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The Fermi surface in niobium

By G. B. Scott† and M. Springford
School of Mathematical and Physical Sciences, University of Sussex

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The low-frequency field modulation technique has been employed to study the de Haas–van Alphen effect in single crystals of niobium in fields up to 10 tesla. The frequency determination of the oscillations was performed by computer-based Fourier analysis and gave five sets of frequencies, which were studied in {100} and {110} planes. Effective masses and Dingle temperatures of some orbits were measured in the symmetry directions ⟨100⟩, ⟨110⟩ and ⟨111⟩. Interpretation of the results has been based on the results of a recent augmented plane wave band structure calculation of Mattheiss (1970). Three of the observed frequency branches can be explained in terms of, and are in good agreement with, the Fermi surface predicted by this calculation. The remaining frequencies can be accounted for, if a slight distortion of the proposed model is made. Comparison of the measured effective masses with those calculated from the band structure gives a value of 2.14 ± 0.17 for the mass enhancement factor due to many body effects. Using the theory of McMillan (1968) we evaluate the superconducting isotope shift coefficient to be 0.24.

1. Introduction

Despite the existence since 1965 of a model for the Fermi surface in niobium (Mattheiss 1965), a systematic experimental study of this Fermi surface has awaited the availability of single crystals of sufficient purity. de Haas–van Alphen (dH–vA) signals were first observed in niobium in 1961 (Thorsen & Berlincourt 1961), but little information on the Fermi surface was available until the galvanomagnetic measurements of Fawcett, Reed & Soden (1967) and of Reed & Soden (1968). The results of these experiments are generally in good accord with the model for the Fermi surface of the group V B transition metals proposed by Mattheiss (1965) and based upon his band structure calculation for tungsten. More recently Mattheiss (1970) has used the augmented plane wave (a.p.w.) method to calculate directly the band structures for both niobium and tantalum. The results of this calculation were a confirmation of the previously proposed Fermi surface and also yielded the angular variation of extremal areas and 'bare band' effective masses for some extremal orbits. Deegan & Twose (1967) have formulated a modified version of the orthogonalized plane wave method for calculating the energy bands of transition metals and applied it to the case of niobium. Whilst they have not estimated a Fermi level and a corresponding Fermi surface, the overall agreement of the energy band results of these two independent calculations for niobium is excellent, the average difference being about 0.003 Ry.

† Present address: Physics Division, National Research Council of Canada, Ottawa, Canada.

This present work was undertaken in the climate of interest in the electronic structures and Fermi surfaces of the transition metals. The lack of detailed information for niobium, coupled with the availability of single crystals of adequate purity and perfection provided the motivation for a detailed investigation of the dH–vA effect in this material. After our experimental work had begun we were informed of a parallel investigation of the Fermi surface in niobium by the group at the Bell Telephone Laboratories (Halloran *et al.* 1970). These workers, however, have employed principally magnetothermal oscillations, although the dH–vA effect has also been studied by means of a torque balance in magnetic fields not exceeding 3 tesla, and our results are in excellent agreement with their work.

We present in § 3 the frequency results and in § 4 their interpretation in terms of a model for the Fermi surface in niobium based on that recently proposed by Mattheiss (1970). Cyclotron effective masses have been measured for the magnetic field applied in the principal symmetry directions. These results are compared with other measured values and with the calculated 'bare band' masses in § 5. Based on measurements of Dingle temperatures, evidence is presented in § 6 for a pronounced anisotropy of the total scattering cross-section for electrons on the different sheets which comprise the Fermi surface in niobium. A preliminary report on some aspects of these studies has been given elsewhere (Scott, Springford & Stockton 1968).

2. Experimental procedure

These experiments were performed in a 10 T niobium-tin superconducting magnet. The magnetic field was monitored by means of a magnetoresistor which consisted of two astatically wound coils of copper wire situated in the liquid helium bath in the bore of the magnet. The voltage developed across these coils, which carried a constant current of 30 mA was a measure of the magnetic field appearing at the specimen. Calibration was achieved in a separate experiment by employing nuclear magnetic resonance in ^{27}Al (Scott *et al.* 1969) and the overall precision achieved was of order 0.3 %.† Instrumentation for the detection of the dH–vA effect by the field modulation method (Shoenberg & Stiles 1964) in its low-frequency version, was conventional and is well documented in the literature (see, for example, Goldstein, Williamson & Foner 1965). By means of a data acquisition system, the dH–vA data together with the voltage appearing across the magnetoresistor was recorded on punched paper tape, and the important parameters such as the dH–vA frequencies and their amplitudes could then be readily evaluated by computer program.

The specimens were spark cut from four electron beam zone refined single crystals and etched to final dimensions of 3 mm × 1.4 mm × 1.4 mm. Most of the crystals used in this work were from an ingot of residual resistance ratio, as defined for a superconductor by Fawcett *et al.* (1967), of about 800; spectrographic analysis of this ingot showed that the main impurities were Ta($100/10^6$), Fe ($3/10^6$), Si ($3/10^6$) and

† Later improvements in the magnetoresistor calibration, not available at the time of these experiments, increased the precision by a factor of 10 or so (Springford & Stockton 1970).

Mg ($1/10^6$). No gas analysis was carried out, but it is probable that a few parts per million of oxygen was also present.

3. Frequency results

Experimental results are discussed separately for the observed frequency branches $\alpha, \alpha', \beta, \nu_1$ and η. Where possible the notation is that of Mattheiss (1970). The dH–vA frequencies, which have been examined for magnetic fields lying in {100} and {110} planes have been converted to extremal areas A_0 by using the relation

$$A_0 = \frac{2\pi^2 eF}{\hbar} = 0.9546 \times 10^{-2} F$$

where F is expressed in tesla and A_0 in nanometre^{-2}.

The η oscillations

These oscillations of highest frequency were observed in {110} planes over an angular range of *ca.* 42°, starting at 33° from ⟨100⟩ and extending to within 15° of ⟨110⟩. The extremal area variation is shown in figure 1 where it is seen to have a minimum value of 186 nm^{-2} at ⟨111⟩. The distribution of data points is such that they do not lie on one smooth curve but rather a serious of curves; this distribution is real and is not experimental scatter. A plot of the amplitude of these oscillations versus magnetic field direction (figure 2*a*) shows strong correlation with the extremal area plot, in that, at the positions of discontinuity on the area plots, there exist minima in the amplitude plots. To establish that the amplitude behaviour was not due to change of sample magnetoresistance with orientation, an amplitude plot of the ν oscillations, which span the η oscillations in angular extent, was also made. The result is shown in figure 2*b*, where the dissimilarity in amplitude behaviour of the two branches is clear and on these grounds it was accepted that the observed amplitude variation was a property of the orbit under investigation.

