\|a$ and $\theta_b=0°$ and $\pm 60°$ due to open orbits in the bc plane but the measured magnetoresistance saturates only at $\theta_b=0°$. One way of modifying the surface so that it agrees with the data is to raise the "roof" at III high enough that orbits entering at IV cannot go across the cell and must remain closed. A second way of preventing open orbits in this direction is to shrink back the surface so that it does not touch any of the "3" type faces but remains in contact with the "2" type faces. This, however, would require the existence of an unusual lattice potential in the real metal. Because there is no reason to suppose that such a potential does exist, this method of removing open orbits is unlikely.

The subsidiary minima for the field in the bc plane require another modification of the OPW surface. For θ_b near 0°, 15°, 30°, 40°, 60°, 75°, and 90° the model predicts a considerable number of open orbits parallel to k_a which enter at the "star" on top, run down along an arm and out the "star" on the bottom whereas the data indicate that the number of open orbits is quite small. As observed (Fig. 2 and Table I) subsidiary minima occur in the rotation curves at θ_b approximately 18°, 30°, 40°, and 74°. These are very deep when $I\|b$ and $I\|c$ but are barely visible when $I\|a$, indicating that these orbits are parallel to k_a but there are not enough open orbits to cause saturation. Thus the "star" at face "1" must be shrunk down so that the number of open orbits parallel to k_a is reduced but not completely eliminated.

The problem in the interpretation of the data for the field in the ac plane is that very pronounced subsidiary minima are observed when $I\|b$ and none is observed when $I\|a$ and $I\|c$. Even if the open orbits lie in the ac plane, the transition from quadratic rise due to $n_e=n_h$ to quadratic rise due to open orbits should be seen in one of the two longitudinal rotation curves. At present this anomaly is unexplained. The minimum observed when $I\|b$ and $\theta_a=37°$ [Fig. 4(a)] is probably due to open orbits in the ac plane, but the number of such orbits is small enough that the magnetoresistance does not saturate. At this field direction, the minimum may be due to an orbit which enters at the "star" in the "1" face and leaves by the "arms" at V. The surface does not seem to support open orbits in any direction for $\theta_a=18°$ or 60°. A possible explanation for this is that these minima are a result of a change in the compensation of the number of holes and electrons due to the occurrence of elongated orbits at these angles, and not a result of open orbits.

In the case where the magnetic field is in the ab plane and $I\|c$ (Fig. 5), the modified surface does not seem to permit any open orbits other than those parallel to k_c for $\theta_a=0°$, 67°, or 72°. The minima at these angles are possibly caused by a decrease in the thickness of the layer of these open orbits.

The area of contact of the Fermi surface with the zone boundary at the edges (places like V) cannot be estimated as in the case of the "star" since there are no major open orbits created by them other than those parallel to k_c. For this reason these contact areas are left unaltered in the modified surface, although the contact area is probably smaller than that predicted by the OPW model. The exact area will have to be determined by a de Haas-van Alphen measurement.

The subsidiary minima which appear in the planar Hall rotation curves near $\theta_c=50°$, 60°, and 70° (Fig. 7) are probably due to open orbits parallel to k_a for these field directions. For B in the ac plane (Fig. 8), no subsidiary minima appear as in the case of the corresponding magnetoresistance.

The Hall effect data are very dependent upon the direction of the magnetic field but in the absence of a detailed theoretical analysis do not furnish much additional information about the Fermi surface. In the case where there is compensation of the number of holes and electrons, the leading term in the resistivity tensor for the ρ_{xy} element is proportional to B^2 in the high-field limit. Since the Hall voltage is defined as the transverse voltage which is odd in the magnetic field, it does not contain the leading term of ρ_{xy} but only lower order terms and is not related to the Fermi surface in a simple way. The transverse even voltage, which represents the leading term of ρ_{xy} when $n_e=n_h$, is related to the general

[12] It should be noted that although gallium has a base-centered-orthorhombic lattice, the cell in k-space is almost hexagonal due to the particular values of the lattice constants, the angles of the "hexagonal" face being 59° and 61° instead of 60°.

anisotropy of the Fermi surface but cannot be interpreted. For those magnetic-field directions where there is a single direction of open orbits, the Hall voltage does represent the leading term of the ρ_{xy} element, but again is not related to the Fermi surface in a simple way. For these reasons, the Hall voltage may only be used to establish the field directions where open orbits occur in more than one direction.

In addition to a transverse even voltage due to $n_e=n_h$, there is also a transverse even voltage associated with open orbits. Klauder and Kunzler[13] have shown how this voltage along with the magnetoresistance can be used to help determine the direction of open orbits if the exact alignment of the crystal and specimen axes were known. However, in our research the crystal axes were misaligned from the specimen axes by one degree and the error in the alignment angle was also one degree. Since the error in the angles between the crystal and specimen axes must be small compared to the value of the angles themselves, the transverse even voltages measured cannot be used to define the Fermi surface.

