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PHYSICAL REVIEW A VOLUME 4, NUMBER 6 DECEMBER 1971

The de Haas-van Alphen Effect in Lutetium†

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(Received 22 July 1971)

de Haas–van Alphen oscillations have been observed in lutetium single crystals using high impulsive magnetic fields. A single-frequency branch is reported which has a minimum value of 3.75 MG along the c axis and extends ~22° in both the $(1\bar{2}10)$ and $(\bar{1}100)$ planes. Comparison of the experimental results with the relativistic-augmented-plane-wave Fermi surface of Loucks suggests that the electron columns are pinched off at the symmetry point H.

The de Haas–van Alphen (dHvA) effect in Lu single crystals has been studied in pulsed fields up to 200 kG. It is believed that the data presented here are the first direct experimental information related to the Fermi surface (FS) of any trivalent heavy-rare-earth metal.[1] The experimental procedure and data-reduction techniques used in the present investigation are essentially the same as those reported by Girvan *et al.*[2] and will not be discussed here.

The crystal structure of Lu is hexagonal close packed (hcp) and single crystals were prepared by the electrotransport technique.[3] The starting material had a resistivity ratio ($\rho_{300}/\rho_{4.2K}$) of ~21 and consisted of a $\frac{1}{8}$-in. rectangular rod 4 in. long. This rod had been spark cut from a single-crystal slab of Lu prepared by the arc-zone-melting technique[4] and annealed in a high vacuum for several hours. During the transport process the Lu bar was held at a temperature of 1120 °C in a vacuum of 10^{-10} Torr for 166 h. Two rectangular samples $\frac{1}{2}$ mm on a side and 4 mm long were cut from the transported rod, which had a resistivity ratio of ~60.

Figure 1 shows the angular dependence of the observed dHvA frequency branch, which has a minimum value of $F = 3.75$ MG and an effective mass of 0.38 ± 0.05 (in units of the free-electron mass) when the field is along [0001]. The oscillations are only observed for field directions within 22° of [0001] and disappear abruptly at this angle. Such behavior indicates that, due to the geometrical features of the FS, the orbit exists only within 22° of [0001]. The solid curves in Fig. 1 are a calculated fit to the data using the equation

$$F = F_0/(1 - D\tan^2\theta)^{1/2}, \quad (1)$$

where $F_0 = 3.75$ MG and $D = 1.83$ for the $(\bar{1}100)$ plane and 2.12 for the $(1\bar{2}10)$ plane. This equation expresses the angular dependence of a dHvA frequency

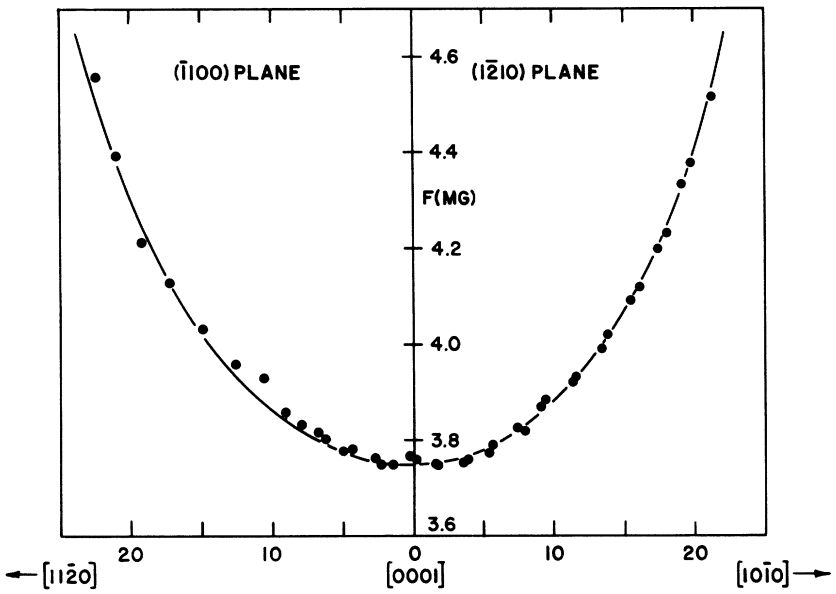

FIG. 1. Variations of the dHvA frequency in Lu for field directions in the $(1\bar{2}10)$ and $(\bar{1}100)$ planes. Solid circles: data points; solid line: calculated fit to the data.

corresponding to the area[5] defined by a plane intersecting a hyperboloid of revolution at its center of symmetry, where θ is the angle between the plane's normal direction and the hyperboloid's axis of revolution.

