OPEN CROSS SECTIONS OF CADMIUM, ZINC, AND THALLIUM FERMI SURFACES

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Submitted to JETP editor July 24, 1962

J. Exptl. Theoret. Phys. (U.S.S.R.) 43, 2094-2104 (December, 1962)

The anisotropy of the electrical resistance of Cd, Zn, and Tl single crystals in a magnetic field was investigated. The results indicate that all three metals possess open Fermi surfaces. In Cd the open conduction-electron trajectories in a magnetic field are parallel to the [0001] direction. In Zn the open trajectories are parallel both to [0001] and to the (0001) plane. In Tl the open trajectories are located only in the (0001) plane. The topological features of the Fermi surfaces are discussed from the standpoint of current theoretical concepts.

ONE of the characteristic indications that a metal possesses an open Fermi surface is strong anisotropy of its electrical resistance in a magnetic field.^[1] By studying resistance anisotropy as a function of both the electric-current and the magnetic-field directions (with $H \perp J$) we can determine the average direction of open electron trajectories on the Fermi surface.^[2] The angle interval of magnetic-field directions associated with open electron trajectories makes it possible in the cases of some metals to determine the size of the open Fermi surface.^[3]

Measurements of the galvanomagnetic properties of Cd and Zn single crystals^[4,5] indicate that these metals possess open Fermi surfaces. Results obtained for a Tl single crystal have also indicated an open Fermi surface.^[6] The present paper discusses detailed measurements of the anisotropy of electrical resistance performed on Cd, Zn, and Tl single crystals in large effective magnetic fields.

I. SAMPLES AND MEASUREMENT PROCEDURE

The Cd, Zn, and Tl single crystals, grown by the Obreimov-Shubnikov method, were ~ 1.5 mm in diameter and ~ 30 mm long. Samples cut in the form of thin $1 \times 3 \times 20$ -mm plates were used to measure the Hall effect. The ratio of the resistance at room temperature to that at 4.2°K was about 10,000 for Cd and Tl, and about 15,000 for Zn. Sample orientations were determined optically and were checked by means of x rays.

The measurements were obtained at liquid helium temperatures in magnetic fields up to 33 kOe. The axes of the samples were usually oriented perpendicular to the magnetic field, but in some instances they deviated from this direction by angles up to 14°. It was therefore possible to reduce the required number of samples and to determine the exact dimensions of two-dimensional regions and special lines in the stereographic projections of especially significant magnetic-field directions. The measurements showed that small angular deviations of the current direction from the $J \perp H$ position do not affect conclusions regarding the topological properties of the Fermi surface of a metal.

In order to investigate the angular dependence of resistance in a constant magnetic field $\rho_{\rm H=const}(\vartheta)$ (where ϑ is the rotation angle of the magnetic field) emf's were registered automatically on the tape of an ÉPP-09 recorder, the emf's first being amplified (116:1) by an "F" device. The electromagnet was rotated continuously at the rate 6.7° per minute.

II. RESULTS OF MEASUREMENTS

1. <u>Cadmium</u>. The Cd samples, with axes parallel to the [1010], [2010], and [0001] directions, exhibited angular dependences agreeing with earlier investigations. ^[4,5,7] The angular dependences of the first two samples are almost completely identical; in polar coordinates they have the appearance of a two-leaved rosette with a deep minimum in the [1210] or [0110] direction. In these directions the magnetic-field dependence $\rho(H)$ of the resistance is an inflected curve; the resistivity increases quadratically in small fields, approaches saturation in moderate fields. In other directions (including [0001]) the resistivity is observed to increase almost quadratically. The Cd sample having its axis parallel to the [0001] direction exhibited almost no magnetoresistance anisotropy; its resistance increased quadratically for all field directions.

