Further Results on the Fermi Surface of Beryllium*

T. L. Loucks†
North American Aviation, Tulsa, Oklahoma
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Following the methods presented in an earlier paper, the conduction eigenvalues for beryllium at the equivalent of over 80 000 points in the first Brillouin zone (all in the immediate vicinity of the Fermi surface) were calculated. The constant energy surfaces were constructed for several values of the energy near the Fermi energy. The hole and electron volumes were calculated for each case, and the Fermi energy was determined by the requirement that the two volumes be equal. This is the first time that this well-known result has actually been used to determine the Fermi energy in a band calculation. The corresponding Fermi surface was defined by about ten cross sections perpendicular to the [0001] direction. The agreement between these results and experiment is generally good and slightly improved over the previous results.

INTRODUCTION

In a previous article[1] the Fermi surface of beryllium was determined theoretically and compared with the experimental results of Watts.[2] The surface was constructed from conduction electron eigenvalues at the equivalent of 5184 general points in the first Brillouin zone (BZ). These eigenvalues were calculated by expanding the wave functions in a linear combination of 23 orthogonalized plane waves (OPW's). The crystal potential used in these calculations was self-consistent and its construction was fully described in the original article.

The same program which was developed for the earlier calculations has been used to calculate the conduction electron eigenvalues at the equivalent of over 80 000 points in the first BZ. All of these points were in the immediate vicinity of the Fermi surface. From these eigenvalues the Fermi energy was determined for the first time by the well-known requirement that the hole and electron volumes be equal. The Fermi surface corresponding to this Fermi energy was constructed and is presented in this report. It differs only slightly from the previous results, but tends to bring the theoretical and experimental results into closer agreement. The interesting feature here is not the new results, but rather the reminder that there is available, through the application of a well-known conservation requirement, a method of determining the Fermi energy which requires the calculation of energy eigenvalues only in the vicinity of the Fermi surface.

DETERMINING THE FERMI ENERGY

In the work of Loucks and Cutler[1] the Fermi energy was determined in the usual way by arranging in increasing value the energy eigenvalues which were calculated for representative points throughout the BZ. The energy corresponding to the highest occupied state was taken to be the Fermi energy. This method, although correct in principle, suffers in that it is difficult to get a representative sample of points (particularly near the zone edges) without calculating the eigenvalues at an extremely large number of points throughout the zone. Many of these points are not near the Fermi surface and hence are of little value except in the counting procedure for the determination of the Fermi energy.

The method proposed here has the advantage that all eigenvalues are calculated at points in the immediate vicinity of the Fermi surface. Thus, they serve not only to determine the Fermi energy but also to define more accurately the surface itself. In addition it provides enough information about the other energy surfaces near the Fermi surface to enable one to calculate first and second derivatives for use in determining such parameters as the density of states at the Fermi energy and the effective mass.

Essentially, the method employed is based on the obvious conservation requirement that the hole volume in the first double zone must equal the volume of the electron pockets in the second double zone. Since the electrons spill out of one zone into the next in order to

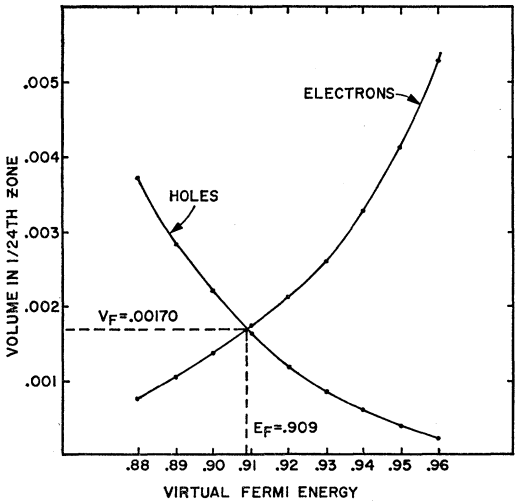

FIG. 1. Dependence of electron and hole volume on virtual Fermi energy.