The lower-half of the primitive Brillouin zone for the hcp structure is shown in Fig. 2, indicating the points of high symmetry. It has been customary to display the FS of hcp metals in the double-zone scheme. However, according to the relativistic-augmented-plane-wave (RAPW) calculations of Keeton and Loucks,[6] the third-zone hole and fourth-zone electron surfaces no longer touch on the *AHL* face. Because of this splitting the FS of Lu will be considered to consist of separate hole and electron pieces. Intersections of the RAPW FS of Loucks and Keeton with symmetry planes of the Brillouin zone are presented in Fig. 3 in the repeated-zone scheme. With the magnetic field along the *c* axis (i.e., in the direction ΓA) there are several extremal orbits which are expected to give rise to a dHvA signal. The smallest dHvA orbits predicted from the model are an electron orbit around the electron column at *H* and a slightly larger electronlike orbit also centered at *H* arising from the hole surface. The shapes of these two orbits are shown in Fig. 4. The minimum dHvA frequency calculated for the smallest orbit is 6–7 MG. Other contributions to the dHvA effect are also expected from much larger orbits centered at Γ (see Fig. 3).

Since the smallest orbits expected from the model are at *H*, the observed frequency branch has been tentatively assigned to this region. The fact that only one low-frequency branch is observed instead of two as predicted from Figs. 3 and 4 can be understood as follows. The FS of Lu is very similar to that of Y (see Ref. 6) and Loucks[7] has noted for Y that the energy bands are very flat near the symmetry points *H* and *L*. Because of this flatness, small changes in the potential used in the RAPW calculations could alter the shape of the FS near *H* considerably and it is possible that the electron columns along *KH* are not present.[7] Assuming that a similar argument holds for Lu, the observation

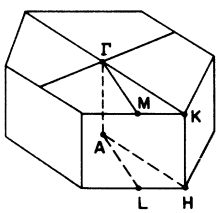

FIG. 2. Lower half of primitive Brillouin zone for the hcp crystal structure.

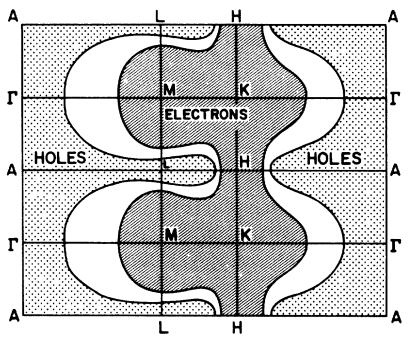

FIG. 3. FS cross sections for lutetium using the RAPW results of Keeton and Loucks. The third-zone holes are shown dotted, the fourth-zone electrons, lined.

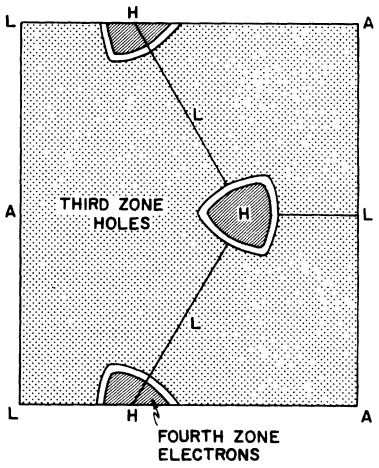

FIG. 4. Shapes of the two smallest orbits expected at H from the RAPW model.