We supplemented the foregoing results by investigating $\rho_{H=const}(\mathfrak{F})$ for samples having the following orientations (in degrees):

Sample:	Cd-1	Cd-2	Cd-3	Cd-4	Cd-5
Orientation, φ; ϑ':	15;30	15;60	15;90	10;90	20;90

Here φ is the angle between the (2110) plane and the plane passing through the sample axis and [0001]; ϑ' is the angle between the sample axis and [0001].

Samples Cd-3, Cd-4, and Cd-5 exhibit mutually similar angular dependences agreeing with $\rho_{\text{H=const}}(\vartheta)$ for Cd samples having axes parallel to [1010] and [2110]. The resistance minimum is observed when the magnetic field direction lies in the basal plane (0001). When the sample axis deviates from the (0001) plane (for Cd-1 and Cd-2) the resistance minimum is always observed parallel to the line of intersection of the (0001) plane with the plane of magnetic-field rotation. The depth of the minimum is reduced with diminishing angle between the sample axis and [0001]. Other less pronounced, flatter, minima exhibit less dependence on the orientation of the crystal axis.

2. <u>Zinc</u>. Unlike the case for Cd, the angular dependences of resistance for Zn samples having axes along $[10\overline{1}0]$ or $[\overline{2}110]$ exhibit a second deep and narrow minimum in a field parallel to [0001]. A zinc sample having its axis parallel to [0001] exhibits almost no resistance anisotropy. In any direction the resistance increases quadratically with the magnetic field. ^[4,5]

In the present work about 40 samples were investigated, most of which had the following orientations: $\vartheta' = 90^{\circ}$ with $\varphi = 0, 5, 10, 15, 20, 25, and$ $<math>30^{\circ}$; $\varphi = 0, 15$, and 30° with $\vartheta' = 80, 70, 65, 60, 55,$ $50, 45, 40, 35, and 30^{\circ}$. The results obtained for Zn are essentially as follows.

The angular dependences $\rho_{H=const}(\vartheta)$ for samples with axes lying in the basal plane are mutually similar. We here observe two principal deep and narrow minima: one in the [0001] direction, and the other parallel to the (0001) plane. One additional less pronounced minimum is also observed at an angle of 50-60° from the [0001] direction. Figure 1 shows one of these angular dependences.

In the [0001] direction the magnetoresistance curve approaches saturation and is modulated by quantum oscillations of the resistance (the Shub-



FIG. 1. Angular dependence of resistance of Zn single crystals in a constant magnetic field H = 22.6 kOe. Curve 1-for sample Zn-1 ($\varphi = 10^{\circ}$, $\vartheta' = 90^{\circ}$) (with ordinate scale on the right); curve 2-for sample Zn-2 ($\varphi = 30^{\circ}$, $\vartheta = 70^{\circ}$) (with ordinate scale on the left). $\vartheta = 0^{\circ}$ for H || (0001).

nikov-de Haas effect). Quantum oscillations are not observed in the second principal minimum $\rho(H)$ having a small saturation region followed by growth in large fields. (The true behavior of resistance in a magnetic field for this direction can possibly be a curve approaching saturation, although the imperfection of the sample prevented a full development of this effect. The same comment applies to the Cd samples.)

In other directions there is approximately quadratic growth of resistance in a magnetic field. The depth of the minimum observed for $H \parallel (0001)$ decreases smoothly with a diminishing angle between the current and [0001]. The behavior of the second principal resistance minimum is a more complicated function of sample axis orientation.

For angles $\vartheta' > 50^{\circ}$ of samples having axes lying in the (1010) plane ($\varphi = 30^{\circ}$) a minimum is observed in the direction parallel to the intersection of the (1010) plane with the plane of magneticfield rotation (Fig. 1). As ϑ' decreases from 90° to 50° the minimum narrows, but its depth remains almost constant. At $\vartheta' \approx 50^{\circ}$ the minimum disappears abruptly; a resistance maximum then appears in the (1010) plane. Replacement of a minimum by a maximum can be observed either by using several samples with different values of ϑ' and by inclining a single sample in a magnetic field. The latter procedure is illustrated by the results obtained with sample Zn-3 (Figs. 2 and 3).



