Fermi Surface for the 3*d* Band of Chromium

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The Fermi surface for the 3*d* band in chromium has been deduced from previously calculated $E(\mathbf{k})$ curves, which were obtained in the tight-binding approximation. It turns out that the filled electronic states occupy the regions around the Γ point and the Δ and F lines of the Brillouin zone.

THE electronic structure of the 3*d* band in chromium has been calculated in a previous paper[1] in the tight-binding approximation, taking into account interactions between nearest and second-nearest neighbors. Some idea of the shape of the Fermi surface can be deduced from the calculated $E(\mathbf{k})$ curves, even if it may be expected *a priori* that the shape of the Fermi surface is more critically dependent on the starting assumptions than is the case of other general conclusions which were deduced in the above-mentioned calculation.

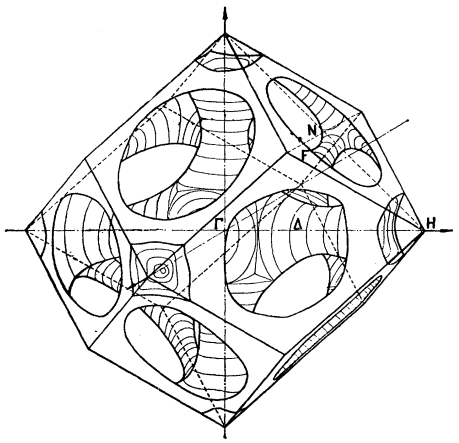

FIG. 1. The Fermi surface for the 3*d* band of Cr.

For each value of the wave vector $\mathbf{k}$, Eq. (4) of reference 1 has five roots, which have to be collected into five sets, each of which being associated with an energy band belonging to one Brillouin zone.

The attribution of the energy values to each set was done by intercombining the solutions at each degeneracy point in such a way that for each value of $\mathbf{k}$ the highest value of the energy belongs to the first Brillouin zone, the next highest one belongs to the second Brillouin zone, and so on.[2]

With the value of the Fermi energy E_F which was previously attributed to chromium (see reference 1), the Fermi surface turns out to lie entirely within one Brillouin zone.

The shape of the Fermi surface is given in Fig. 1.

The filled electronic states occupy the regions around the Γ point and the Δ and F lines, while large empty interconnected regions show around the N point on the external faces of the dodecahedron. Small empty regions appear also around the H point.

Moreover, it is worth while to point out that if a different value of E_F were assumed, namely, if a slightly different number of electrons were assigned to the 3*d* band, the Fermi surface would be modified a little and new portions of it would appear in the other Brillouin zones.

[1] M. Asdente and J. Friedel, Phys. Rev. **124**, 384 (1961).

[2] L. P. Bouckaert, R. Smoluchowski, and E. P. Wigner, Phys. Rev. **50**, 58 (1936); G. Fletcher, Proc. Phys. Soc. (London) **65**, 192 (1952).