transition were to occur, the mode of occurrence would be quite different. Our results definitely indicate that this is true; the transition in the liquid is not discontinuous as in the solid and begins to occur much earlier in pressure. The calculations of Alekseev and Arkhipov,[8] which disregard structure, would seem to indicate no difference between liquid and solid, but this does not seem to be in accord with the present experimental findings.

Cesium IV

The structure of Cs IV has not been resolved. Hall *et al.* have apparently had difficulty in indexing their pattern taken after the Cs III-IV transition. The three structures that appear to be most probable in this connection are the hexagonal close-packed arrangements encountered in the rare-earth metals, bcc structure (this bcc is a collapsed version) and the so-called ω phase encountered at high pressures in the hcp metals Ti and Zr.[26] If the first of these possibilities is true, it is quite puzzling why the Cs III-IV phase change is accompanied by a large decrease in resistance, since a phase transition of the type fcc $\rightleftarrows$ hcp $\rightleftarrows$ dhcp is not usually followed by any such drastic resistivity change. On the other hand, if Cs IV had the bcc structure (bcc could possess a higher density relative to fcc)[27–29] there should have been no difficulty in indexing the pattern.

Cesium IV behaves like a normal metal in that its resistivity decreases gradually with pressure. A determination of the structure of Cs IV would greatly aid in understanding at least in a qualitative way the resistivity behavior of this phase.

[26] J. C. Jamieson, Science **140**, 72 (1963).

ACKNOWLEDGMENTS

We wish to thank Dr. T. M. Rice for illuminating discussions, Dr. D. B. McWhan for commenting on the manuscript, and P. H. Schmidt for some high-purity Cs. It is a pleasure to acknowledge the assistance of R. G. Maines in the pressure runs.

[27] H. T. Hall, J. D. Barnett, and L. Merrill, Science **139**, 111 (1963).
[28] A. Jayaraman, Phys. Rev. **135**, A1056 (1964).
[29] D. B. McWhan and A. Jayaraman, Appl. Phys. Letters **3**, 129 (1963).

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High-Field Galvanomagnetic Properties of Niobium and Tantalum

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The galvanomagnetic properties of niobium and tantalum were measured at 4.2°K in fields up to 100 kG for single crystals having residual resistivity ratios of 1500 (niobium) and ~10 000 (tantalum). The two metals exhibit very similar anisotropy of their galvanomagnetic properties. Each is uncompensated, with a net number of carriers equal to one hole per atom. The strong anisotropy of the magnetoresistance results from open orbits on a surface which is topologically similar to a set of intersecting cylinders along the cube axes. Measurements of the Hall coefficient with the field along the symmetry axes show this to be an open hole surface, and provide a measure of two of its dimensions. This surface is consistent with that proposed by Mattheiss for the group-VB metals on the basis of his energy-band calculations for tungsten.

1. INTRODUCTION

THE Fermi surfaces of niobium and tantalum have not previously been explored experimentally in any detail because of the unavailability of samples with long carrier relaxation times. We have measured the anisotropy of the magnetoresistance of oriented tantalum single crystals, for which $\langle\omega_c\tau\rangle_{av}\sim 30$ at 100 kG, the largest magnetic fields used. Here ω_c is the cyclotron frequency eB/m^*c of a carrier with charge e and effective mass m^*, τ is its relaxation time, and the average is taken over all cyclotron orbits on the Fermi surface.

The magnetoresistance of tantalum shows strong anisotropy resulting from open orbits on a surface which is topologically similar to a set of intersecting cylinders along the cube axes. The Hall coefficient for a general field direction corresponds to one hole per atom. The increase of the Hall coefficient when the field is along the $\langle 100\rangle$ and $\langle 111\rangle$ symmetry axes is consistent with the connectivity of the open surface deduced from the magnetoresistance anisotropy, and shows this to be a hole surface.[1]

We have measured also one sample of niobium in the medium-field region ($\omega_c\tau\sim 4$ at $B=100$ kG), and find the anisotropy of its galvanomagnetic properties to be very similar to that of tantalum. We conclude that its Fermi surface has one open sheet, like tantalum, which also has a hole character. This open hole surface in

[1] I. M. Lifshitz and V. G. Peschanskii, Zh. Eksperim. i Teor. Fiz. **35**, 1251 (1958) [English transl.: Soviet Phys.—JETP **8**, 875 (1959)]; I. M. Lifshitz, M. Ya. Azbel, and M. I. Kaganov, *ibid.* **31**, 63 (1956) [*ibid.* **4**, 41 (1957)].

niobium and tantalum is identified with that suggested for the group-VB metals by Mattheiss[2] on the basis of his band-structure calculations for tungsten.

