CALCULATED SHAPE OF THE FERMI SURFACE OF COPPER

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(Received July 12, 1961)

The electronic properties of copper have recently become the subject of intensive study by a wide variety of experimental methods.[1] One important result of these investigations has been the general verification of the Pippard model[2] for the Fermi surface, which is nearly spherical over the main part of the surface (called the "belly") and which is pulled out in the ⟨111⟩ directions to form eight "necks" which contact the Brillouin zone surface. It is the purpose of this Letter to note that our recently completed band-structure calculations[3] on Cu not only have led to results consistent with the Pippard model but have also predicted interesting distortions of the "belly" which have just been observed experimentally.[4] Also we will present an explanation for the distortions and will discuss the importance of this effect for the other noble metals.

The calculations were carried out by the Green's function method[5] using two different crystal potentials. The first one, which is perhaps most appropriate for the d bands, was used initially by Chodorow.[6] For the second potential, we computed the Coulomb and exchange contributions separately for the different angular momenta from renormalized Cu Hartree-Fock functions. Only the results for the latter potential, which we believe to be somewhat more realistic than the former, will be discussed here although the other results are in semiquantitative agreement with them and lead to similar conclusions about the Fermi surface.[7]

Our results[3] show that the Fermi surface associated with the calculated energy bands contacts the hexagonal zone surface and the calculated ratio of neck to belly radii is 0.22 ± 0.02 in good agreement with the experimental ratio[1,4] of about 0.20. Also, for these bands, the onset of interband optical transitions would occur for transitions between the d bands around the upper L_3 state and the Fermi surface at about 2.6 ev in fair accord with the observed 2.2-ev value.

To study the Fermi surface in more detail, we have determined the intersections of the constant energy surfaces with a (110) plane (Fig. 1). The estimated Fermi energy is -0.19 ry. Aside from the sizable region of contact with the zone surface (for $E = E_F$), the principal feature of interest in these curves is that the belly is pulled out in the ⟨100⟩ directions and is contracted in the ⟨110⟩ directions. The occurrence of these appreciable distortions is at variance with the generally held belief that the main section of the surface is very nearly spherical.

Bearing out these results are the recently reported studies of the shape of the Cu Fermi surface by Morse et al.[4] using the magnetoacoustic effect which clearly show these deviations from sphericity. It is clear from their diagram that their observed and our calculated distortions are comparable. We find $k_F(100)/k_F(110) \approx 1.09$.

The explanation for the occurrence of these distortions involves the "repulsion" of conduction band states by the relatively high-lying d-band states of the same symmetry. In Fig. 2 are shown some of the bands of interest for this discussion. Now, the calculations[3] show that the lowest conduction band state at the end of the [100] axis has the p-like symmetry X_4'. As d-band states of this symmetry cannot occur, this state is not "re-

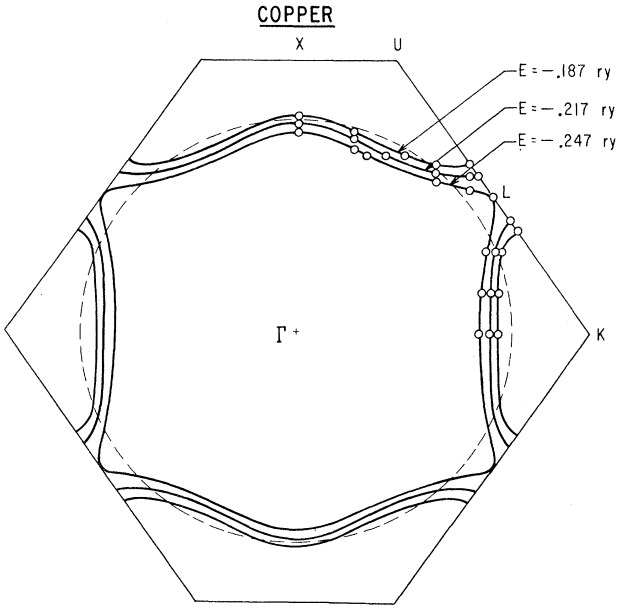

FIG. 1. The intersections of a (110) plane with calculated constant energy surfaces for Cu and with a free electron Fermi sphere (dashed curve). The estimated Fermi energy is -0.19 ry.

