TOPOLOGY OF THE FERMI SURFACE FOR GOLD

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The resistance anistropy of gold single crystals in a magnetic field has been investigated. It has been found that for certain directions of the magnetic field relative to the crystallographic axes of the single crystals the resistance increases as the square of the field, while for other directions it reaches complete saturation for values of the field $H \gg H_0$. It can thus be concluded that an open Fermi surface exists in the case of gold. A stereographic projection of preferred directions of the magnetic field has been constructed, and an analysis of it shows that the Fermi surface in the case of gold is a "spatial net" formed by "corrugated cylinders" whose axes are parallel to the [110] and [111] directions of the reciprocal lattice. The resistance of gold single crystals has been averaged over the angles. The values of the averaged resistance depend linearly on the magnetic field, thus explaining Kapitza's law.

1. INTRODUCTION

THE theory of galvanomagnetic phenomena based on the assumption of the quadratic form of the dispersion of the conduction electrons in a metal $\epsilon(\mathbf{p}) = \mathbf{p}^2/2m^*$ (ϵ is the energy, $\mathbf{p}$ is the quasi-momentum, m^* is the effective mass of electron[1,2]) was unable to explain such well known experimental facts as the linear increase in the resistance of polycrystalline samples (Kapitza's law[3]) and the pronounced resistance anisotropy of single crystals in a magnetic field.[4-6]

In 1955 I. Lifshitz, Azbel', and Kaganov[7] carried out a theoretical investigation of galvanomagnetic phenomena in metals with an arbitrary dispersion law. A very important aspect of this investigation was the treatment of the conduction electrons in the metal as a gas of quasi-particles with a complex anisotropic dispersion law $\epsilon(\mathbf{p})$ which may correspond to both closed and open isoenergetic surfaces $\epsilon(\mathbf{p}) = \zeta_0$. It was shown that in the region of strong magnetic fields $H \gg H_0$ (H_0 is the field for which $l/r = 1$, l is the mean free path, r is the radius of curvature of the electron trajectory in the magnetic field) the characteristic features of the galvanomagnetic properties of metals are determined by the topology of the Fermi surface $\epsilon(\mathbf{p}) = \zeta_0$ and do not depend on the interaction between the electrons and the lattice imperfections.

In the case of metals with open Fermi surfaces the theory[7] established in principle the possibility of saturation of the resistance of single crystals for some orientations of the magnetic field, and the quadratic increase of the resistance for other orientations. In the case of metals with closed Fermi surfaces we should not expect pronounced anisotropy of the resistance in a magnetic field, and, moreover, for metals with $n_1 \neq n_2$ (n_1 and n_2 are the densities of electrons and of "holes") the resistance will tend to saturation, while in the case $n_1 = n_2$ the resistance will increase quadratically with the magnetic field.

Thus, experimental study of galvanomagnetic phenomena enables us to obtain valuable information on the topology of Fermi surfaces in metals. However, this possibility was rendered doubtful as a result of the work of Chambers.[8] By extrapolating the experimental results to $H = \infty$ he concluded that the linear increase of resistance in the case of polycrystalline samples of Au, Cu, and Ag will occur only at very high values of the magnetic field, while, according to Lifshitz, Azbel' and Kaganov,[7] the resistance in this case must either increase quadratically with the field, or must be independent of the field.

It should be emphasized that Chambers carried out his measurements using polycrystalline samples. It appeared to us to be probable that an investigation of single crystals would lead to an essentially different picture. In connection with this we undertook an investigation of the resistance of single crystals of gold in a magnetic field, for which the linear growth of resistance in the case of polycrystalline samples[4] and the pronounced anisotropy of resistance in the case of single crystals[9] have been established most clearly. A preliminary communication of the results obtained by us has been given earlier.[10]

2. SAMPLES AND THE MEASUREMENT METHOD

As we have noted already, the modern theory of galvanomagnetic phenomena in metals has been developed for the case of large fields $H \gg H_0$. In the case of monovalent metals H_0 may be estimated from the condition $l/r = H/\rho_0 nec = 1$, where e is the electron charge, n is the electron density, c is the velocity of light in vacuo, ρ_0 is the specific resistance at $H = 0$.