2. EXPERIMENTAL PROCEDURE

The samples of niobium and tantalum were prepared from a $\frac{1}{8}$-in.-diam electron-beam float-zoned bar. The starting material for the niobium and tantalum were obtained from Metals Hydrides, Inc., and Cibia Corporation, respectively. After several passes of the molten zone, each crystal was seeded to grow with its axis within 2° of a symmetry axis. A sample of the required length (about 15 mm) was spark-cut from each crystal and subjected to a degassing treatment[3,4] to increase its residual resistivity ratio, which is a measure of the carrier relaxation time in the normal state at liquid-helium temperatures.

Three pairs of mutually perpendicular potential leads were soldered to each sample so that all components of the electric field could be measured. The Hall (transverse) leads were placed in a plane perpendicular to the sample axis and the magnetoresistance leads were placed above and below the Hall leads, separated by about 6 mm. The diameter of each sample in the plane of the Hall leads was measured with a traveling microscope; to within the accuracy of measurement, about $\pm 5\%$, each sample had a circular cross section in this plane.

The galvanomagnetic measurements were carried out at a temperature of 4.2°K in a Bitter solenoid magnet in fields up to 100 kG. Each sample was mounted in an assembly which permits it to be either tilted $\pm 90°$ about a horizontal axis (the field is vertical), or rotated $\pm 90°$ about its own axis.[5] The angle of tilt between the sample axis and the horizontal plane and the angle of rotation about the sample axis are denoted by φ and θ, respectively.

The residual resistivity ratio (RRR) is not easily measured in superconducting metals for which the critical magnetic field is sufficiently high to produce an appreciable magnetoresistance in the normal state at the lower temperature (which should be low enough for temperature-dependent phonon scattering to be much less than impurity scattering). For our samples of tantalum, phonon scattering is negligibly small at 4.2°K, and at this temperature the critical field is only ~60 G, which produces an insignificant magnetoresistance. The RRR is therefore defined as the ratio between the resistivity at room temperature and the resistivity in a field just large enough to drive the sample normal at 4.2°K. For niobium the critical field at 4.2°K is ~2.7 kG, and the RRR is defined as the ratio between the resistivity at room temperature and the resistivity in the normal state at 4.2°K in zero field, the latter value being obtained by extrapolating the curve showing the field dependence of the magnetoresistance. The values of the RRR's defined in this way are listed in Table I.

TABLE I. Orientation and residual resistivity ratio of tantalum and niobium samples.

Metal	Orientation of axis	RRR
Ta	[100]	7100
	[110]	11 000
	[111]	6900
Nb	[110]	1560

3. EXPERIMENTAL RESULTS

A. Tantalum

The experimental data for the magnetoresistance of tantalum may be summarized as shown in the stereogram of Fig. 1. When the field **B** lies in a general direction, which does not coincide with any of the symmetry planes or symmetry axes of the cubic single crystal, the magnetoresistance saturates, showing tantalum to be an uncompensated metal. When **B** is rotated through one

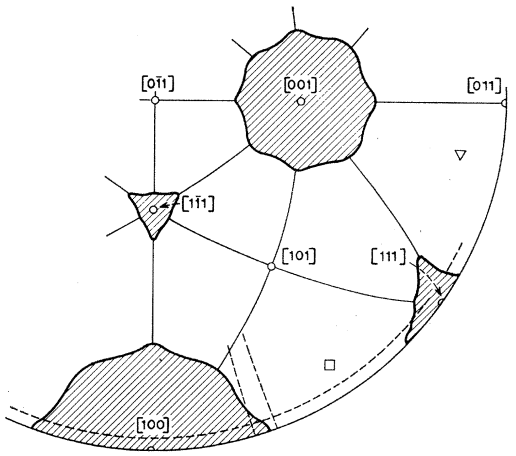

FIG. 1. Stereogram showing the occurrence of open orbits in tantalum.

[2] L. F. Mattheiss, Phys. Rev. **139**, A1893 (1965).

[3] This treatment was suggested by the work of D. P. Seraphim, J. I. Budnick, and W. B. Ittner, Trans. Met. AIME **218**, 527 (1960), who by a similar process produced samples of tantalum having values of RRR up to 8000 starting from 10-mil polycrystalline wires. We are deeply indebted to Professor J. I. Budnick for supplying us with one of his samples. He and D. Nowick made some preliminary measurements of the magnetoresistance of a similar sample in fields up to 20 kg. Our own preliminary measurements in fields up to 100 kG on a short, single-crystal section showed that the high-field magnetoresistance of tantalum is strongly anisotropic, which provided additional incentive for the work described in this paper.