The ν oscillations

These oscillations, observed to be continuous in the {100} and {110} planes, consisted of six branches, two of which were doubly degenerate. Any misalinement of sample, causing it to rotate out of the symmetry planes, removed the degeneracy and this accounts for the scatter on the $\nu_{3,4}$ branch (see figure 3). The gaps in the branches, in particular the ν_2 branch, are attributable to a high effective mass of one orbit relative to the others. The continuity of the branches implies that the surfaces from which they originate are closed and, by symmetry arguments similar to those used by Watts (1964), must lie along the ΓN directions of the b.c.c. Brillouin zone. The symmetry and degeneracy of the branches is consistent with assigning them to distorted ellipsoidal pockets situated at N in the Brillouin zone and having semi-axis dimensions in NP, NΓ and NH directions of 5.7, 4.8 and 4.2 nm^{-1} respectively. Because the axes NΓ and NH of any one of the ellipsoids are respectively

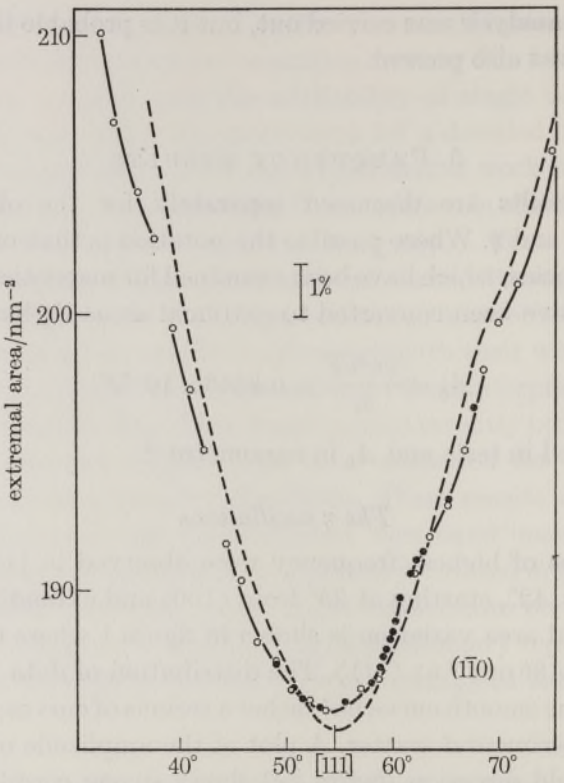

FIGURE 1. Extremal Fermi surface areas derived from the η oscillations in niobium, for field directions in the (1$\bar{1}$0) plane. The field orientation is measured from [001], ○ and ● are taken from different experiments. The full lines indicate several sets of data points. The dashed curve corresponds to the a.p.w. calculation (Mattheiss 1970) for extremal areas of the 'jungle gym' centred at the H point in the Brillouin zone.

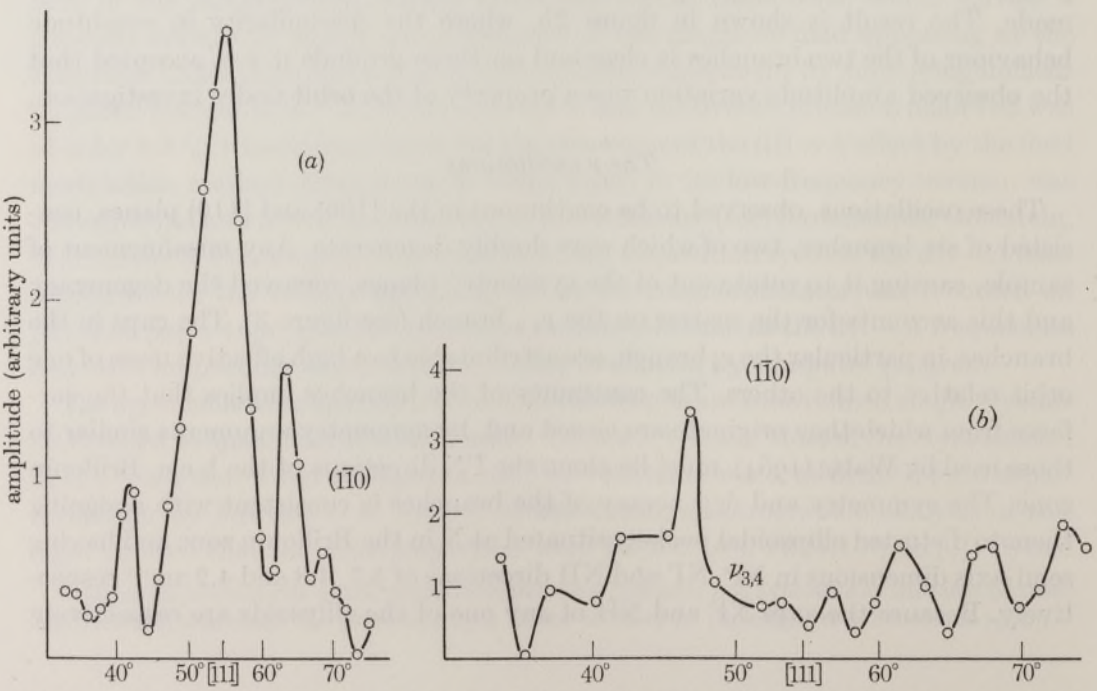

FIGURE 2. Amplitude variation of (*a*) η and (*b*) $\nu_{3,4}$ dH–vA oscillations in niobium for field directions in the (1$\bar{1}$0) plane. The field orientation is measured from [001].

always parallel to the axes NH and NΓ of one of the other five ellipsoids in the Brillouin zone, it is not possible experimentally to assign the two corresponding semi-axis values. We have therefore used the result of the a.p.w. calculation which is that NΓ > NH. The largest discrepancy between ν oscillations and the calculated