The validity of the condition $H \gg H_0$ improves as ρ_0 becomes smaller. Therefore, it is necessary to carry out the measurements at low temperatures utilizing samples of high purity.

a) Samples. The material used for the preparation of the samples was gold of purity 99.9999% (the impurities were Ag ≈ 0.00008% and Cu ≈ 0.00002%).

Gold single crystals were prepared by a method due to Bridgman.[11] The initial material in a quantity sufficient for obtaining one sample was melted under high vacuum in the wide portion of a quartz flask at the end of which there was a capillary of the required diameter and length (usually of 0.5 mm diameter and of length ~ 20 mm).

After melting and outgassing, the metal under a small pressure (≈ 1 atm) of gaseous helium was made to fill the capillary. The capillary was detached from the flask and was placed inside a quartz tube which could be pulled through an oven. The oven temperature was of the order of 1200°C. A clockwork mechanism pulled the oven along the quartz tube. The length of time that the sample remained in the oven was varied from 2 to 60 min.

After crystallization the quartz capillary was dissolved in hydrofluoric acid, and the sample was subjected to etching in aqua regia. A five minute etching period was sufficient to make the crystal sides produce sharp reflections, which permitted the optical method to be used for the determination of the orientation of the samples. The determination of orientations was carried out by means of a two-circle reflecting goniometer. As measurements have shown, in the case of gold which has a cubic face-centered lattice the planes giving the most intense reflections are the (111) planes. The shape of the reflected spots was that of three-pronged stars. Only the reflections from the (111) planes were used for the determination of the orientation. The accuracy of measurement was ~ 1°.

The determination of the orientation of a large number (~ 20) of single crystals showed that with such a method of preparation the axes of the samples were situated primarily in the binary plane of the crystal. In this plane the direction of the sample axes was random.

Eight samples were selected for the measurements. The characteristics of these samples are given in Table I (one can also infer the orientation of the samples from Fig. 5).

b) Mounting the samples. Particular attention was paid to the mounting of the samples. In reference 12 it was shown that the relative position of the sample electrodes may significantly affect the results of the measurements. It is also necessary to take precautions against the deformation of the samples.

We soldered the current electrodes (copper wire of 0.15 mm diameter) by means of Wood's alloy to the ends of the sample. The potential electrodes (copper or gold wire of 0.05 mm diameter) were mounted at a distance of ⅓ of the sample length from its ends.

The wire encircled the sample by a single loop and was drawn tight. The ring formed in this manner was in tight contact with the sample and was then soldered.

The sample was then mounted in an ebonite holder which had the shape of a hollow half-cylinder. One end of the sample was glued to the inner wall of the half-cylinder while the other was completely free. A long metal needle could be inserted into the holder perpendicular to its axis (and to the sample axis), and a second determination of the directions of the crystallographic axes could be carried out with respect to it. By fixing the direction of the

TABLE I

Samples*	Au-1	Au-2	Au-3	Au-4	Au-5	Au-6	Au-7	Au-8
Orientation φ, ϑ', in degrees	23; 85	45; 90	45; 50	42; 4	45; 17	45; 28	40; 84	42; 84
$\rho(300°)/\rho(4°,2)$	1650	304	1456	945	1022	896	1178	1670
H_0, koe	1.4	7.6	1.56	2.44	2.25	2.6	1.95	1.38

*φ and ϑ' are polar coordinates of the sample axes in the stereographic projection of the gold lattice (Fig. 5); φ is the angle measured from the (010) plane, ϑ' is the angle between the [001] axis and the sample axis.

needle with respect to the magnetic field it was possible to determine the direction of the projections of the principal crystallographic axes on the plane in which the magnetic field was rotated and which was perpendicular to the sample axis. The error in determining the orientation with respect to the magnetic field could amount to not more than 2°.

c) Measurements. For the measurement of resistance we utilized a potentiometer KL-48 with a galvanometric two-stage photoelectric amplifier FEOU-15. The sensitivity of this arrangement was 1×10^{-9} V/(mm/m). The measuring current through the sample was usually equal to 0.5 amp.