[4] For Nb the RRR's increase with *decreasing* amounts of carbon and oxygen as measured by a mass spectrometer, whereas for Ta the RRR's increase with *increasing* amounts of carbon and oxygen. We have not observed any carbide or oxide precipitates in our samples and the possibility of these impurities ordering in the lattice is being investigated. A detailed description of the purification procedure will be the subject of a separate publication.

[5] G. F. Brennert, W. A. Reed, and E. Fawcett, Rev. Sci. Instr. **36**, 1267 (1965).

of the {100} or {110} planes, shown by continuous lines in Fig. 1, and the current direction is *not* perpendicular to this plane, the plot of the magnetoresistance versus the rotation angle exhibits a maximum. Provided the angle between the current direction and the plane is not too small, the magnetoresistance at the maximum approaches a quadratic field dependence at the highest fields.

These results show there are sets of one-dimensional periodic open orbits with their net directions along ⟨100⟩ and ⟨110⟩. We also observe two-dimensional regions of aperiodic open orbits when the field is near either a ⟨100⟩ or ⟨111⟩ axis, but not when the field is near ⟨110⟩. The shaded regions in Fig. 1 show the extent of the two-dimensional regions.

A typical curve showing the anisotropy of the magnetoresistance for the [110] sample of tantalum is illustrated in Fig. 2. The two-dimensional regions of open orbits give rise to the prominent features of this curve. The small peaks near $\theta=\pm 30°$ result from open orbits of higher order than the ⟨100⟩- and ⟨110⟩-directed

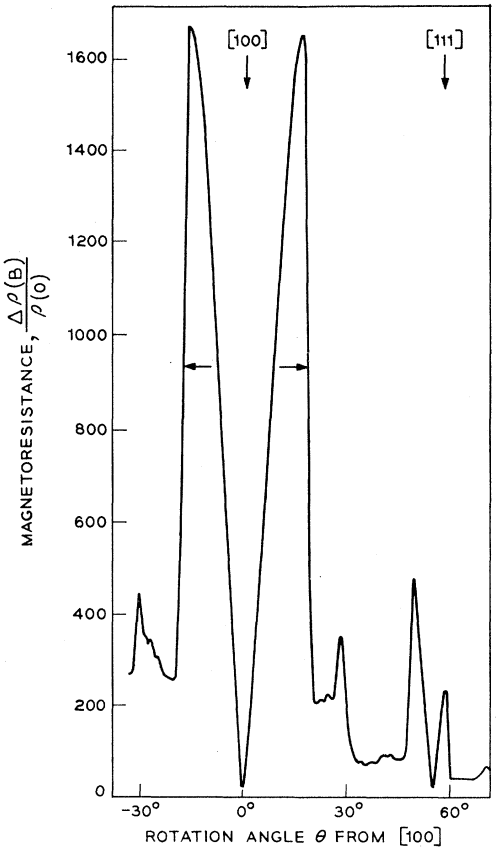

FIG. 2. Magnetoresistance for the [110] sample of tantalum in a field $B=85$ kG as the sample is rotated about its axis (the [0$\bar{1}$1] axis at the center of the stereogram in Fig. 1), which is inclined at 88° to B. The locus of **B** on the stereogram is indicated by the dashed line in Fig. 1. The horizontal arrows show how the extent of the two-dimensional regions was defined for the purpose of constructing Fig. 1.