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† Present address: Iowa State University, Ames, Iowa.
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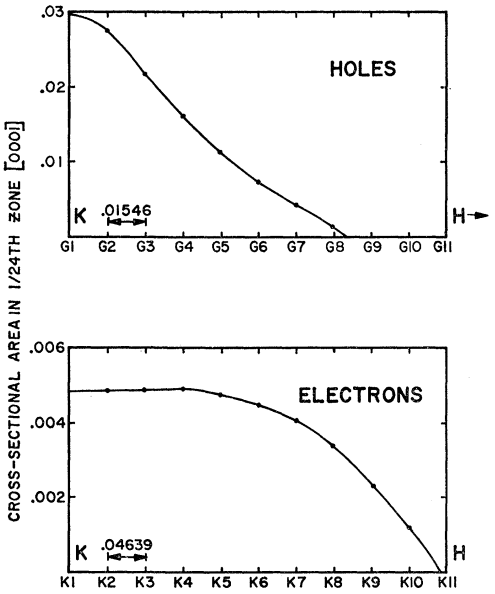

FIG. 2. Cross-sectional area of electron and hole surfaces in 1/24th zone for planes perpendicular to the [0001] direction.

minimize the energy, the vacated volume must be exactly equal to the volume occupied by the electrons. This is an admittedly obvious fact. However, it has never been used in practice to determine a theoretical value of the Fermi energy from a band calculation. The reason it has been avoided is perhaps because of the large number of calculations necessary to determine the electron and hole volumes. In this work they were determined for each of several constant energy surfaces near the Fermi surface. The results are plotted in Fig. 1. The curves of the hole volume and electron volume were found to intersect at $E_F=0.909$ Ry. The Fermi energy presented in the original paper was $E_F=0.901$ Ry.

FERMI SURFACE OF BERYLLIUM

The constant energy surface was constructed at $E_F=0.91$, as well as at other points, in constructing the curves shown in Fig. 1. Since we have found that the true Fermi energy is $E_F=0.909$, it is within the accuracy of the procedure used in constructing the surfaces to consider the one for $E_F=0.91$ to be the Fermi surface. These results are presented in Figs. 2, 3, and 4. In Fig. 2 the cross-sectional area perpendicular to the [0001] direction is shown for the holes and the electrons. In both drawings the left-hand side represents the symmetry point K, and the abscissa corresponds to distances measured along the symmetry edge KH. The identifications such as G1, G2, etc., correspond to the cross sections shown in Fig. 4. It should be noticed that in the lower curve of Fig. 2, corresponding to the electron cigars, the abscissa extends from K to H. However, in the upper curve, corresponding to the hole coronet, the distance between G1 and G11 extends only $\frac{1}{3}$ of the distance from K to H. Figures 3 shows the intersection of the Fermi surface with the 1/24th zone faces.

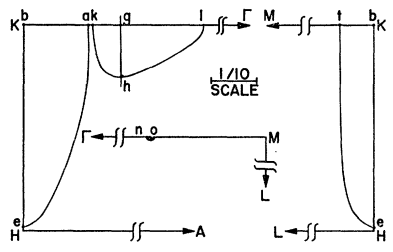

FIG. 3. Intersections of Fermi surface with faces of the 1/24th zone.

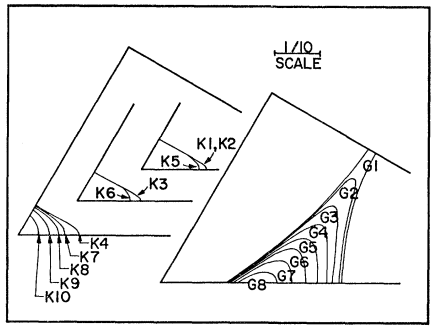

FIG. 4. Intersections of Fermi surface with planes perpendicular to the [0001] direction.

DISCUSSION

The Fermi surface which corresponds to the Fermi energy determined by the above method is compared to the previous theoretical results and the experimental results in Table I. It is seen that the agreement between the present theory and experiment is very good, especially for the bottom four entries which correspond to the coronet. However, the theoretical cigar is still shorter than the experimental one and almost triangular, rather than circular in cross section. This almost triangular shape also yields extremal cross-sectional areas

TABLE I. Comparison of representative dimensions of the Fermi surface as determined by the present work, the de Haas–van Alphen measurements, and the previous theoretical work.