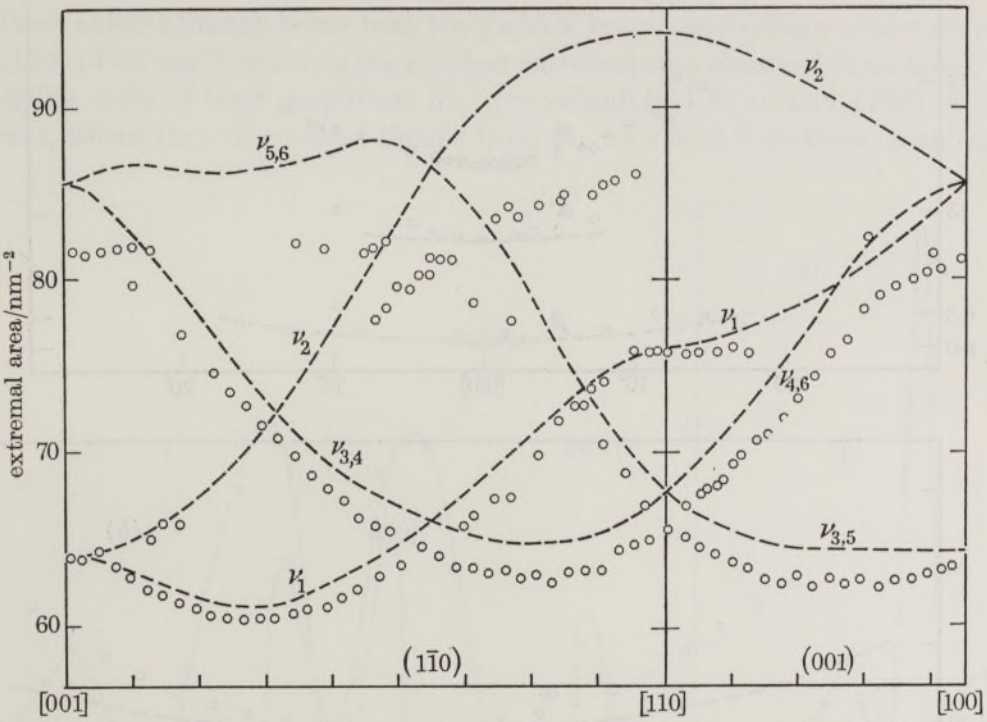

FIGURE 3. Extremal Fermi surface areas derived from the ν oscillations in niobium, for field directions in the (1$\bar{1}$0) and (001) planes. The dashed line is from the a.p.w. calculation of Mattheiss (1970) and refers to the pseudo-ellipsoidal surfaces centred at N in the Brillouin zone.

variation for general ellipsoids occurs in the {110} planes at about 30° from ⟨100⟩ where the ν_1 branch has a minimum. Such a calculation also reveals that both NHP and ΓNH cross-sections of the real surfaces are closely elliptical.

The α oscillations

These oscillations have been observed in {100} and {110} planes up to 23° and 29° from ⟨100⟩ respectively, at which orientation there exists a minimum in the extremal area of 13.9 nm^{-2}. The angular variation of extremal area is shown in figure 4 and for the {100} planes, is compared with the behaviour of a cylindrical surface having a cross-sectional area of 13.9 nm^{-2}. The measured area increases more rapidly than cylindrical behaviour and is therefore associated with a concave surface. The amplitude behaviour of the α, α' and β oscillations (the α' and β oscillations are discussed in the following subsections) in {100} and {110} planes is presented in figure 5.

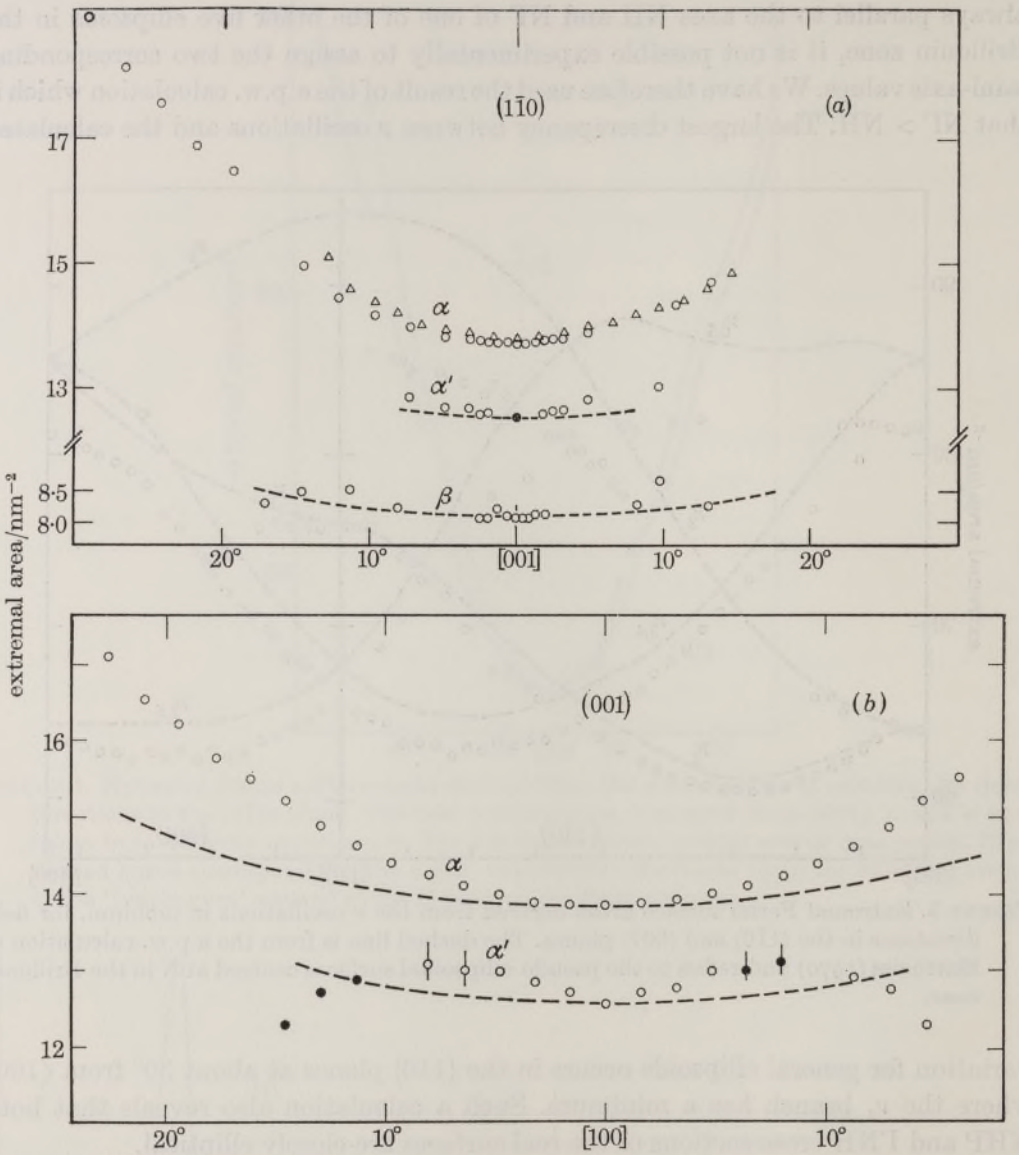

FIGURE 4. Extremal Fermi surface areas derived from the α, α' and β oscillations in niobium for field directions in the (*a*) (1$\bar{1}$0) plane and (*b*) (001) plane. The dashed curves represent the angular variations for cylindrical surfaces.