To eliminate the effect of thermoelectric and Hall emfs both the measuring current and the magnetic field were chopped. The magnetic field was provided by means of an electromagnet which enabled us to obtain field intensities up to 24,000 oe in a 20 mm gap, and up to 34,000 oe in a 12 mm gap. Most of the measurements were carried out at T = 4.2°K, since when the temperature was lowered further the decrease in the resistance of the samples was insignificant.

3. RESULTS OF MEASUREMENTS

The dependence of the resistance $\rho(\vartheta)$ on the angle was measured for all eight single crystals in a constant magnetic field of H = 23,500 oe. The angle ϑ through which the magnetic field was rotated was varied from 0° to 180°, and the resistance was measured at intervals of 2.5°. Figures 1 — 4 show rotation diagrams for four gold single crystals:

$$\frac{\Delta\rho_H}{\rho_0} = \frac{\rho_H(\vartheta) - \rho_0}{\rho_0}.$$

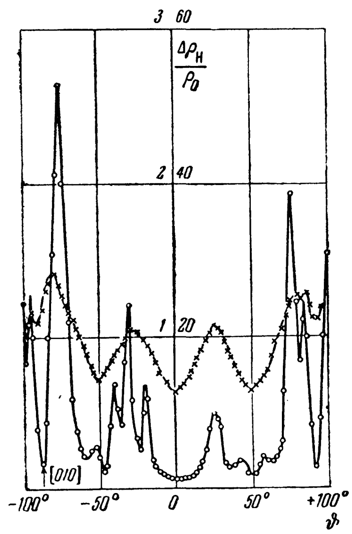


FIG. 1. Angular dependence of the resistance of the single crystal Au-1: H = 23,500 oe; o — T = 4.2°K (the values of $\Delta\rho_H/\rho_0$ are shown on the right); × — T = 20.4°K (the values of $\Delta\rho_H/\rho_0$ are shown on the left).

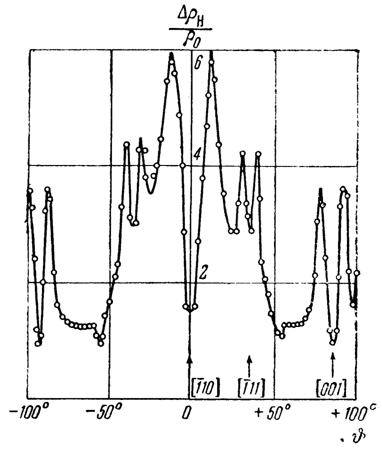


FIG. 2. Angular dependence of the resistance of the single crystal Au-2: H = 23,500 oe; T = 4.2°K.

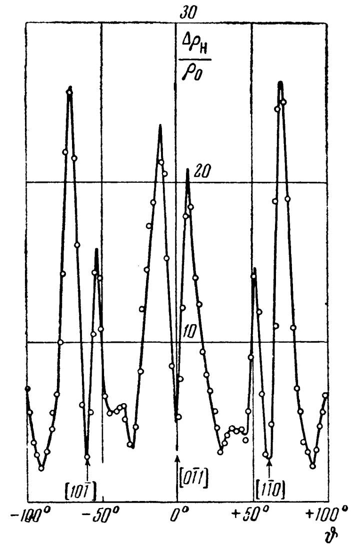


FIG. 3. Angular dependence of the resistance of the single crystal Au-3: H = 23,500 oe; T = 4.2°K.

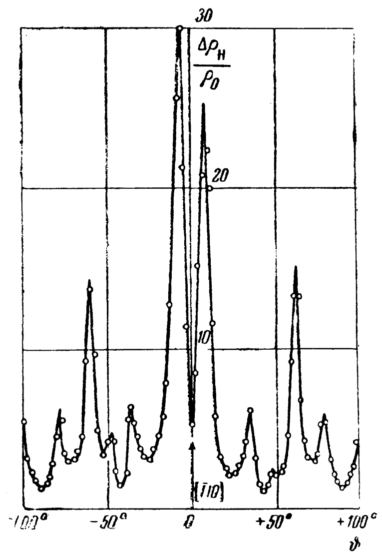


FIG. 4. Angular dependence of the resistance of the single crystal Au-5: H = 23,500 oe; T = 4.2°K.