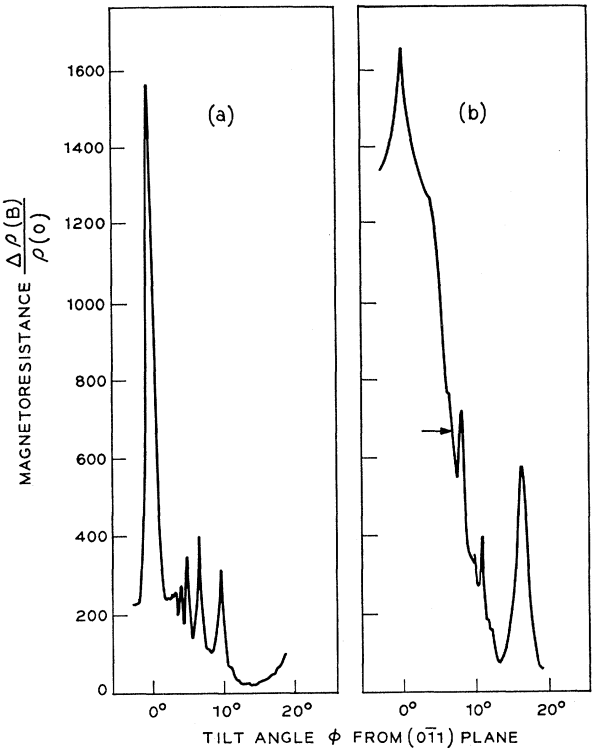

FIG. 3. Magnetoresistance for the [110] sample of tantalum in a field $B=85$ kG as the sample is tilted about axes perpendicular to **B** and the sample axis (the [0$\bar{1}$1] axis at the center of the stereogram in Fig. 1). Curves (a) and (b) correspond, respectively, to a locus of **B** which intersects the (0$\bar{1}$1) plane at point 1° *outside* the perimeter of the two-dimensional region, and to a locus of **B** which intersects the (0$\bar{1}$1) plane at a point 3° *inside* the perimenter. These loci are indicated by dot lines in Fig. 1. The horizontal arrow shows how the extent of the two-dimensional region was defined for the purpose of constructing Fig. 1.

open orbits. Several such peaks resulting from higher-order open orbits appear on the magnetoresistance curve when the field moves on a locus skirting the perimeter of the two-dimensional region of open orbits, as shown in Fig. 3. The "whiskers" corresponding to the directions of B for which these higher-order open orbits appear are not shown in the stereogram of Fig. 1. The strong peak at $\varphi=16°$ in Fig. 3(b) results from [0$\bar{1}$0]-directed open orbits.

The field dependence of the transverse magnetoresistance is shown in Fig. 4 for two different general-field directions[6] and with the field along the three symmetry axes in the [110] sample of tantalum. The magnetoresistance saturates for the general-field directions at values which differ from one general field direction to another in the same sample, but this anisotropy of the *saturating* magnetoresistance was not

[6] A general field direction is a nonsymmetry direction for which the Fermi surface supports no open orbits. Since the Fermi surface of tantalum supports ⟨100⟩- and ⟨110⟩-directed open orbits, the transverse magnetoresistance cannot, strictly speaking, be measured in a general field direction for the [110] and [100] samples; for these two samples the general field direction was chosen to lie ~10° from the transverse plane.

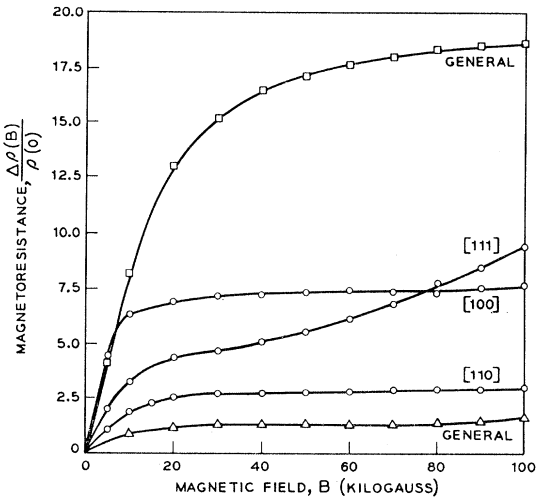

FIG. 4. Field dependence of the magnetoresistance in tantalum. The symbols □ and ▽ for the two general field directions are also used to represent these directions in the stereogram of Fig. 1.

studied systematically. The curves of Fig. 4 for the field along the symmetry axes also approach saturation, but for the field along [111] turns upwards at the highest fields. The latter effect probably results from imperfect alignment of the field along the axis, so that a small number of open orbits occur which begin to contribute significantly to the conductivity tensor at the highest fields.

The Hall coefficient of tantalum for a general field direction corresponds to a carrier density of one hole per atom to within the experimental accuracy of about ±5%. The main limitation on the absolute accuracy is the difficulty in measuring the cross-sectional area of the sample and the distance between the Hall leads. The cross-sectional area varies due to undulation in the surface of the as-grown sample, and the exact point at which each Hall lead is attached is difficult to define precisely because of the finite size of the solder spot.

The *relative* accuracy of measurements of the Hall coefficient for different field directions in the same sample was found to be considerably higher, of the order of ±1%. Nevertheless, when the Hall coefficient was measured along corresponding symmetry axes for different samples of tantalum, and the value for each sample expressed as a ratio of the number of carriers per atom to the number unity for the general-field direction, e.g.,

$$R_{\langle 100\rangle}=\frac{\text{Hall coefficient for } \mathbf{B} \text{ along } [100]}{\text{Hall coefficient for a general field direction}},$$

the numbers thus obtained were found not to agree to this high accuracy (see Table II). The discrepancies may result from imperfect alignment of the field along the symmetry axes, but in any case the average value of $n_{\langle 100\rangle}$ and $n_{\langle 111\rangle}$ in the singular-field directions given in Table II are seen to have an accuracy of about ±5%. The decrease of these values of n from the value unity for a general field-direction results from the occurrence of electron orbits on an open hole surface. This hole surface is identified with the open surface which gives rise to the anisotropy of the magnetoresistance.