The α' and α'' oscillations

The α' oscillations were observed in both {100} and {110} planes up to 15° and 10° from ⟨100⟩ respectively. The area variation in the {100} planes (see figure 4*b*) initially varies more rapidly than for a cylindrical surface but beyond *ca.* 8° from ⟨100⟩ the extremal area decreases out to 15° from ⟨100⟩ beyond which we have not observed oscillations. Halloran *et al.* (1970) did not observe this over more than *ca.* 9° from ⟨100⟩ in either plane, but reported seeing oscillations between 14 and 20° from ⟨100⟩ in the {100} planes which they designate α''. In these planes our data

and those of Halloran *et al.* (1970) overlap at *ca.* 15° from ⟨100⟩, lending credence to the theory that the α' and α'' branches are parts of the same branch. The amplitude behaviour of the α' and α'' oscillations in the {100} planes, shown in figure 5*a*, also support the above idea.

The β oscillations

There exists a branch below both the α and α' branches, having a minimum value at ⟨100⟩ of 8.1 nm^{-2}, which is the smallest extremal area observed in niobium. The β signals were of large amplitude for approximately 1.5° around ⟨100⟩ in {110} planes, where they dominated signals from the α, α' and ν surfaces. Although β

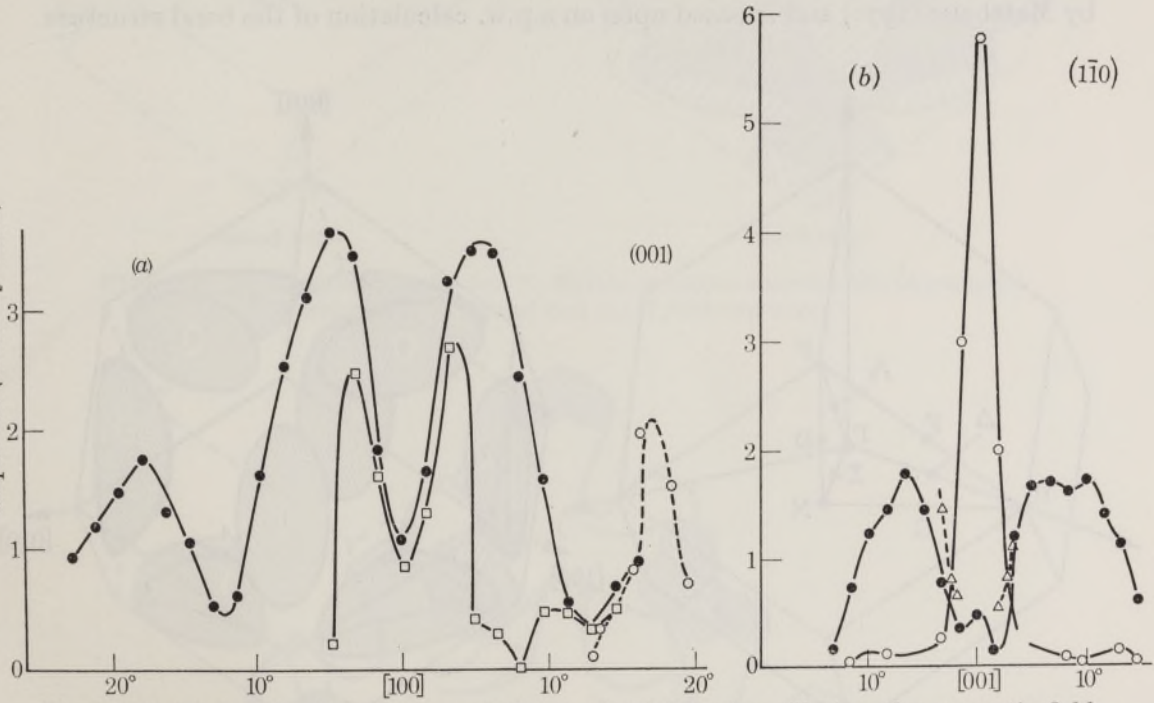

FIGURE 5. (*a*) Amplitude behaviour of the α, α', α'' dH–vA oscillations for magnetic field directions in the (001) plane. ●, α oscillations; □, α' oscillations; ○, amplitude data on α'' oscillations taken from Halloran *et al.* (1970) and scaled to fit our data for α' at 15° from [100]. (*b*) Amplitude behaviour of the α, α' and β oscillations in the (1$\bar{1}$0) plane. ○, β oscillations; ●, α oscillations; △, α' oscillations.

oscillations were observed in {100} planes, they were of low amplitude and no systematic angular variation of extremal area could be recovered. The strong correlation of the amplitude behaviour of β, α and α' oscillations (see figure 5*b*) is suggestive of magnetic breakdown where the amplitudes of the oscillations formed or degraded by the breakdown are strongly orientation dependent. The failure of Halloran *et al.* (1970) to observe β oscillations was probably due to (i) the low fields of less than 3.1 T that they employed with the torque balance (we never observed β signals below ~ 3.5 T), (ii) close to ⟨100⟩ where we found the β oscillations to be strongest the torque signal, which is proportional to $\partial F/\partial\theta$, would be small, vanishing at

⟨100⟩ where the frequency has a stationary value, (iii) in the magnetothermal effect, signals from orbits of high mass tend to be enhanced (Blatt 1967) and since the β oscillations have an effective mass of 0.27 at ⟨100⟩ compared with α and ν masses *ca.* 1.5, it is possible that this causes the β signal amplitude to become much less than that of the α and ν oscillations.

4. The Fermi surface

We describe in this section the interpretation of the preceding topological experiments in terms of a model for the Fermi surface in niobium which has been proposed by Mattheiss (1970) and is based upon an a.p.w. calculation of the band structure.