A very sharp anisotropy characterizes the angular dependence of the resistance of gold single crystals. In the range of angles 5 — 10° the resistance varies by a factor of 10 or more. Very sharp maxima and minima occur in the rotation diagrams. Their position corresponds to the crystallographic symmetry of the samples.

The directions of the narrow minima coincide with the special crystal directions [001], [110], and [111]. Narrow maxima are situated symmetrically with respect to these directions at small distances from each other (not exceeding 26°). Very broad minima also occur (for example, in Fig. 1 at 0°). Considerable anisotropy showing all the characteristic features is also observed in the other gold samples. Table II gives the angular coordinates (with an accuracy of ± 0.5°) of all the maxima and the narrow minima occurring in the rotation diagrams.

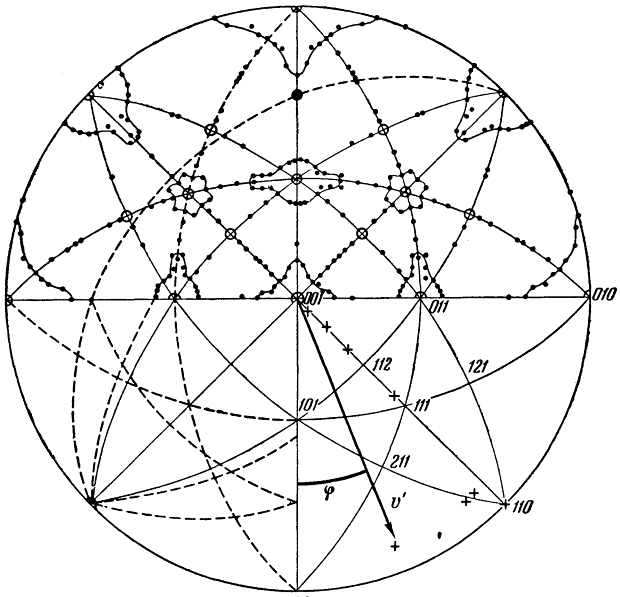


FIG. 5. The stereographic projection of the directions of the maxima (●) and of the narrow, deep minima (o), observed for all eight gold single crystals. Dotted lines show the traces of the planes of rotation of the magnetic field for some samples (Au-2, Au-3, and Au-6), + – orientations of the sample axes.

On the basis of all the rotation diagrams a stereographic projection was constructed of those directions of the magnetic field at which maxima occur (Fig. 5). The directions of the narrow minima are also indicated in the same diagram. Such a projection enables us to obtain a qualitative picture of the angular dependence of the resistance of a gold sample with an arbitrary crystallographic orientation. The experimental points on the projection are grouped in a twofold manner: the directions of the maxima of the first type are situated on lines which surround small regions in the stereographic projection. The centers of these regions coincide with the directions of the crystal axes [001], [110], and [111]. The basic dimensions of the regions are as follows: regions 001 and 110 — 26° and 15°, region 111 — 12° and 10°. The directions of the maxima of the second type lie in the (110) and (111) planes. The rotation diagram for the Au-1 sample (Fig. 1, $\vartheta = 0$) enables us to conclude that there are no maxima in directions lying in the (001) plane.

Two characteristic features of the stereographic projection should be noted: 1) if the directions of the current and of the magnetic field both lie in the binary plane then, instead of there being a maximum in the rotation diagram, a minimum occurs (for example, Fig. 4, $\vartheta = 90°$). It is quite likely that the same is also true for current and field directions lying in the (111) plane. 2) In the direction of the intersection of the (110) and (111) planes the maxima also disappear, and the minimum occurring in this case, in contrast to the minima in the directions [001], [110] and [111], is not surrounded by a line of maxima (Fig. 2, $\vartheta = +55°$ and Fig. 3, $\vartheta = \pm 30°; \pm 90°$).

The dependence of the resistance on the magnetic field was investigated for the directions corresponding to the minima and the maxima of the rotation diagrams.

As may be seen from Figs. 6 and 7, complete saturation of resistance is observed in the directions of the minima; in the directions of the maxima the resistance increases without limit: $\Delta\rho_H/\rho_0 \sim H^n$, where n varies from 1 to 1.8 for different maxima (cf. Table II).