FIG. 2. Angular dependence of resistance in a constant magnetic field H = 18 kOe for sample Zn-3 ($\varphi = 30^{\circ}, \vartheta' = 41^{\circ}$). Curve 1-crystal axis perpendicular to the magnetic field (with ordinate scale on right); curve 2-crystal axis rotated 14° (in the (1010) plane toward [0001]) from a direction perpendicular to the field.



FIG. 3. Angular dependence of resistance for sample Zn-3. The conditions are the same as in Fig. 2. The angles labeling the curves are the deviations in the (1010) plane from a perpendicular to the magnetic field. The plus and minus signs denote inclination toward or away from [0001].

As ϑ' decreases from 90° to 84° in the ($\overline{2}110$) plane the discussed minimum undergoes no appreciable change. Beginning at $\vartheta' \approx 84°$ the minimum divides into two minima, each of which is observed in the ($10\overline{10}$) plane (Figs. 4 and 5). For samples with axes at angles φ from 0° to 30° the minima in ($10\overline{10}$) planes have different depths. These minima are also observed up to $\vartheta' \approx 50°$, after which they disappear (Fig. 6).

The Hall effect was measured on a Zn sample having the axis orientation $\varphi = 0^{\circ}$, $\vartheta' = 90^{\circ}$. The Hall emf was extremely small in all directions except those close to [0001] (e.g., for H = 23.5



FIG. 4. Change in the character of the resistance minimum as the sample axis in the $(\overline{2}110)$ plane departs from an orientation perpendicular to the magnetic field, for sample Zn-4 $(\vartheta' = 90^{\circ})$ in the field H = 18 kOe at T = 4.2° K. $\vartheta' = 0^{\circ}$ for H || $(\overline{2}110)$. The curves are spread out arbitrarily in the vertical direction and are labeled with the angles of deviation.



FIG. 5. Angular dependence of resistance for sample Zn-5 ($\varphi = 4^\circ$; $\vartheta' = 58^\circ$); H = 22.6 kOe, T = 4.2°K.

kOe, I = 1 A, and plate thickness 0.87 mm the Hall emf was ~ 5×10^{-8} V). The Hall emf increased by a factor of about 50 in the [0001] direction; its dependence on the magnetic field is linear in this direction. The Hall constant has the "hole conduction" sign and the value 8×10^{-4} electromagnetic cgs units.

3. <u>Thallium</u>. The only angular dependence $\rho_{\text{H}=\text{const}}(\vartheta)$ for Tl is that previously obtained in our earlier work^[6] on a sample having its axis in



FIG. 6. Depth of minimum vs. deviation of sample Zn-5 axis in ($\overline{2}110$) plane from an orientation perpendicular to the magnetic field (H = 18 kOe).



FIG. 7. Angular dependence of resistance for Tl single crystals in a constant magnetic field H = 22.6 kOe. Curve 1for sample Tl-1 ($\varphi = 19^\circ$; $\vartheta' = 90^\circ$); curve 2-sample Tl-2 ($\varphi = 19^\circ$; $\vartheta' = 50^\circ$). $\vartheta = 0^\circ$ when the magnetic-field direction is in a plane passing through the sample axis and [0001].

the (0001) plane. This function was well described by the expression $\rho(\vartheta) \sim \cos^2 \vartheta$ ($\vartheta = 0^\circ$ for H || [0001]). In the direction H || [0001] we observed approximately linear growth of resistance with increasing magnetic field strength, whereas in other directions the increase was quadratic.

In the present work about 30 thallium single crystals having different orientations were investigated.¹⁾ The principal results are as follows.



FIG. 8. Angular dependence of resistance for Tl single crystals in a constant magnetic field H = 22.6 kOe. Curve 1 for sample Tl-3 ($\varphi = 10^\circ$; $\vartheta' = 7^\circ$) (ordinate scale on the left); curve 2-sample Tl-4 ($\vartheta' = 0$; [0001] axis) (ordinate scale on the right).