TABLE II. Number of holes per atom determined from Hall coefficients.

Sample	$n_{\langle 100\rangle}$	$n_{\langle 111\rangle}$
Ta [100]	0.40	...
Ta [110]	0.45	0.61, 0.71
Ta [111]	...	0.64
Ta (av)	0.425	0.65
Nb [110]	0.62	...

Since the transverse magnetoresistance saturates in all samples of tantalum when the field lies along a ⟨110⟩ axis (see Fig. 4), one might expect each such axis to be the center of a two-dimensional region of open orbits, since it lies at the instersection of two one-dimensional regions of open orbits. But the shape of the magnetoresistance anisotropy curve shows that there is no such two-dimensional region. The fact that the Hall coefficient at a ⟨110⟩ axis is very small, less than 2% of the value for a general direction, shows that instead, for this field direction, the ⟨100⟩- and ⟨110⟩-directed open orbits must lie in different planes and so do not intersect.[7]

The Hall angle θ_H with the field in a general direction is a rough measure of $\langle\omega_c\tau\rangle_{\text{av}}$ for an uncompensated metal. For a metal having a spherical Fermi surface with an isotropic relaxation time we have

$$\frac{\text{transverse Hall field}}{\text{transverse resistive field}}=\tan\theta_H\equiv\langle\omega_c\tau\rangle_{\text{av}}.$$

However, for a nonspherical (but still closed) Fermi surface or an anisotropic relaxation time, the use of this equation yields an incorrectly low value of $\langle\omega_c\tau\rangle_{\text{av}}$ because of the enhanced value of the saturating magnetoresistance.[8] The *saturating* magnetoresistance of tantalum for general field directions exhibits a marked anisotropy (see Fig. 4), and we propose that in such a case the best estimate of $\langle\omega_c\tau\rangle_{\text{av}}$ is obtained by using in the above equation the resistive field for the direction in which the metal exhibits the *lowest* value of the magnetoresistance. This direction is indicated by the symbol ▽ in the sterogram of Fig. 1, and the corresponding magnetoresistance shown in Fig. 4 yields a value $\langle\omega_c\tau\rangle_{\text{av}}=32$, in a field $B=100$ kG, for the [110] sample of tantalum.

[7] See, for example, E. Fawcett, Advan. Phys. **13**, 139 (1964); we refer here to case IV in Table I, p. 160.

[8] See, for example, R. G. Chambers, Proc. Roy. Soc. (London) **A238**, 344 (1956).

B. Niobium

The anisotropy of the magnetoresistance of the niobium sample is shown in Fig. 5, which is to be compared with the corresponding curve shown in Fig. 2 for the [110] tantalum sample. The region of quadratic magnetoresistance associated with the two-dimensional region of open orbits surrounding the [100] axis appears to be wider for niobium than for tantalum and extends out almost to the [111] axis. The cause of the irregular structure of the maxima in the neighborhood of $\theta=\pm 20°$ is not known.

It is not possible to map out in detail the two-dimensional regions of open orbits in niobium since this sample is still only entering the high-field region at the highest fields due to its relatively low RRR. It is not clear, for example, whether the expected two-dimensional region of open orbits surrounding each ⟨111⟩ axis even exists. The threefold symmetry about this axis would necessitate the existence of such a region only provided that the ⟨110⟩ directed open orbits occur for field directions in the (110) plane on both sides of the ⟨111⟩ axis.

The field dependence of the magnetoresistance for the field along the [100], [110], [111] axes and also a general field direction ($\theta=10°$, $\varphi=10°$) is shown in Fig. 6. These curves are similar to the corresponding curves for tantalum (Fig. 4) except that the saturation is not as complete due to the lower RRR in niobium. The lack of saturation for the field along [111] is probably due to our inability to align the field exactly parallel to this axis. The lack of saturation is our best evidence for the existence of a two-dimensional region at ⟨111⟩.

The Hall coefficient determined in two independent measurements for a general field corresponds to 0.938 and 0.942 holes per atom. Again, as in tantalum, the relative accuracy of the two measurements is high and the deviation of the average value from unity is thought to result from inaccurate measurement of the geometry of the sample. The value of $n_{\langle 100\rangle}$ is given in Table II, but $n_{\langle 111\rangle}$ was not measured since for niobium no sharp singularity in the magnetoresistance or the Hall voltage was observed as **B** moved through this axis.

The Hall coefficient at a ⟨110⟩ axis is about 70% of its value for a general direction. This result suggests that when the field is in a ⟨110⟩ direction, the ⟨100⟩- and ⟨110⟩-directed open orbits lie is different planes and do not intersect. But the evidence for a singularity of this nature is much less convincing for this niobium sample than in the case of tantalum.