The proposed surface shown in Fig. 14(b) fits the basic features of the galvanomagnetic data. It is the OPW surface to which a minimum number of modifications have been made. Only the major topological features of this surface are significant since the galvanomagnetic effects only supply general information about the topology. The specific details, such as the small undulations, are left unaltered in the figure so that this surface may be directly compared with the unmodified surface, or with other types of measurements such as the de Haas-van Alphen effect,[14] cyclotron resonance, anomalous skin effect or magnetoacoustic attenuation, but they should not be considered a result of these measurements.

ACKNOWLEDGMENTS

We would like to thank J. H. Condon for his assistance with the experimental problems and discussions of the data, and Dr. J. R. Klauder for the discussions on the theoretical interpretations of the results.

APPENDIX A: TRANSVERSE EVEN VOLTAGE

The transverse even (TE) voltage is defined as that voltage which is even in the magnetic field and measured on the transverse or Hall probes. Since it does not possess the same dependence upon the magnetic field direction as the magnetoresistance and it may have both positive and negative values on the same rotation curve, this voltage is not a scaled down magnetoresistance caused by the misplacement of the probes along the current direction.

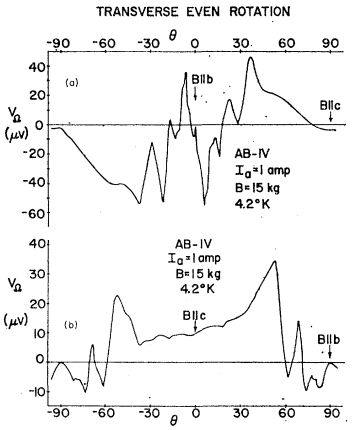

FIG. 16. Transverse even voltage rotation curves for gallium single crystals. B is rotated in a plane perpendicular to the a axis. $I\|a$. (a) $V\|c$, (b) $V\|b$.

Although Shoenberg[15] recognized its possible existence, the first detailed discussion of TE was made by Mason, Hewett, and Wick.[16] They showed that for germanium in the low field region, where a phenomenological relation for the galvanomagnetic data is valid, a TE voltage is possible when the current and magnetic field are not along crystallographic directions. Yahia and Marcus[6] later reached this same conclusion for gallium. The TE voltage found by this method is not highly dependent upon the magnetic field direction. It is due to the misalignment of the crystal and specimen axes and can be considered as the projection of the magnetoresistance along the crystal axes onto the specimen axes.

Connell and Marcus[17] first recognized that at 4.2°K TE was not simply a component of the magnetoresistance. They observed that in bismuth the even voltage measured on the transverse probes did not scale with the magnetoresistance measured on the longitudinal probes. Since then, TE has been observed by Yahia and Marcus in gallium,[6] Kunzler and Klauder in copper,[13] Kachinskii in tin,[18] as well as by the authors in this research on gallium (see Fig. 16).

Lifshitz *et al.*[1,2] predict such a voltage in the high-field region. They show that when $n_e=n_h$ the leading term in the ρ_{xy} element of the resistivity tensor is even in the magnetic field. It is also implicit in their work that a transverse even voltage exists when there are open orbits. The explicit relations for open orbits have been derived by Kunzler and Klauder.[13] All of these predictions are made for arbitrarily aligned crystals. However, if well aligned crystals are used so that the current is exactly along a crystal axis and the magnetic field is in a plane exactly perpendicular to the current, crystal symmetry requires that TE be zero.

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[13] J. Klauder and J. Kunzler, Phys. Rev. Letters **6**, 179 (1961).
[14] The DHVA measurements of D. Shoenberg [Phil. Trans. Roy. Soc. (London) **A245**, 1 (1952)] cannot be used for comparison since they are low-field measurements which measure only the small sections of the Fermi surface.
[15] D. Shoenberg, Proc. Cambridge Phil. Soc. **31**, 271 (1935).
[16] W. P. Mason, W. H. Hewitt, and R. F. Wick, J. Appl. Phys. **24**, 166 (1953).
[17] R. A. Connell and J. A. Marcus, Phys. Rev. **107**, 940 (1957).
[18] V. N. Kachinskii, Doklady Akad. Nauk S.S.S.R. **135**, 818 (1960) [translation: Soviet Phys.—Doklady **5**, 1260 (1961)].