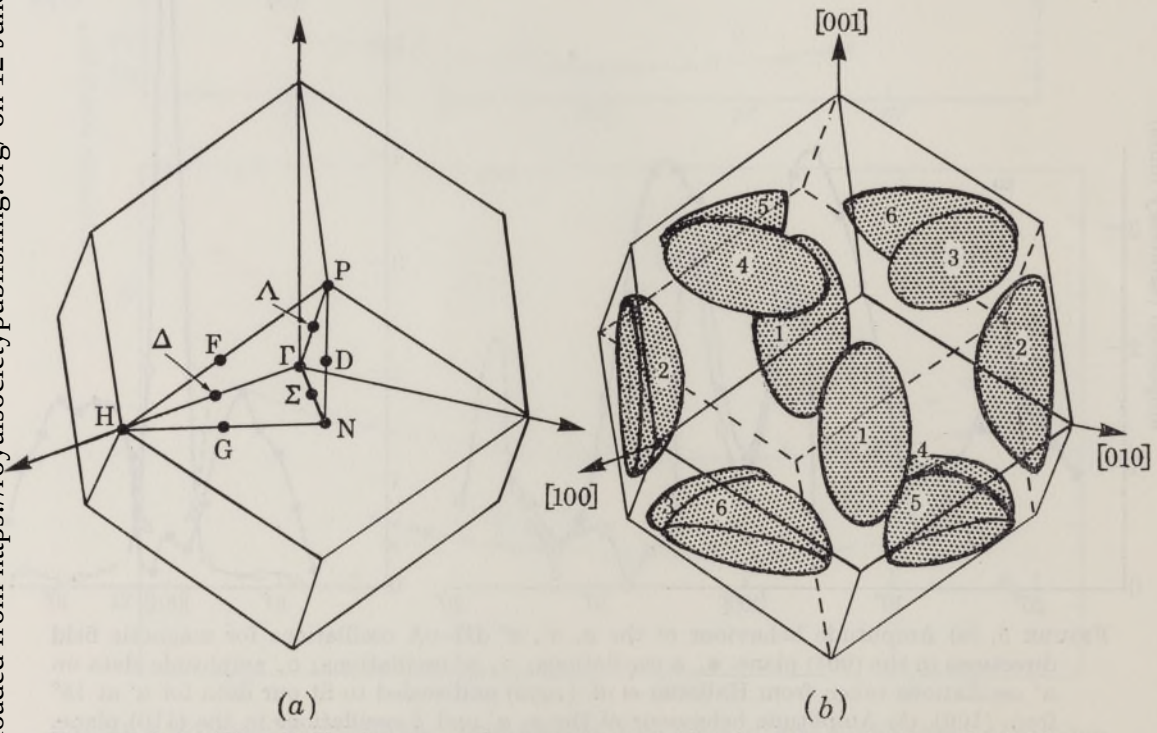

Figure 6. (*a*) First Brillouin zone and symmetry notation for a b.c.c. lattice. (*b*) Arbitrary numbering scheme (Mattheiss 1970) for distinguishing between the six equivalent distorted ellipsoids situated at N in the Brillouin zone.

We shall first describe this model which is similar to that originally proposed for the vanadium group transition metals by Mattheiss (1965) based upon his energy band calculations for tungsten.

Niobium contains five conduction electrons (one less than tungsten) and crystallizes in the b.c.c. structure. The first Brillouin zone and symmetry notation are depicted in figure 6. In terms of the tungsten band structure, the first band is filled, the second almost filled and the third zone is rather more than half filled. The Fermi surface sheets that enclose the unoccupied regions in the second and third bands are

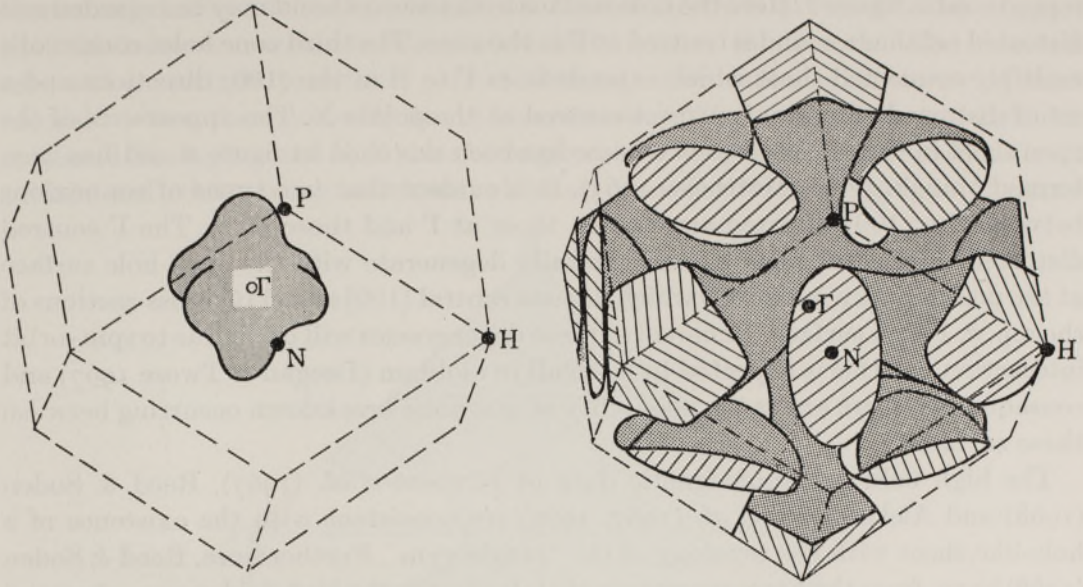

FIGURE 7. Fermi surface model due to Mattheiss (1970) showing the unoccupied portions of the second and third Brillouin zones.

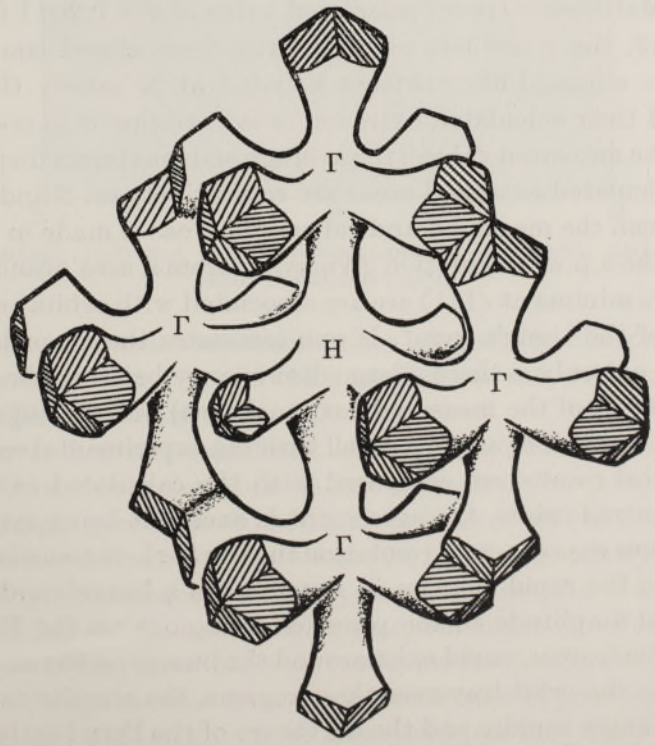

FIGURE 8. Sketch of the 'jungle gym' Fermi surface sheet in the repeated zone scheme, showing the different types of connexion at Γ and H. The existence of electron orbits for field directions near ⟨100⟩ is clear from this diagram.

reproduced in figure 7. Here the hole surface in the second band may be regarded as a distorted octahedron and is centred at Γ in the zone. The third zone holes consist of a multiply connected sheet which extends from Γ to H in the ⟨100⟩ directions and a set of distorted ellipsoidal surfaces centred at the points N. The appearance of the open sheet in the repeated zone scheme has been sketched in figure 8 and has been termed 'jungle gym' (Mattheiss 1965). It is evident that two types of connexions between the ⟨100⟩-directed arms exist, those at Γ and those at H. The Γ-centred distorted octahedral surface is accidentally degenerate with the open hole surface at the points shown in figure 9 which depicts central {100] and {110} cross-sections of the a.p.w. Fermi surface. Removal of these degeneracies will occur due to spin–orbit interaction but this is expected to be small in niobium (Deegan & Twose 1967) and consequently there exists the possibility of magnetic breakdown occurring between these surfaces.