Measurements in the region of low fields have shown that the difference in the character of the

TABLE II

Samples	Direction $\vartheta=0°$	Directions of the maxima in degrees. Brackets contain the power index n $\Delta\rho_H/\rho_0 \sim H^n$	Direction of the narrow, deep minima in degrees
Au-1	Intersection with the plane (001)	+85 (1.5); +78 (1.75); +58; +43 (1); +25 (1.25) −75 (1.8); −52; −40; −30 (1.5); −18 (1.35)	−87
Au-2	$[\bar{1}10]$	±13 (1.8)±30; +38: +82; −40; −81	0; ±35?; ±55;±90
Au-3	$[0\bar{1}1]$	±8; ±35; ±53; ±70	0; ±60
Au-4	[010]	+10; ±38; ±55; ±82; −7	0; ±45
Au-5	$[\bar{1}10]$	±8 (1.7); +35 (1)±48; ±60 (1.5); −37; ±80 (1)	0
Au-6	$[\bar{1}10]$	±7 (1.7); ±33 (1.15); ±50; +72; +78 (1.5)	0
Au-7	$[\bar{1}10]$	±7 (1.7); ±25; ±40; +55; ±82; −62	0; ±90
Au-8	$[\bar{1}10]$	+8; +30; +80; −15 (1.7); −32; ±40; ±63; −82	0; ±35

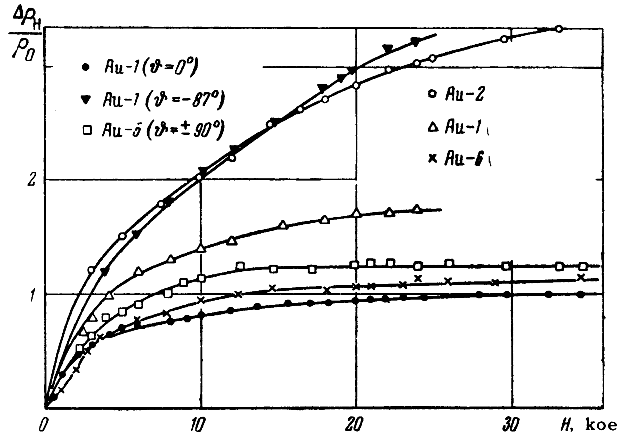


FIG. 6. Dependence of the resistance on the magnetic field in the direction of the minima in the rotation diagrams; ○ – ϑ = ± 35°, Δ – ϑ = – 45°, × – ϑ = ± 42°.

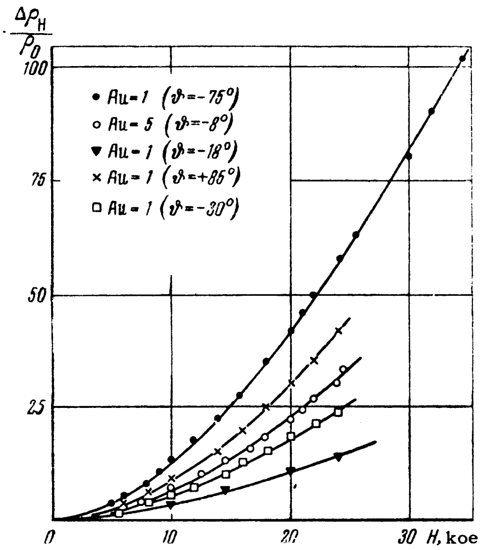


FIG. 7. Dependence of the resistance on the magnetic field in the direction of the maxima.

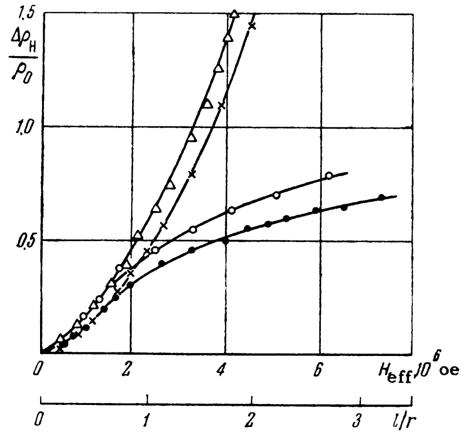
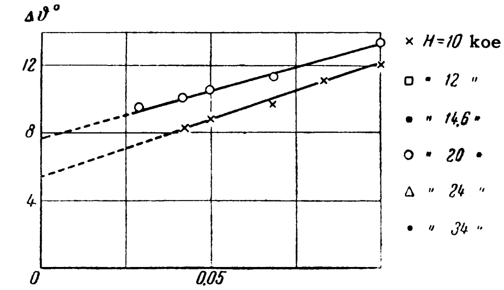