For samples with axes in the (0001) plane $(\vartheta' = 90^{\circ}, \varphi = 0 - 30^{\circ})$ the function $\rho_{H=const}(\vartheta)$ has a form close to $\cos^2 \vartheta$ (Fig. 7). Saturation of resistance in a magnetic field is observed in the [0001] direction. The form of the angular dependence is preserved as the axes of samples depart from the basal plane by angles up to $\vartheta' \approx 50^{\circ}$. However, the coefficient A in $\rho(\vartheta) = A \cos^2 \vartheta$ gradually decreases. The resistance minimum in these cases is always observed in the direction parallel to the line of intersection of the plane passing through the sample axis and [0001] with the plane of magnetic-field rotation (Fig. 7). Saturation in the magnetic field was observed in these directions for all samples.

Beginning at about $\vartheta' \approx 50^{\circ}$ several narrow minima appear in the smooth angular dependence of the resistance (Fig. 8).

Finally, for a sample having its axis parallel to [0001] the angular dependence exhibits considerable anisotropy (Figs. 8 and 9). Measurements performed on this sample at $T = 4.2^{\circ}$ K in fields up to 23.6 kOe showed that in any direction of the magnetic field except [2110] the growth of resistance is more rapid than linear. Saturation was observed in the [2110] direction.

It was of interest to determine the variation of resistance for different crystallographic directions in large effective magnetic fields. For this purpose measurements were performed at 1.34°K in fields

¹⁾The authors are indebted to G. É. Karstens for preparation of the Tl single crystals.



FIG. 9. Angular dependence of resistance for sample Tl-4. a - H = 22.6 kOe, $T = 4.2^{\circ} \text{ K}$; b - H = 22.6 kOe, $T = 1.34^{\circ} \text{ K}$; c - H = 31 kOe, $T = 1.34^{\circ} \text{ K}$.

up to 33 kOe. The results are shown in Figs. 9 and 10. Two results are noteworthy:

1. The appearance of new narrow resistance minima. Figure 9 shows clearly the origination and development of these minima. For the resistance ratio $\rho(300^{\circ}\text{K})/\rho(1.34^{\circ}\text{K}) \approx 12,000$ at $T = 1.34^{\circ}$ and H = 31 kOe minima of $\rho_{\text{H}=\text{const}}(\vartheta)$ are observed at the following angles ϑ (in order of decreasing depth of the minimum): $30^{\circ}([\bar{2}110]$ direction), $0^{\circ}([10\bar{1}0]$ direction), 11.5° , 18.5° , and 4.5° .

2. Resistance saturation is reached both at the minimum and the maximum of the angular dependence; for different values of ϑ saturation is reached with different magnetic field strengths (Fig. 10).



FIG. 10. Resistance of sample Tl-4 as a function of the magnetic field for different crystallographic directions. (The curves are labeled with the values of ϑ in degrees.)

III. DISCUSSION OF RESULTS

According to our measurements, in the case of Cd quadratic increase of resistance occurs for any direction of the electric current and for any direction of the magnetic field that is not parallel to the (0001) plane. This behavior of the resistance occurs when for the given magnetic-field directions no open trajectories of conduction electrons exist on the Fermi surface, and $V_e = V_h$, where V_e and V_h are the respective "electron" and "hole" volumes of the Fermi surface.^[3] The behavior of resistance for $H \parallel (0001)$ as a function of current orientation is accounted for by the existence of open trajectories on the Fermi surface of Cd with their average direction parallel to [0001]. In accordance with the foregoing, Figure 11 shows the stereographic projection of significant magneticfield directions for the Cd Fermi surface.