The high field galvanomagnetic data of Fawcett *et al.* (1967), Reed & Soden (1968) and Alekseevskii *et al.* (1967, 1969) are consistent with the existence of a hole-like sheet with the topology of the 'jungle gym'. Furthermore, Reed & Soden (1968) have, from their measurements of Hall effect in the high field region, observed a decrease in the number of holes per atom when the magnetic field is changed from a general direction to [100]. This decrease is related to the minimum 'jungle gym' arm diameter d from which they deduce that $d = 0.21\,\Gamma\mathrm{H}$ which is in excellent agreement with Mattheiss's (1970) calculated value of $d = 0.207\,\Gamma\mathrm{H}$.

As stated in §3, the ν oscillations must arise from closed convex surfaces in {110} planes. The ellipsoid-like surfaces situated at N satisfy these qualitative requirements and their calculated extremal area variation is in good quantitative agreement with the measured values; the average and maximum disparities between measured and calculated extremal areas are respectively *ca.* 5 and 10 %. A direct comparison between the measured and calculated areas is made in figure 3.

The results of the a.p.w. calculation give two extremal area branches in the {110} planes which have minima at ⟨111⟩ are are associated with orbits around the Γ and H intersections of the 'jungle gym'. If one associates the η oscillations with the Γ centred orbits, not only is there a large discrepancy between the areas (at ⟨111⟩ the difference is 60 % of the measured extremal area) but the angular extent and variation of this branch does not agree well with the experimental results. However, if the experimental results are compared with the calculated extremal area behaviour for H centred orbits, the agreement is excellent being typically 1 % (see figure 1). Within our experimental resolution the η branch was continuous and hence we may attribute the rapid changes in slope of the η branch and the associated decrease in signal amplitude to the presence of regions on the Fermi surface of high curvature. Such areas would exist around the bumps on the arms predicted by the model and, as the orbit traverses these regions, the angular rate of change of extremal area changes rapidly and the curvature of the Fermi surface at the extremum, $\partial^2 A/\partial k_H^2$, causes a reduction in signal amplitude. However, Halloran *et al.* (1970), using the technique of crystal rotation in a constant magnetic field, find that

there exist definite discontinuities at *ca.* 38 and 61° from ⟨100⟩ and they suggest that this behaviour is due to non-central orbits on the 'jungle gym'. The observed area and amplitude variations cannot be completely explained in terms of non-central orbits and are probably due to a combination of both the above explanations. It should be emphasized that the above phenomena represent detail on the Fermi surface and whilst being of intrinsic interest they derive from features of minor

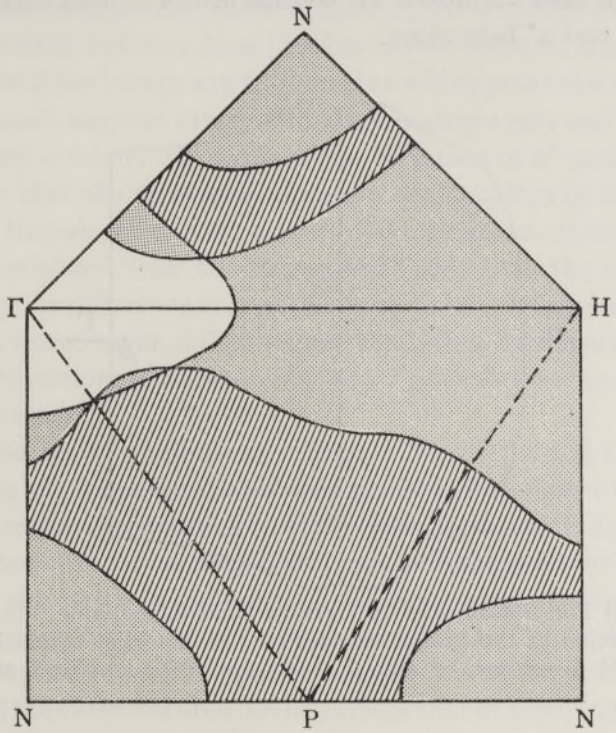

FIGURE 9. Central {100} and {110} cross-sections of the Fermi surface of niobium, after Mattheiss (1970).

significance. At no orientation is the difference between the observed and calculated central orbits greater than 4 % and the η oscillations can with confidence be associated with the H intersection of the open hole sheet.

Mattheiss (1970) has not calculated any extremal area variations which are consistent with the α branches, but he has estimated the ⟨100⟩ minimum cross-section of the 'jungle gym' arms to be 11.7 nm^{-2}. At ⟨100⟩ the α and α' orbits have extremal areas close to this value (13.9 and 12.6 nm^{-2} respectively) but variation of the α' branch is not consistent with a hyperboloid sheet and it would appear that the α oscillations derive from the 'jungle gym' arm minimum. Further justification of this assignment is that Reed & Soden (1968) predict a minimum arm diameter of 0.21 ΓH and assuming that this cross-section is circular (a good approximation, see Reed & Soden (1968, p. 678)) our ⟨100⟩ area corresponds to 0.22 ΓH arm diameter. Although the amplitude behaviour of the α oscillations (figure 5) is suggestive of magnetic breakdown, the linearity of the Dingle temperature plots refute this

explanation and we can only suggest that the observed amplitude behaviour is due to variations in effective mass, curvature of the Fermi surface, etc.

The α' and α'' areas are too small to be associated with the quasi-ellipsoids, and since the minimum area of the 'jungle gym' arms is greater than the $\langle 100 \rangle$ α' and α'' areas, the α' and α'' areas cannot derive from the 'jungle gym'. The remaining surface of the model to be considered is the Γ-centred distorted octahedron but the calculated extremal area variations for central orbits on this surface are not consistent with the α' and α'' behaviour.

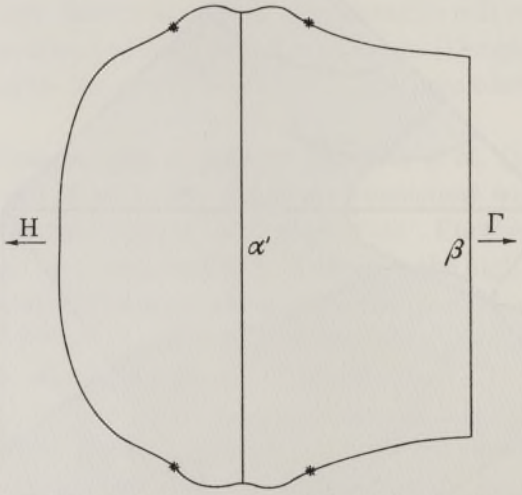

FIGURE 10. Proposed Fermi surface in the second band in niobium. The diagram shows a central (001) section of the protruberances on the distorted octahedral surface which occur in the ΓH directions, α' and β oscillations originate from the extremal areas indicated.