FIG. 8



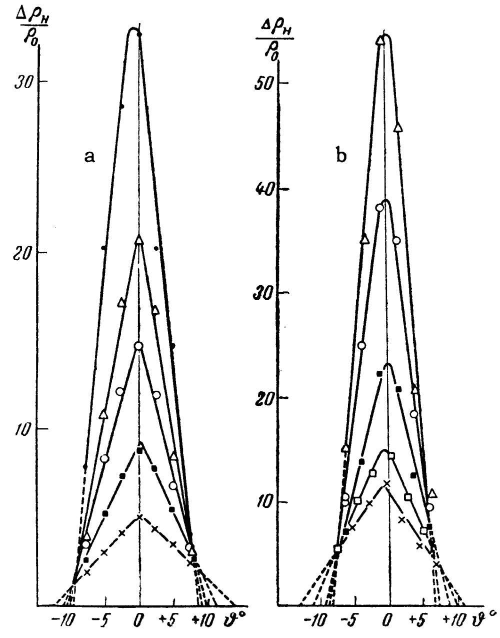


FIG. 9

variation of the resistance corresponding to a minimum and a maximum sets in at fields close to H_0. It may also be seen from Fig. 8 that measurements at a temperature of 20.4° do not differ in any essential way from measurements carried out at 4.2°K (naturally, the measurements at higher temperatures are equivalent to measurements in smaller effective fields).

It was of interest to study the change in the shape of the maxima as the magnetic field was varied. From Fig. 9 it is seen that the width of a maximum of the first type decreases approximately as 1/H with increasing field. It was also established qualitatively that the width of the maxima of the second type also decreases as the magnetic field is increased.

The increase of resistance in a magnetic field in the direction of the maxima and a corresponding decrease in their width must lead to a decrease in the power of the dependence of the resistance on the field after averaging over the angle ϑ has been carried out. This was checked on samples Au-1 and Au-5. In the case of these samples rotation diagrams were obtained at several values of the magnetic field (from 5000 to 24,000 oe). For each value of the field the resistance was averaged over the angle ϑ. It turned out that the averaged resistance depends linearly on the magnetic field. The averaging of the resistance for an individual maximum of the first type (sample Au-1, $\vartheta = -75°$ in the interval from $-85°$ to $-69°$) also leads to a decrease in the power index n, however, we do not obtain a linear dependence as a result ($n \approx 1.4$). The results of averaging are shown in Fig. 10. Here are also given for purposes of comparison the curves for $\Delta\rho/\rho_0$ obtained by Kapitza[3] and Justi[4] for polycrystalline gold samples.

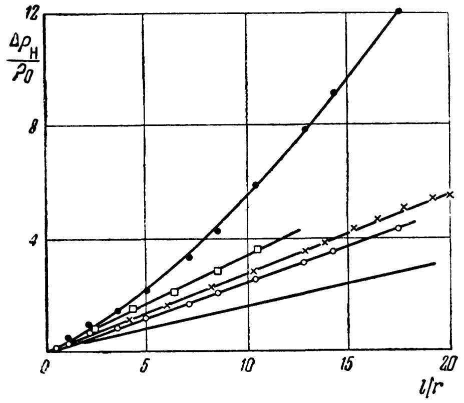


FIG. 10. Dependence on the magnetic field (in units of l/r) of the resistance averaged over the angle ϑ: o – Au-1 (from –87° to 93°); □ – Au-5 (from 0° to –106°); • – Au-1 (maximum of the first type from –87° to –69°); × – Justi's results[4] for polycrystalline gold samples. The lowest straight line is an extrapolation of Kapitza's results[3] for polycrystalline gold samples.