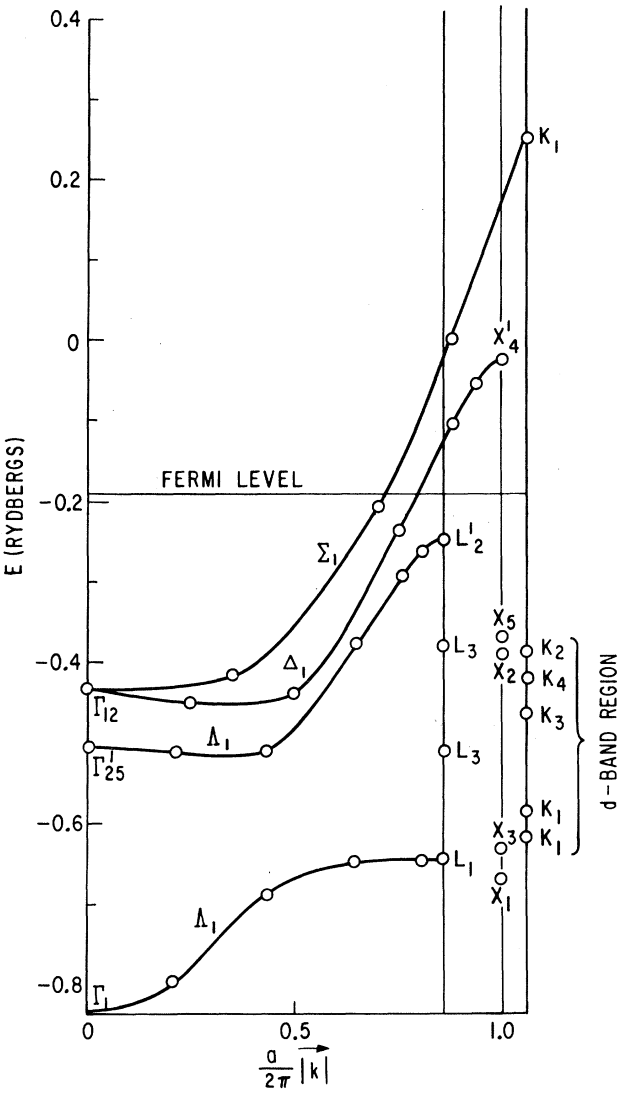

FIG. 2. The Cu energy bands in the conduction and d-band regions for the Λ_1, Δ_1, and Σ_1 states in the [111], [100], and [110] directions, respectively. For clarity, most of the calculated d-band curves were not drawn in.

pelled." Conduction band states "near" X_4' will, of course, have very small admixtures of d functions and consequently will only be affected weakly by the lower states. In the [110] direction, on the other hand, the conduction band (Σ_1 symmetry) "interacts" fully with the d band all the way out to the zone surface where it has K_1 symmetry. The argument also applies to the other noble metals as our calculations for them[8] also indicate that the lowest conduction band states at X and L are p-like. It is interesting to note that Morse et al. have also observed these distortions in Au. Inasmuch as the d bands in Ag are expected to be lower than in Cu and Au, we would predict smaller distortions in that metal.

It is thus seen that, contrary to opinions often expressed in the past about the possibility of calculating meaningful energy bands for such a metal, the calculated bands lead to a Fermi surface in good agreement with the one determined by experiment. Of course, as the many-electron effects have not been treated adequately and the electron-phonon coupling has been neglected, we cannot expect these bands to describe all the electronic properties of this metal without the introduction of corrections for these correlation effects.

The details of the calculations will be published shortly.

The author wishes to thank Miss E. L. Kreiger for her invaluable help with the numerical computations.

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[1]This work is reviewed in The Fermi Surface, edited by W. A. Harrison and M. B. Webb (John Wiley & Sons, Inc., New York, 1960), in the articles by D. Shoenberg, p. 74; J. R. Klauder and J. E. Kunzler, p. 125; A. F. Kip, p. 146; G. E. Smith, p. 172; and R. W. Morse, p. 214.

[2]A. B. Pippard, Phil. Trans. Roy. Soc. London A250, 325 (1957).

[3]The essential results and conclusions discussed in this paper were given in B. Segall and E. L. Kreiger, Bull. Am. Phys. Soc. 6, 10 (1961), and in B. Segall, Bull. Am. Phys. Soc. 6, 231 (1961). The latter talk has been written up as General Electric Research Laboratory Report No. RL-2785G which is available upon request. Also, see B. Segall, reference 1, p. 314.

[4]R. W. Morse, A. Myers, and C. T. Walker, J. Acoust. Soc. Am. 33, 699 (1961).

[5]W. Kohn and N. Rostoker, Phys. Rev. 94, 1111 (1954), and F. S. Ham and B. Segall (to be published).

[6]M. Chodorow, thesis, Massachusetts Institute of Technology, 1939 (unpublished).

[7]More recently G. A. Burdick (private communication) has also calculated $E(\vec{k})$ for Chodorow's potential and his results agree with ours.

[8]B. Segall, Bull. Am. Phys. Soc. 6, 145 (1961); 6, 231 (1961).