Three possible sources of the α' and α'' were considered: (i) magnetic interaction, (ii) magnetic breakdown and (iii) non-central orbits on the Γ centred octahedron. Magnetic interaction effect can 'mix' dH–vA frequencies giving sum and difference frequencies and hence there was the possibility that the α' and α'' oscillations did not originate from extremal orbits on the Fermi surface. However, neither the α' nor the α'' frequency was a simple arithmetic combination of other observed frequencies. Magnetic breakdown between the distorted octahedron and the 'jungle gym' at the points of accidental degeneracy was considered as a cause of the remaining dH–vA frequencies. Breakdown between the central $\langle 100 \rangle$ octahedron orbit and the four electron orbits on the 'jungle gym' would give orbits of area much larger than the α' orbits. The other possible breakdown junctions involving extremal orbits were those between the α orbit on the 'jungle gym' and non-central orbits on the $\langle 100 \rangle$-directed protrusions of the octahedron. However, there is no experimental evidence of magnetic breakdown involving the α orbit over the present magnetic field range and consequently this source of new dH–vA frequencies was rejected. Our final consideration of the source of the low-frequency oscillations involves a slight

distortion of the octahedral surface. The distortions we propose are shown in figure 10 where a (100) section of part of the protrusion is shown with the α' orbit originating from a minimum on the protrusion. The form of the distortion was suggested by assuming the protrusions to have cylindrical symmetry about $\langle 100 \rangle$ and converting the extremal areas to radii. This procedure gave the form between the asterisks, the remaining shape being dictated by closure of the surface and connectivity to the main body of the octahedron. If the α' oscillations originate from the minimum, a movement of the field direction from [100] in an (001) plane will cause the extremal area to increase until the bumps are traversed at which point the extremal area will decrease over a small angular range before increasing again and finally becoming non-extremal. Such a model can explain the variation of α' and α'' branches and supports the view that the α'' oscillations are a continuation of the α' oscillations. It would appear though, that with a [001] field direction, there should be three extremal areas associated with the ridges while only one, the α' orbit, has been observed. Possibly the difference in areas between these orbits is such as to give large beat packets and hence make difficult their resolution by experiment. The origin of the amplitude behaviour of these oscillations is probably due to changes of curvature and effective mass.

We propose that the β oscillations originate from extremal orbits around the regions connecting the ridges to the octahedron body (see figure 10). The observed extremal area variation is consistent with this interpretation, following closely that of a cylindrical sheet of surface near $\langle 100 \rangle$ and increasing faster than this further from $\langle 100 \rangle$. This similarity to cylindrical behaviour would explain the amplitude variation of the β oscillations in the $\{110\}$ planes; close to $\langle 100 \rangle$ where the surface is cylindrical the amplitude of the signals is large, but as the field direction moves farther from [100] the extremal area deviates from that of a cylindrical sheet and the amplitude rapidly decreases.

Table 1 contains a summary of the extremal cross-sectional areas of the Fermi surface deduced from both the present dH–vA experiments and also from magneto-thermal oscillations (Halloran *et al.* 1970). It is seen that there is excellent agreement between these two experiments which are in good accord with the a.p.w. calculation. The largest discrepancy between the measured and calculated areas of *ca.* 16 % occurs for the $\langle 100 \rangle$ minimum cross-section of the 'jungle gym' arms.

In the course of these experiments, unsuccessful attempts were made to observe the central $\langle 100 \rangle$, $\langle 110 \rangle$ and $\langle 111 \rangle$ orbits on the octahedron, $\langle 111 \rangle$ orbits on the Γ intersection of the 'jungle gym' and $\langle 100 \rangle$ electron orbits along the 'jungle gym' arms. Our failure to observe these orbits may be explained in terms of the high effective mass values. In particular the enhanced mass of the $\langle 111 \rangle$ orbit on the Γ intersection of the 'jungle gym' is expected to be 5.2 and the enhanced masses of central orbits on the octahedron to lie between 3.4 and 5. Clearly experiments in the ^{3}He temperature range performed on crystals of improved quality would be most valuable in this respect.

TABLE 1. COMPARISON OF EXTREMAL AREAS OF THE FERMI SURFACE AND EFFECTIVE MASSES IN NIOBIUM DEDUCED FROM MAGNETOTHERMAL OSCILLATIONS (HALLORAN *et al.* 1970), THE PRESENT dH–vA EXPERIMENTS AND THE A.P.W. CALCULATIONS (MATTHEISS 1970)

		area/nm^{-2}			effective mass, m^*/m		
	orbit	m.t.o.	dH–vA	a.p.w.	m.t.o.	dH–vA	a.p.w.
⟨100⟩	JG(α)	0.138	0.139	0.117	1.12	1.6 $\pm$0.4	0.57
	OCT(α')	0.125	0.126	—	—	< 4	—
	Oct(β)	—	0.081	—	—	0.27 $\pm$ 0.02	—
	ELL (1, 2)	0.636	0.638	0.642	—	—	0.83
	ELL (3, 4, 5, 6)	0.815	0.813	0.855	1.60	1.97 $\pm$ 0.09	0.97
⟨111⟩	ELL (1, 3, 4)	0.647	0.644	0.663	1.28	1.56 $\pm$ 0.08	0.73
	ELL (2, 5, 6)	0.813	0.811	0.863	—	—	1.12
	JG(H)	1.862	1.860	1.881	—	3.1 $\pm$ 0.1	1.17
⟨110⟩	ELL (3, 4, 5, 6)	0.657	0.658	0.677	1.22	1.40 $\pm$ 0.06	0.70
	ELL (1)	0.757	0.757	0.762	—	1.54 $\pm$ 0.06	0.79
	ELL (2)	0.857	0.857	0.944	—	—	0.97

5. EFFECTIVE MASSES

From the temperature dependence of the dH–vA signal amplitude we have measured the effective masses of most of the observed orbits for the magnetic field along [100], [110] and [111]. Measured masses and those obtained from the a.p.w. calculation are collected in table 1. The mass enhancement factor $(1+\lambda)$ is given by the ratio of the measured mass to the calculated or bare band mass and from our measurements we find the value 2.14 ± 0.17. Also in table 1 are given effective masses derived from the magnetothermal experiments by Halloran *et al.* (1970), and these lie consistently below the dH–vA masses and yield a value of 1.75 for the mass enhancement in niobium. It is interesting that in tantalum also Halloran *et al.* (1970) obtained effective masses from magnetothermal oscillations which were *ca.* 10 % lower than the values obtained using a torsion balance. The origin of the difference is not understood but in the case of niobium the discrepancy between dH–vA and magnetothermally measured masses is larger at *ca.* 15 %. The error quoted for the dH–vA masses in the table refer only to the random errors of measurement and do not include any systematic errors; however, these are presumed to be small in view of the close agreement between the values obtained for the noble metals using the present equipment and the accepted values quoted by Halse (1969). We may also derive a value of the mass enhancement in niobium from the measured electronic specific heat. Using the value $\gamma = 7.80\,\mathrm{mJ\,mol^{-1}\,K^{-2}}$ (Heininger Bucher & Muller 1966) we obtain for the enhanced density of states $N_e(E_F)$,

$$N_e(E_F) = \frac{3\gamma}{2\pi^2 k^2} = 1.65 \text{ states of one spin/eV atom.}$$

Comparing this with the bare band density of states 0.73, obtained by Mattheiss (1970) gives a value for the enhancement (being an average over the Fermi surface) of 2.26 which is in good agreement with our result of 2.14 ± 0.17.

