Fermi Surface of Aluminum

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Calculated cross sections of the aluminum Fermi surface relevant to the magnetoacoustic measurements of Kamm and Bohm are presented. The nature of the agreement between the calculated and measured dimensions of the surface is considered. On the basis of this and comparisons with other experimental data, it is concluded that the calculated surface, the features of which are similar to those of Harrison's nearly-free electron surface, is in quantitative accord with experiment. The only important unresolved question concerns the connectivity of the third band arms in the vicinity of the Brillouin zone corners.

IN the preceding paper, Kamm and Bohm[1] presented the results of their study of the Fermi surface (F.S.) of Al by the magnetoacoustic method. They compared dimensions of the Al Fermi surface determined from their measurements with the corresponding values calculated by the present author. We wish in this note to discuss briefly the calculations and to present the results of the relevant cross sections of the Fermi surface and finally to make a few comments about the comparison of the data and the theory.

The present work is an extension of the author's earlier band structure calculations on Al.[2] In that study the energy bands for Al were calculated for wave vectors in the principal symmetry directions. The results were obtained from "first principle" in the sense that they were based on a potential determined from atomic wave functions for the core and from physically reasonable assumptions about the distribution of the conduction electrons (later shown consistent with the results).[3] While the results were not explicitly made self-consistent (in the sense used in atomic calculations), it was clear from the free-electron character of the results that they were in fact rather close to being self-consistent.

Using the same potential and the same calculational procedure as in I except where noted below, the $E(\mathbf{k})$ was calculated for $\mathbf{k}$ near the F.S. in a number of (110) and (100) planes. The intersections of the second zone surface (which encloses holes) with (110) and (100) planes through the center of the zone (Γ) are shown in Figs. 1(a) and 1(b), respectively. It is evident from these figures that the shape of the second band surface is quite similar to that obtained from the nearly free electron (or one OPW) model of Harrison.[4] The dimensions of the calculated second zone contours are, in general, only a few percent smaller than the free electron surface. One difference between the two sections is that corners of the surface in (110) plane are rounded by the "residual" lattice interaction while those in the (100) are not. This is due to the fact that the corners in the (100) planes (near W) are points of contact.[4] That is, the relevant bands in that region cross. When the spin-orbit interaction is included, it is found that the corresponding states of the double group interact so that the corners are rounded and the point of contact is removed. A significant feature of these results is that the second zone surface does not intersect the zone boundary for the value of the Fermi energy, E_F, that we have used. For the latter we have taken the free-electron value which should be a very good approximation since the $E(\mathbf{k})$ is so free-electron-like over so much of the zone. To produce contact with the zone surface, a decrease in E_F by more than 0.03 Ry would be required. The shift in E_F due to deviation from free electron $E(\mathbf{k})$ should be significantly less than that amount.

Three different sections through the third band arms are given in Fig. 2. The cross sections in (110) and (100) planes through the points K or U [i. e., $\mathbf{k}=(\pi/a)$ $(\frac{3}{4}, \frac{3}{4}, 0)$, etc.], which are at the center of the arms, are shown in Figs. 2(a) and 2(b), respectively. Due to a limitation of our current computer program which restricts us to certain symmetry planes, the $E(\mathbf{k})$ used in constructing Fig. 2(b) were not obtained from the detailed band calculations used for the other results. For this calculation, the pseudopotential approach with the

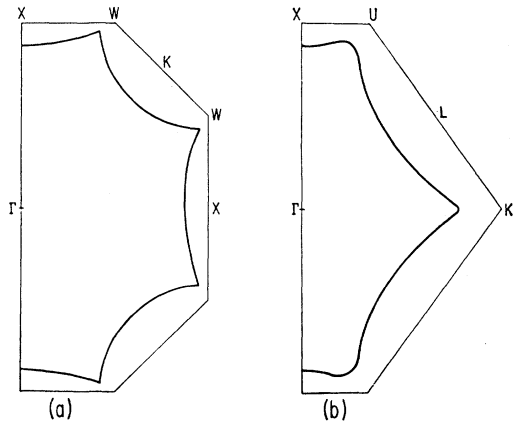

FIG. 1. Intersections of the second band Fermi surface with (a) a (100) plane and (b) a (110) plane through the center of the zone (Γ).