C. Niobium and Tantalum

The Hall angle for niobium with the field in a general direction ($\theta=60°$, $\varphi=10°$) yields a value $\langle\omega_c\tau\rangle_{\rm av}=4$, in a field $B=100$ kG. If we compare this value of $\langle\omega_c\tau\rangle_{\rm av}$ with the value $\langle\omega_c\tau\rangle_{\rm av}=32$, at the same field for the [110] sample of tantalum, we can estimate the relative average mobilities $\bar{\mu}$ of the carriers in these samples at

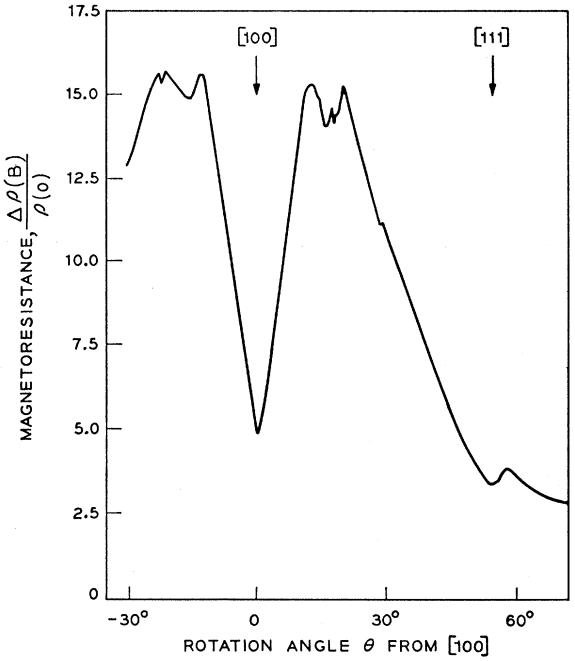

FIG. 5. Magnetoresistance for the [110] sample of niobium in the field $B=85$ kG as the sample is rotated about its axis, which is inclined at 88° to **B**.

4.2°K. Since for each sample the mobility is inversely proportional to the resistivity, we can use the values of RRR for these two samples given in Table I to estimate the relative mobilities of the carriers in niobium and tantalum at room temperature:

$$\frac{\bar{\mu}_{\rm Nb}}{\bar{\mu}_{\rm Ta}}=\frac{4}{32}\times\frac{11\,800}{1\,560}\sim 1.$$

Figure 7 shows how the size of the magnetoresistance peak associated with ⟨110⟩-directed open orbits varies with the rotation angle of **B** in the (110) plane of the [110] samples of niobium and tantalum. We define the

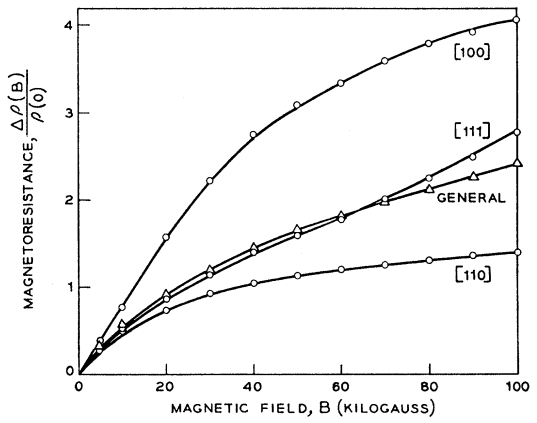

FIG. 6. Field dependence of the magnetoresistance in niobium.

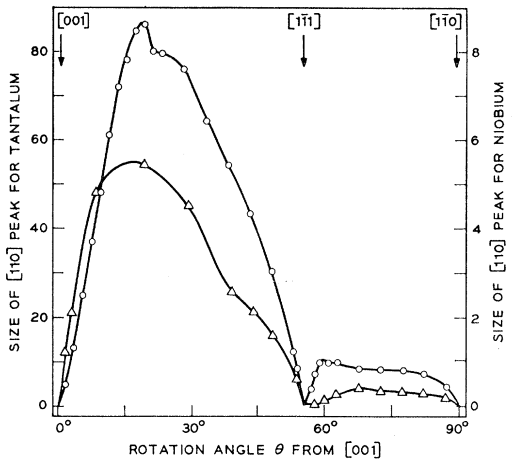

FIG. 7. Angular dependence of the size of the magnetoresistance peak associated with ⟨110⟩-directed open orbits in a field, $B=85$ kG. Each point in the curve is obtained by tilting the [110] sample so that **B** passes through the (110) plane at the corresponding rotation angle θ. 0—Ta [110], left-hand scale; ▽=Nb [110], right-hand scale.