For Zn, besides the minima in the (0001) plane, we observe a resistance minimum for $H \parallel [0001]$ and minima for $H \parallel (10\bar{1}0)$ (with the magnetic field departing by not more than 42° from [0001]). The minimum for $H \parallel [0001]$ remains unchanged for any current direction, whereas the depth of minima for $H \parallel (10\bar{1}0)$ depends on the current direction. A minimum reaches its greatest depth when the current is parallel to (10\bar{1}0) and is less deep for other directions. For all other magnetic-field directions the behavior of Zn resistance coincides with that of Cd.

The existence of the foregoing resistance minima in the angular dependences for Zn can be accounted for by open electron trajectories parallel



FIG. 11. Stereographic projections of significant magneticfield directions for Fermi surfaces: a - Cd, b - Zn, c - Tl. Region I – two-dimensional regions of magnetic-field directions for which open electron trajectories appear on the Fermi surface. The open trajectories disappear for H \parallel [0001] and on the boundary of the two-dimensional region. Regions II – magneticfield directions for which there are no open trajectories, but the "electron" and "hole" volumes of the Fermi surface compensate each other. Regions III – magnetic-field directions for which extremely elongated electron trajectories exist (regions III are shown with arbitrary boundaries). The central line of a region III is a special line. Open electron trajectories appear in the directions of special lines.

to the (0001) plane. Indeed, for $H \parallel [0001]$ we should in this case observe resistance saturation that is independent of current direction. Close to the [0001] direction minima of the function $\rho_{H=const}(\vartheta)$ should be observed. For large de-viations of the magnetic field from [0001] resistance minima can be observed only in rational planes.^[3] The experimental results for Zn are represented by a stereographic projection of significant magnetic-field directions (Fig. 11b).

The stereographic projection shown in Fig. 11c can explain the behavior of resistance anisotropy in Tl single crystals. Before comparing the experimental results for Tl with this projection, it should be noted that the behavior of resistance in the presence of greatly elongated closed electron trajectories on the Fermi surface should not differ qualitatively from that in the case of open trajectories, i.e., the magnetic-field dependence of resistance for extremely elongated closed orbits depends essentially on the current orientation with respect to the largest orbital diameter. When the current is perpendicular to this diameter the resistance should not depend on the field. For current directions parallel or almost parallel to the diameter the resistance increases with the square of the field. Greatly elongated trajectories always appear close to special lines in the stereographic projection. The given stereographic projection of significant magnetic-field directions for Tl consists of a two-dimensional region (with its radius determined only very approximately) and special lines. The separation of the special lines does not exceed 12°; therefore the regions between special lines can comprise regions of extremely elongated trajectories.

According to the stereographic projection for Tl samples having axes in the range $90^{\circ} > \vartheta > 45^{\circ}$ the angular dependence of the resistance should be of the form $\rho = A \cos^2 \vartheta$ (where ϑ is measured from a plane passing through the sample axis and [0001]). For $\vartheta' < 45^{\circ}$ the magnetic field will intersect the special lines, with extrema appearing on the resistance curves. Special lines in the stereographic projection for Tl form with the trace of the (1010) plane the angles $\varphi' = 0$, 4.5, 11.5, 18.5, and 30°. For a sample having its axis parallel to [0001] resistance saturation should be observed in large magnetic fields at all angles ϑ .

IV. TOPOLOGICAL TYPES OF OPEN Cd, Zn, AND T1 FERMI SURFACES

In our discussion of the forms of open Cd, Zn, and Tl Fermi surfaces we shall made the reasonable assumption that our earlier investigation^[3] of the topological properties of constant-energy electron surfaces in tetragonal metals can be applied qualitatively to hexagonal lattices.

Figure 12 shows the most general case of an open constant-energy electron surface which intersects all faces of the first Brillouin zone. We assume that the tubes formed here around the [0001] and $[\bar{2}110]$ edges have diameters such that all possible open electron trajectories are parallel to the (0001) plane and to the [0001] axis. According to the stereographic projection (Fig. 11b) Zn should possess a surface of this type. Since the "electron" and "hole" volumes compensate each other

FIG. 12. System of open directions for the Fermi surface of a hexagonal metal. Arbitrary dimensions are shown for the Brillouin zones and surfaces.



on the Zn Fermi surface, the sign of the Hall constant measured in the [0001] direction indicates that the open Fermi surface corresponds to electrons.