4. DISCUSSION OF RESULTS

a) The Fermi surface for gold. A comparison of the results obtained by us with theory[7] shows that the Fermi surface for gold is open. This finds its expression in the fact that the resistance increases in the magnetic field in quite a different manner (quadratic increase and saturation) for the different crystallographic directions.

The galvanomagnetic properties of metals having open Fermi surfaces have been treated in the paper by Lifshitz and Peschanskiĭ.[13] One of the principal conclusions of this paper is that on the basis of an experimental study of the resistance anisotropy of a metal it is possible to determine those directions in which the Fermi surface is open.

Figure 11 gives a stereographic projection of the special directions of the magnetic field in the case of gold which was constructed on the basis of the projection of the maxima (Fig. 5). For the directions of the magnetic field lying within the two-dimensional regions I of this projection and in the (111) and (110) planes one should observe according to the theory[13] a quadratic increase in resistance

$$\Delta\rho_H / \rho_0 \sim H^2 \cos^2 \alpha, \qquad (1)$$

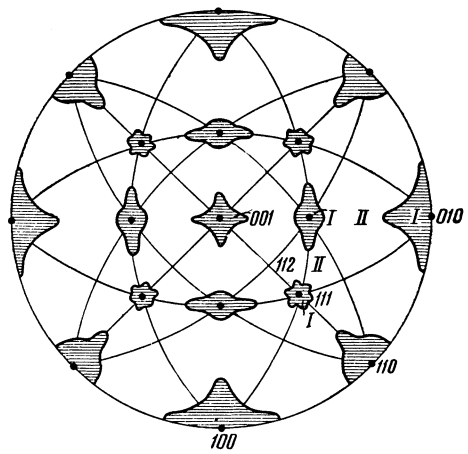


FIG. 11. The stereographic projection of special directions of the magnetic field for the Fermi surface for gold. The shaded regions (I) and the lines joining the regions I are directions for which the resistance increases quadratically with the magnetic field. In regions II the resistance does not depend on the field for $H \gg H_0$ (saturation). Points denote the directions of narrow deep minima.

where α is the angle between the current and the direction of the open sections of the Fermi surface. However, the dependence of the resistance on the field observed experimentally for these directions is somewhat less than quadratic. This circumstance may be explained by the averaging of the resistances associated with the narrow maxima as the result of the single crystals not being perfect, the magnetic field not being homogeneous, etc. As has been shown earlier, an averaging of this type leads to a decrease in the power dependence of the resistance on the field.

On taking this into account we may assume that the Fermi surface for gold, in accordance with the stereographic projection (Fig. 11), is represented (in a topological sense) by a "spatial net" formed by "corrugated cylinders" whose axes are parallel to the [110] and [111] axes of the reciprocal lattice. Indeed, the special directions situated in the (110) and (111) planes are formed by the "cylinders" [110] and [111]. The two-dimensional regions I arise as a result of the mutual intersection of these cylinders. Thus, the region 001 is formed by the cylinders [110] and [$\bar{1}$10] which intersect in the plane (001); the region 110 is formed by the cylinders [1$\bar{1}$0], [$\bar{1}$11], [1$\bar{1}$1], which intersect in the (110) plane; and, finally, the region 111 is formed by the cylinders [$\bar{1}$10], [0$\bar{1}$1] and [$\bar{1}$01], which intersect in the (111) plane. The dimensions and the shapes of the two-dimensional regions are chosen in accordance with the experimental data. The basic dimensions of the regions 001 and 110 are 15° and 26°, while the corresponding dimensions of the 111 region are 10° and 12°. (It is possible that the actual dimensions of the regions are really somewhat larger, but in any case they cannot be smaller than the values indicated).

In accordance with reference 13, a very narrow minimum should appear for the central direction [001], [110] and [111] of the two-dimensional region in the diagram of the angular dependence of the resistance, and the resistance should tend to saturation in that direction. This finds good experimental confirmation. For all the other directions of the magnetic field (the broad regions II in Fig. 11) lying in the Fermi surface of the type indicated above a saturation of resistance should be observed. This is also confirmed by measurements (in the rotation diagrams broad minima correspond to these directions).