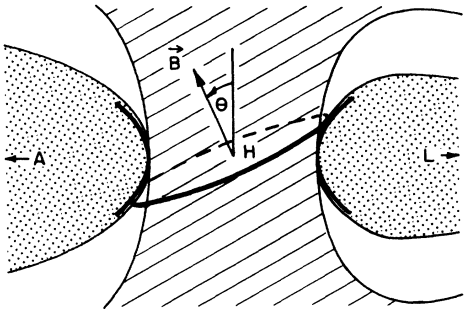

FIG. 5. Expanded view of the RAPW FS shape near the symmetry point H and along the line AHL. Light lines: RAPW FS (the hole and electron surfaces have been displaced symmetrically around H to correspond to the observed minimum area); heavy lines: calculated shape of FS near H assuming hyperboloid of revolution; dotted regions: third-zone holes; lined regions: fourth-zone electrons. Extremal orbit expected when the magnetic field is tipped 22° from the c axis is also indicated.

of only one low-frequency branch suggests that the electron columns are indeed pinched off at H in Lu. Such a modification in the band structure would also seem to move the hole surface closer to H (see Fig. 6 of Ref. 6) and thus reduce the size of the larger orbit shown in Fig. 4. A reduction in the size of this orbit would lead to better agreement with the observed minimum frequency of 3.75 MG. Further support for the absence of the electron surface at H is presented in Fig. 5. This figure is a cross-sectional drawing of the FS at H where the electron and hole pieces have been displaced symmetrically around H to correspond to the observed minimum area (an extremal orbit which agrees with the data is shown for a field direction of 22° from [0001]). The heavy vertical curves in Fig. 5 represent the FS shape corresponding to Eq. (1). Note that the shape of the hole surface near H closely resembles the calculated shape and thus could give rise to the observed dHvA frequency branch with only slight modification. If the observed orbit was from the electron column, then according to Fig. 5 the increase in frequency upon rotation away from the c axis would be much less than actually observed. Furthermore, the limiting angle for which one would expect an extremal orbit at H from the hole surface is ~30° and agrees reasonably well with the data, while the limiting angle from the electron column is near 45°.

No evidence was found in the data for large dHvA frequencies, although such frequencies would be expected from the model Fermi surface. The absence of high-frequency oscillations is undoubtedly due to the low purity of the sample. A second sample was used to search for dHvA oscillations for field directions in the basal plane, but no signals were observed. This is probably also due to the low sample purity, since no low-frequency branches are predicted from the RAPW model for such field directions. Lutetium single crystals of higher quality are presently unavailable and no further experimental results are anticipated at this time.

The Lu metal used in this work was kindly supplied by B. J. Beaudry and Professor F. H. Spedding, and invaluable help in growing the single crystals was given by F. A. Schmidt. Helpful discussions with Dr. S. H. Liu are also greatly appreciated.

†Work performed in the Ames Laboratory of the U. S. Atomic Energy Commission, Contribution No. 3058.

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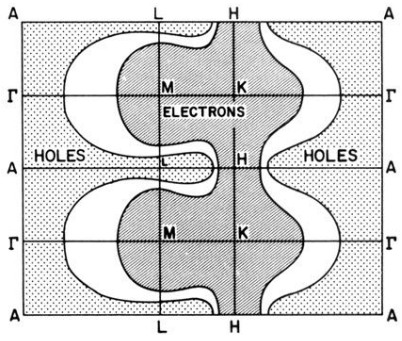

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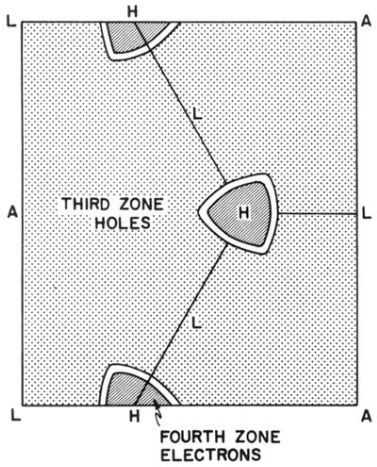

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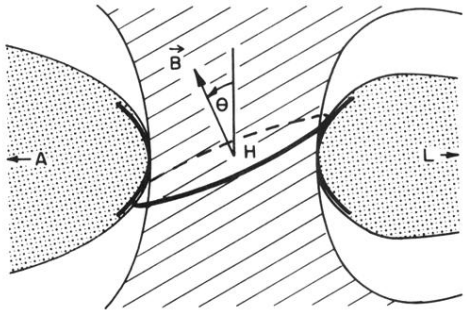

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