The ratio of measured to calculated mass represents the extent to which the bare band mass has been enhanced by many body effects such as electron–electron and electron–phonon interactions. In niobium, however, electron–electron enhancement is expected to be negligible (Lomer 1969). McMillan (1968) has derived an expression for the electron–phonon enhancement, factor $(1+\lambda)$ where λ in strong coupled superconductors ($\lambda \sim 1$) is given by

$$\lambda = \frac{1.04+\mu^* \ln(\theta/1.45T_c)}{(1-0.62\mu^*)\ln(\theta/1.45T_c)-1.04}$$

and

$$\mu^* = (1-2\alpha)^{\frac{1}{2}}/\ln(\theta/1.45T_c)$$

μ^* is the Coulomb coupling constant, T_c the superconducting transition temperature, θ the Debye temperature and α the isotope shift coefficient. Since α has not been measured in niobium, McMillan took a value for $\mu^* = 0.13$ (being an average for the measured transition elements) in order to determine the enhancement $(1+\lambda)$ in niobium to be 1.82. The implied value of α was thus 0.42. If we assume that the correct enhancement factor in niobium is from the present work 2.14, then we find $\mu^* = 0.24$ and $\alpha = 0.24$.

6. Dingle temperatures

We have determined the Dingle temperatures for the α, β and η orbits at $\langle 100\rangle$, $\langle 110\rangle$ and $\langle 111\rangle$ respectively from the field variation of amplitude; the appropriate logarithmic plots show no anomalous effects. The Dingle temperature, T_D (Dingle 1952) is a parameter in the theory of the dH–vA effect which accounts for the finite electron lifetime due to collisions with impurities or other crystal defects. T_D is related to the electron lifetime through the relation

$$\left\langle \frac{1}{\tau} \right\rangle = \frac{2\pi k_B T_D}{\hbar},$$

where $\langle 1/\tau \rangle$ is an orbital average lifetime for electrons at the Fermi energy given by

$$\left\langle \frac{1}{\tau} \right\rangle = \frac{1}{\tau_c} \oint_{\text{Ext}} \frac{dt}{\tau}.$$

Here, τ_c is the cyclotron time and the integral refers to an extremal orbit in the dH–vA effect. A graph of $\ln [AH^{\frac{1}{2}}/J_2]$ against $1/H$ has as its gradient $-C(T+T_D)m^*/H$, where A is the amplitude of the dH–vA signal, C a constant $= 14.68\,T\,\text{K}^{-1}$ and J_2 a second-order Bessel function which enters in view of the particular manner of performing the experiments (Shoenberg & Stiles 1964). Here the dH–vA signal was detected at the second harmonic of the field modulation frequency whose amplitude was maintained constant as the main magnetic field was swept. The values found for the α, β and η orbits were 0.58 ± 0.6, 6.9 ± 0.8 and 0.10 ± 0.05 K respectively. Although these values refer to a very limited portion of the total Fermi surface, they do suggest a pronounced anisotropy of the electron lifetime due to impurity scattering (the chief impurity is tantalum as mentioned earlier).

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References

Alekseevskii, N. E., Bertel', K. Kh., Dubrovin, A. V. & Korstens, K. E. 1967 *Zh. eksp. teor. Fiz., Pisma v Redaktsiyu* **6**, 637. (English translation: *Soviet Phys. JETP Lett.* **6**, 1932 (1968).)

Alekseevskii, N. E., Bertel', K. Kh. & Dubrovin, A. V. 1969 *Zh. eksp. teor. Fiz., Pisma v Redaktsiyu* **10**, 116. (English translation: *Soviet Phys. JETP Lett.* **10**, 74 (1969).)

Blatt, 1967 *Electrons in metals*. London: Gordon and Breach.

Deegan, R. A. & Twose, W. D. 1967 *Phys. Rev.* **164**, 993.

Dingle, R. B. 1952 *Proc. Roy. Soc. Lond.* A **211**, 500.

Fawcett, E., Reed, W. A. & Soden, R. R. 1967 *Phys. Rev.* **159**, 553.

Goldstein, A., Williamson, S. J. & Foner, S. 1965 *Rev. Sci. Instrum*, **36**, 1356.

Halloran, M. H., Condon, J. H., Graebner, J. E., Kunzler, J. E. & Hsu, F. S. L. 1970 *Phys. Rev.* **1**, 366.

Halse, M. R. 1969 *Phil. Trans. Roy. Soc. Lond.* A **265**, 507.

Heininger, F., Bucher, R. & Muller, J. 1966 *Phys. Kond. Mat.* **5**, 243.

Lifshitz, I. M. & Kosevich, A. M. 1955 *J. exp. theor. Phys.* **29**, 730.

Lomer, W. M. 1969 *Progr. Mat. Sci.* **14**, no. 3, 99.

Mattheiss, L. F. 1965 *Phys. Rev.* **139***A*, 1893.

Mattheiss, L. F. 1970 *Phys. Rev.* **1**, 373.

McMillan, W. L. 1968 *Phys. Rev.* **167**, 331.

Onsager, L. 1952 *Phil. Mag.* **43**, 1006.

Reed, W. A. & Soden, R. R. 1968 *Phys. Rev.* **173**, 677.

Scott, G. B., Springford, M. & Stockton, J. R. 1968 *Phys. Letts.* **27***A*, 655.

Scott, G. B., Springford, M. & Stockton, J. R. 1968 *J. scient. instrum.* (*J. Phys.* E) **1** (2), 925.

Shoenberg, D. & Stiles, P. J. 1964 *Proc. Roy. Soc. Lond.* A **281**, 62.

Springford, M. & Stockton, J. R. 1970 *J. scient instrum.* (*J. Phys.* E) **3**, (2), 55.

Thorsen, A. C. & Berlincourt, T. G. 1961 *Phys. Rev. Letts.* **7**, 244.

Watts, B. R. 1964 *Proc. Roy. Soc. Lond.* A **282**, 521.