Let us now discuss the two peculiar features of the stereographic projections (Figs. 5 and 11) noted above.

1. Since the [112] direction is not surrounded by a two-dimensional region of special directions of the magnetic field (in contrast to the [001], [110] or [111] directions) we can conclude that some of the "corrugated cylinders" of the Fermi surface for gold do not intersect (for example, for the [112] direction such "cylinders" will be [$\bar{1}\bar{1}$1] and [$\bar{1}$10]).

2. Expression (1) enables us to explain the absence of maxima in the rotation diagrams of samples Au-5 and Au-6 in the directions $\vartheta = 90°$, which are perpendicular to the axes of the "cylinders" [1$\bar{1}$0]. In the case of these samples the direction of the current, as well as the direction of the field, lies in the (1$\bar{1}$0) plane. As a result of this angle $\alpha = 90°$, and minima should indeed arise in the rotation diagrams.

An investigation of the resistance anisotropy in a magnetic field enables us to draw conclusions only with respect to the direction of the open sections of the Fermi surface.

The shape of the Fermi surface for a metal can be constructed on the basis of results obtained by other experimental methods (oscillation of susceptibility, anomalous skin-effect, cyclotron resonance). Pippard[14] has constructed the Fermi surface for copper on the basis of a study of the anomalous skin-effect. Peschanskiĭ[15] has generalized the analytic expression for the Fermi surface for copper proposed in reference 16 and has investigated the possible types of open Fermi surfaces for metals with a face-centered cubic lattice. The stereographic projection of the special directions of one of the Fermi surfaces discussed by him agrees very well with the stereographic projection for gold. On taking into account the results of these papers it becomes natural to represent the Fermi surface for gold in the form of "cubes." In the space of the reciprocal lattice the "cubes" are joined at their vertices in such a way that open directions occur along the [111] and [110] axes, while the direction along the [001] axis remains closed.*

b) Kapitza's law. In the case of gold single crystals both a quadratic increase and a complete saturation of resistance in a magnetic field are observed. The resistance of polycrystalline samples of gold, as is well known,[3,9] depends on the field linearly. This forces us to conclude that Kapitza's law is a result of the averaging of the resistance over the variously oriented (with respect to the field) crystallites which make up the polycrystalline sample.[10] This conclusion is confirmed by averaging over the angle ϑ the resistance of the single crystal samples Au-1 and Au-5.

A theoretical explanation of Kapitza's law (using as an example a metal with a Fermi surface of the "corrugated cylinder" type) is given in reference 13. From the same paper it may also be seen that the resistance of the single crystals averaged over the angles lying in the two-dimensional region I (Fig. 11) will not depend linearly on the magnetic field ($\overline{\Delta\rho_H}/\rho_0$ must be proportional to H^2). A confirmation of this is provided by the results of averaging the resistance over a maximum of the first type ($n \approx 1.4$, Fig. 10).

Since the dimensions of the two-dimensional regions are relatively small, then in fields, which exceed H_0 by a factor of only several fold, their contribution to the averaged resistance is not significant. Therefore, averaging of the resistance for single crystals of gold which has a Fermi surface of the "spatial net" type is equivalent to averaging the resistance of single crystals of a metal with a Fermi surface of the "corrugated cylinder" type. However, in the region of very high fields the role played by the two-dimensional regions is significant, and the resistance of single crystals averaged over the whole rotation diagram will no longer depend linearly on the field.

For the reasons stated above one can expect that in the region of very high magnetic fields deviations from Kapitza's law will occur for gold polycrystalline samples (in contrast to the results of reference 8).

In conclusion the author considers it his pleasant duty to thank Academician P. L. Kapitza for

*If we assume that we can use Eq. (1) of reference 13 to estimate the smallest diameter of the "corrugated cylinder" [110], then it is possible to form some idea of the area of mutual intersection of the "cubes" of the Fermi surface for gold. For the [110] "cylinder" the smallest diameter (in units of the reciprocal lattice constant b) is equal to 0.1b.

his close attention to this work and Prof. N. E. Alekseevskiĭ for constant guidance. The author is also grateful to Professor I. M. Lifshitz and V. G. Peschanskiĭ for discussion of the results obtained by him.

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