size of the peak by the expression

$$\frac{\rho_{\text{peak}}(B)-\rho_{\text{sat}}(B)}{\rho_{\text{sat}}(B)},$$

where $\rho_{\text{sat}}(B)$ is the resistivity in the field, $B=85$ kG, at a field direction near the peak where the magnetoresistance saturates. According to this definition, the size of the peak is a rough measure of the number of ⟨110⟩-directed open orbits, which is necessarily zero when **B** lies along a symmetry axis (threefold or greater) at the center of a two-dimensional region of open orbits. The magnetoresistance saturates at all three symmetry axes, as shown in Figs. 4 and 6, and the curves in Fig. 7 accordingly go to zero at the corresponding values of θ. For tantalum the peak in the magnetoresistance reappears as **B** moves away from [1$\bar{1}$1] towards [1$\bar{1}$0] in the (110) plane, while for niobium it is barely distinguishable from zero for several degrees beyond [1$\bar{1}$1]. This may indicate that ⟨110⟩-directed open orbits do not occur over this angular interval in niobium which would imply the absence of a two-dimensional region of open orbits surrounding the [111] axis. Alternatively, there may be a two-dimensional region of open orbits surrounding ⟨111⟩ in niobium as in tantalum, but the number of open orbits may be too small to produce an observable peak with this low RRR sample.

For both niobium and tantalum the ⟨100⟩-directed open orbits occur for *all* field directions in the (100) plane, and a plot corresponding to Fig. 7 shows that the size of the peak is roughly constant, except near the ⟨100⟩ symmetry axes. We conclude that the ⟨100⟩-directed open orbits are primary, i.e., the arms of the Fermi surface connecting the surface which supports the open orbits are along the ⟨100⟩ axes, while the ⟨110⟩-directed open orbits are secondary and arise by alternate use of different arms.

4. DISCUSSION

An open hole surface having a connectivity consistent with the occurrence of the observed open orbits was proposed for the group-VB metals by Mattheiss.[2] He carried out an augmented-plane-wave (APW) energy-band calculation for tungsten and, removing one electron per atom corresponding to the change from Group VIB to group-VB metals, made the appropriate change of the Fermi level assuming a rigid-band model. The resultant Fermi surface is reproduced in Fig. 8.

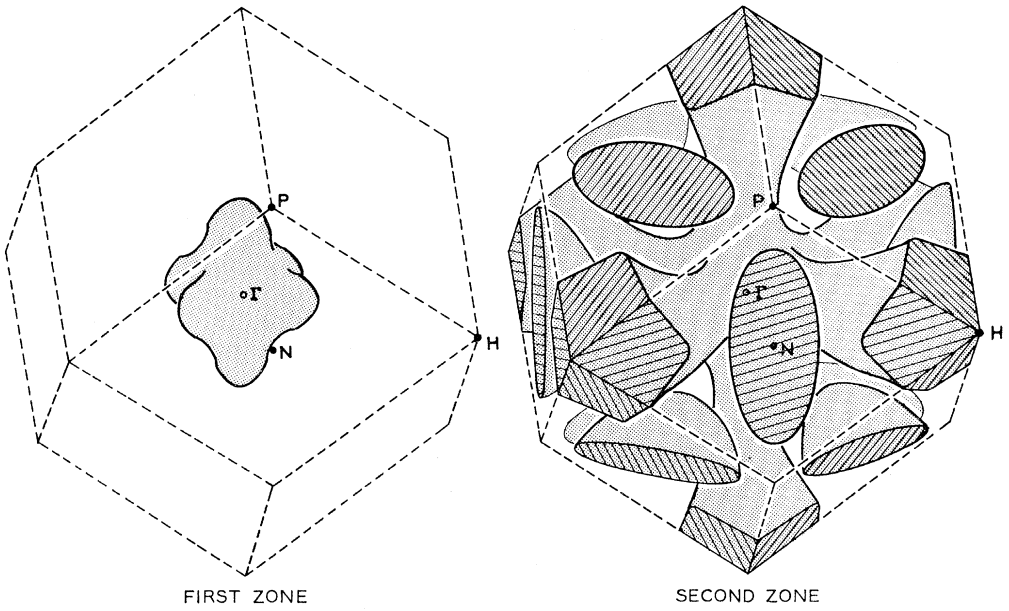

FIG. 8. Proposed Fermi surface for group-VB metals [after Mattheiss (Ref. 2)].