The radius of the two-dimensional region $(\theta_0 \approx 6^\circ)$ and the lengths of special lines $(\theta_{(10\overline{1}0)} \approx 42^\circ)$ in the stereographic projection can be used to calculate the minimum diameter d_{\min} of the tube parallel to $[\overline{2}110]$.

In the $[10\overline{1}0]$ direction $d_{min} \approx 0.03 \text{ b}$; in the [0001] direction $d_{min} \approx 0.1 \text{ b}$ (b = $1.16(2\pi/a)$, a = 2.664 Å). The diameter of the tube parallel to [0001] cannot be determined from our measurements; however, we note that according to Ver-kin's^[8] measurements of the de Haas-van Alphen effect the diameter of this tube must be extremely small (of the order 0.10 b).

For the open Cd Fermi surface tubes parallel to $[\overline{2}110]$ should be absent according to our results, whereas for Tl tubes parallel to [0001] should be absent.

If it is assumed that the Fermi surface of Tl consists of slightly undulating sheets parallel to (0001) and joined in the [0001] direction by cylindrical tubes, we can compute the maximum possible diameter d of these tubes and the distance h between the sheets.^[3] Assuming that the radius of a two-dimensional region in the stereographic projection is $\theta_0 = 45^\circ$ and that the length of a special line for $\varphi' = 4.5^\circ$ is $\theta = 90^\circ$, the calculations yield $h = d \le 0.1b$ [$b = 1.16(2\pi/a)$, a = 3.45 Å].²⁾

The model of a nearly free electron gas has recently received good experimental confirmation for Al, Pb, and Sn.^[9]. It is interesting to compare the foregoing results with this model. Figure 13 shows a central (1010) cross section of the Tl Fermi surface based on Harrison's construction.^[9] This surface agrees qualitatively with experimental results. However, the theoretical diameter d_{th} is several times larger than the experimental value d_{exp} .

The Fermi surface of hexagonal close-packed divalent metals has been considered by other authors.^[9,10] As represented by Fawcett^[10] this surface contains two types of open trajectories dd trajectories lying in the basal plane and aa trajectories parallel to [0001]. This surface thus completely fits the experimental results obtained for Zn.

The dd trajectories have not been observed ex-



FIG. 13. Central section of an open Fermi surface of T1 by the (1010) plane, constructed in accordance with $[^9]$. Dimensions are given in the unit $(2\pi/a)$.

perimentally for the Cd Fermi surface. As reported in the literature the Mg Fermi surface contains only dd trajectories. [11,12] From Borovik's data [13] we can infer that the Be Fermi surface has no open trajectories. While the differences between the topological properties of the Fermi surfaces of Be, Mg, and Cd are not surprising since these metals possess different values of c/a, it is difficult to account for the essential difference in the cases of Zn and Cd on the basis of the free-electron model, since almost identical values of c/a are found for the Zn and Cd lattices.³⁾

The authors wish to thank Academician P. L. Kapitza for his interest in this work.

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Translated by I. Emin 359

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Submitted to JETP editor February 14, 1963

J. Exptl. Theoret. Phys. (U.S.S.R.) 44, 1421 (April, 1963)

A conclusion is drawn in this article that the open Fermi surface in zinc has the same sign as the electron. Unfortunately, an error was made in the sign in the analysis of experimental results on the measurement of the Hall emf. Therefore, it should be concluded that the sign of the Hall constant is "electronic" in zinc in the [0001] direction, at fields from 5 to 22 kOe. This agrees with the much earlier measurements of E. S. Borovik (Dissertation, Physico-technical Institute, Khar'kov, 1954). Thus the open Fermi surface of zinc corresponds to "holes."

Translated by R. T. Beyer