Designation	Loucks	Watts	Loucks & Cutler
be	0.453	0.48	0.44
ba	0.141	0.09	0.13
bt	0.075	0.09	0.07
ak	0.008	0.08	0.01
kl	0.246	0.23	0.26
gh	0.118	0.13	0.13
no	0.017	0.02	0.04
ml	0.574	0.56	0.57

which are consistent with the observed de Haas–van Alphen frequencies. Further experiments or calculations which can distinguish between this model and the circular one proposed by Watts are necessary. It should be noticed in Fig. 2 that there is a waist on the almost triangular cigar. This is also consistent with the de Haas–van Alphen data. The larger cross-sectional area is about 2% greater than that of the waist. The corresponding experimental results predict 3%.

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Specific Heat of Thulium Metal Between 0.38 and 3.9°K*

O. V. LOUNASMAA†
Argonne National Laboratory, Argonne, Illinois
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The specific heat C_p of thulium metal has been measured in a He^3 cryostat. Between 0.38 and 3.9°K $C_p=2.839T^3+17.94T+23.43T^{-2}-1.79T^{-3}-0.066T^{-4}$ (in mJ/mole °K). The last three terms represent the nuclear specific heat C_N. On the basis of earlier estimates, we put $C_L=0.243T^3$ and $C_E=10.5T$ for the lattice and electronic specific heats, respectively. According to the simple spin-wave theory, the magnetic specific heat C_M is proportional to T^3 for a ferrimagnetic metal; experimentally one finds $C_M=6.2T^{5/2}$ for thulium, which has a rather complicated ferrimagnetic structure. Further, there seems to be no evidence in C_M for an exponential factor, to be expected because of magnetic anisotropy. All conclusions on C_M are tentative, however, until data at temperatures between 4 and 20°K become available. C_N does not fit to the simple picture as given by Bleaney either. Since $I=\frac{1}{2}$ for the only stable thulium isotope Tm^{169}, quadrupole interactions are zero and there are only two nuclear energy levels, their separation being determined by the magnetic hyperfine constant a'. This would give a nuclear specific heat with even powers of T only, with a' determining the values of the coefficients. The observed C_N cannot be fitted into an equation of this type which indicates that other interactions, probably nuclear exchange interactions, are present. Formally, the experimental situation may be expressed by writing $a'=a_0-b/T$, instead of treating a' as a constant. Our results are in good agreement with recent Mössbauer data by Kalvius *et al.* who found 22.9 for the coefficient of the T^{-2} term.

I. INTRODUCTION

AT low temperatures, the specific heat of rare-earth metals has four components which, depending on circumstances, can be separated totally or partially from each other. These are the lattice specific heat $C_L=AT^3$, the electronic specific heat $C_E=BT$, the magnetic specific heat C_M, and the nuclear specific heat C_N. In the higher lanthanides, C_M is primarily caused by exchange interaction between the $4f$ electronic spins. At 4.2°K and below, thulium has a unique ferrimagnetic structure, to be described in some detail later (cf. Sec. IV.B).[1] It is interesting to see how well the magnetic specific heat follows the prediction, $C_M=CT^3$, of the simple spin-wave theory.[2]

C_N is due to splitting of the nuclear spin states by interaction with the $4f$ electrons. By far the largest contribution to C_N comes from the magnetic field produced by the orbital angular momentum of the $4f$ electrons. The resulting nuclear specific heat has the familiar appearance of a Schottky curve with its maximum somewhere below 0.1°K. Above the maximum, C_N may be expressed in inverse powers of T, the leading term being proportional to T^{-2}.

According to the above discussion the total specific heat of thulium becomes

$$C_p=AT^3+BT+C_M+C_N, \quad (1)$$

where A and B are constants.

The present measurements on thulium are a part of our research program for studying the heat capacities of rare-earth metals between 0.4 and 4°K,[3–10] with particular emphasis on C_N. The specific heat of thulium has previously been measured by Jennings, Hill, and

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† Present address: Wihuri Physical Laboratory, University of Turku, Turku, Finland.
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