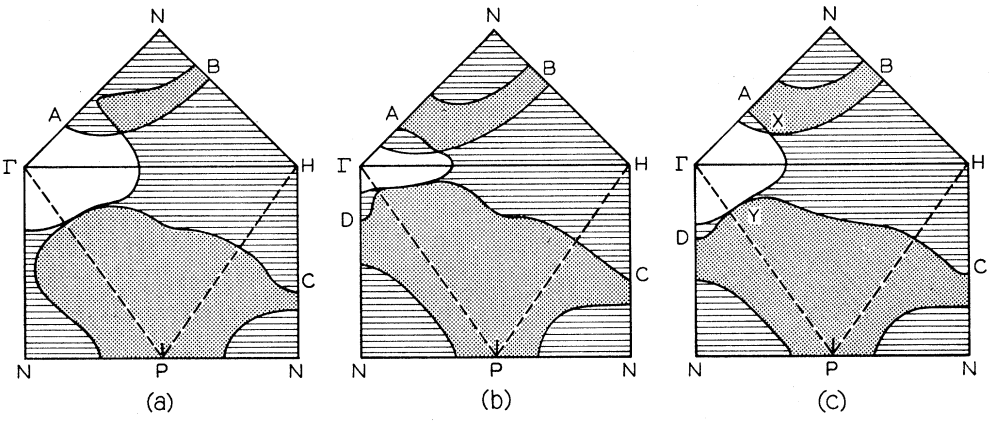

FIG. 9. Central (100) and (110) cross sections of the Fermi surface for group VB metals calculated by Mattheiss[2] using energy bands for iron (a) and for tungsten (b) and (c), corresponding to slightly different potentials.

There is an open hole surface in the second zone, with ⟨100⟩-directed connecting arms. The near-ellipsoidal hole surfaces centered on N in the second zone have been observed in tantalum through the associated de Haas–van Alphen oscillations.[9] The closed hole surface at Γ in the first zone (Fig. 8) has not been observed directly.

We identify the open surface in second zone with the surface which supports open orbits giving rise to the magnetoresistance anisotropy in both tantalum and niobium. The surface clearly supports primary open orbits along the ⟨100⟩ arms ΓH and secondary open orbits directed along ⟨110⟩ may also occur, depending upon the relative dimensions of the regions of the Fermi surface surrounding Γ and H.

Figure 9 is also reproduced from Mattheiss'[2] paper and shows cross sections of the group-VB metals' Fermi surface for three different energy-band structures. In Figs. 9(b) and 9(c) the cross section of the open hole surface is denoted ΓABHCD. In Fig. 9(a) the surface coalesces with the ellipsoids at N to form an open surface with arms along both ΓN and ΓH. The latter surface can be ruled out for both tantalum and niobium, since it would support primary ⟨110⟩-directed as well as primary ⟨100⟩-directed open orbits, and therefore would give rise to either a two-dimensional region of open orbits centered on each ⟨110⟩ axis or a single set of open orbits when the field is along ⟨110⟩.

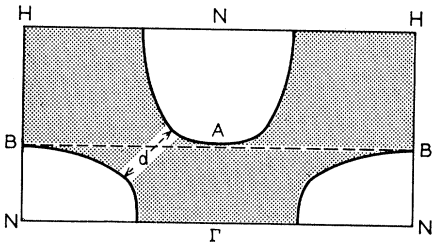

FIG. 10. Extended central (110) cross section from Fig. 9(c). The dashed line is the intersection of a plane, perpendicular to NAΓ, which allows ⟨110⟩ open orbits.

[9] J. H. Condon, Bull. Am. Phys. Soc. **11**, 170 (1966).

Returning to the section ΓABHCD, we see that with the field in a ⟨110⟩ direction (along ΓN) the surface supports secondary ⟨110⟩-directed open orbits only if ΓA>NB. This is shown more clearly in Fig. 10. These secondary open orbits are necessarily in a different plane from the ⟨100⟩-directed open orbits for the same field direction. Since we observe behavior corresponding to this type of singularity in the Hall coefficient at a ⟨110⟩ axis in both niobium and tantalum, we conclude that the cross section shown in Fig. 9(c), for which ΓA≃NB, agrees better with experiment than the cross section shown in Fig. 9(b), for which ΓA<NB. Figure 9(c) corresponds to the larger 6s-5d energy separation of the two potentials used by Mattheiss.[2]

From the difference between the number of holes per atom observed with the field in a general direction and in a ⟨100⟩ direction, we can calculate the minimum dimension d (as defined in Fig. 10) of the ΓH arms. From the average values given in Table II we obtain d=0.18ΓH for niobium and d=0.29ΓH for tantalum.

Mattheiss[2] points out that the accidental degeneracies at X and Y in Fig. 9(c) where the closed hole surface at Γ contacts the open hole surface will be removed by spin-orbit coupling. He suggests that the small energy gap expected for niobium when the spin-orbit coupling is relatively small could lead to magnetic breakdown. We have not observed any such effects, but probably a careful search in higher-purity samples of niobium would be required to see them.

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