[1] G. N. Kamm and H. V. Bohm, preceding paper, Phys. Rev. **131**, 111 (1963), hereafter referred to as K-B.
[2] B. Segall, Phys. Rev. **124**, 1797 (1961), hereafter referred to as I.
[3] For the relationship of the crystal potential used in these calculations to that used by V. Heine, Proc. Roy. Soc. (London) **A240**, 361 (1957), see reference 2.
[4] W. A. Harrison, Phys. Rev. **116**, 555 (1959); **118**, 1182 (1960).

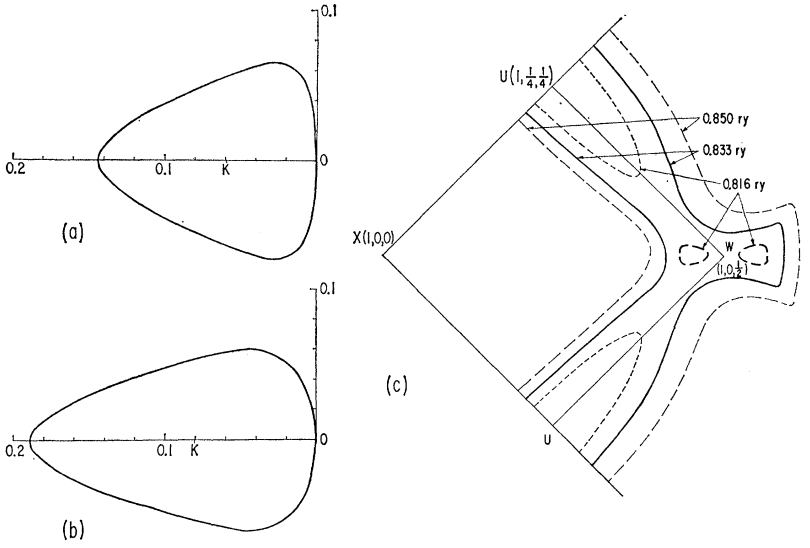

FIG. 2. Intersections of third band arms of the Fermi surface with (a) a (110) plane through the symmetry point K, (b) a (100) plane through K, and (c) a (100) plane through X.

parameters $V(200)$, $V(111)$, and m^* determined in I was employed. As shown in I, this approach leads to reasonably accurate $E(\mathbf{k})$ for Al. The resulting energy contour is, thus, expected to be correspondingly useful, although somewhat less accurate than the contours determined from the detailed band calculation. It is appropriate at this point to note that the shapes of the Fermi surface sections are similar to those obtained by Harrison[4] using the pseudopotential approach. The intersection of the (100) plane through X [i. e., $\mathbf{k}=(\pi/a)(1,0,0)$] with the four arms which lie on the edges of the square face of the Brillouin zone is shown in Fig. 2(c) for three different energies. It is to be noted that the arms of the calculated surface are connected for the E_F employed. However, a relatively small shift in E_F of the order of 0.01 Ry or a comparable modification of the energy bands disconnects the arms. Thus, small changes could produce changes in the topology of the surface in that region. A small change of this magnitude cannot be ruled out. The experiments of K-B, and the previous measurements of the Fermi surface, apparently do not provide definitive information as to whether the arms are connected or not. We believe that the nature of the surface in this region is the only significant unresolved feature of Fermi surface topology.

As was noted by K-B, not all of their data is fully understood. Some of the incompletely understood aspects of their results probably are related to complexities of the magnetoacoustic attenuation itself, in particular, the variation of the electron-phonon coupling for orbits over different parts of the Fermi surface. Nevertheless, much of their data is readily interpretable in terms of the Al band calculations.[2,4] In all cases where unambiguous comparisons between present calculated results and K-B measurements could be made, it has been found that the agreement has been good, generally within the experimental error. The magnetoacoustic experiments thus lend additional support to the picture of the Fermi surface that we have been discussing. Considering the other available experimental information about the surface, it appears that aside from the unsettled question of the connectivity of the third band surface near W, the calculated surface has been fairly well substantiated.

In a subsequent paper a more extensive study of the Al Fermi surface will be undertaken. Other electronic properties, including cyclotron resonance, deHaas–van Alphen effect, and interband optical transitions, will be considered.

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