To experimentally determine that TE does indeed become zero for perfectly aligned crystals would be extremely difficult. This experiment would require that the crystals be aligned to within a tenth or even a hundredth of a degree since the crystals used in this work, which were aligned to within one degree, produced TE voltages as large as 10% of the magnetoresistance voltage. In addition, these crystals would have aligned in the magnetic field with the same accuracy.

The experimental evidence that TE is large for crystals misaligned by only one degree makes it difficult to believe that TE will not be observed when there is complete alignment. However, the very general nature of the crystal symmetry arguments almost forces one to assume that TE will be zero for perfectly aligned crystals.

APPENDIX B: VALUE OF PARAMETERS USED IN THE OPW CONSTRUCTION

Lattice constants for gallium at 4.2°K[19]:

$$a_0 = 4.5103\ \text{Å},$$
$$b_0 = 4.4861\ \text{Å},$$
$$c_0 = 7.6463\ \text{Å}.$$

Valence of gallium: 3.
Bravais lattice: base-centered orthorhombic.
Number of atoms per base-centered cell: 4.

[19] C. S. Barrett (private communication).

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Symmetry and Free Electron Properties of the Gallium Energy Bands*

J. C. SLATER, G. F. KOSTER, AND J. H. WOOD
Department of Physics, Massachusetts Institute of Technology, Cambridge, Massachusetts
(Received December 18, 1961)

Atomic arrangement, unit cell, and Brillouin zone of metallic gallium are described, including notations for the various symmetry directions. The point and space groups are discussed, including character tables, and basis functions in the form of symmetrized plane waves for electronic wave functions of each symmetry type. The free-electron approximation is used as a first step toward finding the energy bands and Fermi surfaces. This work is preparatory toward a study of energy bands which is under way using the augmented-plane-wave method.

1. CRYSTAL STRUCTURE AND BRILLOUIN ZONE OF GALLIUM

A GREAT deal of experimental activity is going on at present with the aim of studying the Fermi surface of gallium.[1] We do not have a suitable theoretical treatment of the gallium energy bands. Consequently, we are preparing to apply the augmented-plane-wave (APW) method to this metal. As a preliminary, we have studied the group-theoretical properties of this substance, and the free-electron approximation to the energy bands and the Fermi surface.[2] It is known[3] that the free-electron approximation has proved to be a successful first approach to the energy bands of a number of elements, so that we may hope that it will give us a good enough indication of the nature of the gallium bands to guide us in interpreting the APW calculations when they are completed.

The crystal structure of gallium is orthorhombic,[4] with eight atoms in an orthorhombic cell. According to recent data of Barrett,[5] the sides of this cell, at 2.35°K, are $a=4.5151$ Å, $b=4.4881$ Å, $c=7.6318$ Å, respectively. It is an accident, without physical importance, that the two sides a and b are so nearly equal. According to earlier work of Bradley,[4] the eight atoms are located at the following positions:

$$(m,0,p,),\quad (m+\tfrac{1}{2},\tfrac{1}{2},\bar{p}),\quad (\bar{m}+\tfrac{1}{2},\tfrac{1}{2},p),\quad (\bar{m},0,\bar{p}),$$
$$(m,\tfrac{1}{2},p+\tfrac{1}{2}),\quad (m+\tfrac{1}{2},0,\bar{p}+\tfrac{1}{2}),\quad (\bar{m}+\tfrac{1}{2},0,p+\tfrac{1}{2}),$$
$$(\bar{m},\tfrac{1}{2},\bar{p}+\tfrac{1}{2}).\quad (1)$$

The values of the parameters m and p, according to Bradley, are $m=0.0785$, $p=0.1525$. These values were determined at room temperature, and we do not know whether they are correct at 2.35°K. However, nothing in our argument will depend on the precise values of these parameters.

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[1] We are indebted to Dr. B. W. Roberts, of the General Electric Company, for pointing out the importance of this problem to us.

[2] The free-electron Fermi surface has also been studied by Jules Marcus and W. A. Reed, preceding paper [Phys. Rev. **126**, 1298 (1962)]. We are indebted to Dr. Roberts and to Professor Marcus for information regarding this work.

[3] Much of the old work on energy bands was based on this approximation; see for instance N. F. Mott and H. Jones, *The Theory of the Properties of Metals and Alloys* (Oxford University Press, New York, 1936), Chap. V. More recent work includes that of F. Herman, Revs. Modern Phys. **30**, 102 (1958); W. A. Harrison, Phys. Rev. **116**, 555 (1959); **118**, 1182, 1190 (1960); contribution in *The Fermi Surface* (John Wiley & Sons, Inc., New York, 1960), p. 28.

[4] A. J. Bradley, Z. Krist. **91**, 302 (1935), who quotes earlier references.

[5] C. S. Barrett (private communication).