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EVIDENCE FOR SPIN-ORBIT SPLITTING IN THE BAND STRUCTURE OF ZINC AND CADMIUM*

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Cohen and Falicov[1] have discussed the effect of spin-orbit coupling on the topology of the Fermi surfaces of the hexagonal close-packed metals. They conclude that spin-orbit splitting lifts the degeneracy between the first and second bands at the corners of the Brillouin zone and separates the small pockets of holes (arm caps) in the first band from the region of holes (arms) in the second. This gives rise to a closed-hole surface (cap surface) in the first band and a second-band surface that is infinitely extended along the hexagonal axis [Fig. 2(b) of reference 1] due to the intersections of arms. Both of these surfaces have extremal cross sections at the hexagonal face of the zone which one would expect to be observable in de Haas–van Alphen, cyclotron resonance, and ultrasonic attenuation experiments.

During the course of detailed de Haas–van Alphen studies of zinc and cadmium, we have observed oscillations in the magnetic susceptibility whose periods correspond to estimated values for the aforementioned extremal cross sections and which we have been unable to account for with Fermi surface models that neglect spin-orbit coupling. The de Haas–van Alphen periods were obtained by a torsion method in magnetic fields up to 23 kilogauss, using a null deflection technique and automatic recording. The angular dependences of the periods essential to this discussion are shown in Fig. 1. θ is the angle between the magnetic field direction and the hexagonal axis.

In Cd, for small θ the values of the Δ and x periods can be determined to within approximately 2% because all of the oscillations present are of comparable amplitude. As θ is increased the amplitude of the main arm oscillation increases rapidly, while effects due to arms in the other symmetry directions [periods indicated by dashed lines in Fig. 1(b)] are hardly observable. The amplitudes of the x and Δ oscillations drop rapidly, with Δ undetectable at $\theta \cong 1°$ and x at $\theta \cong 10°$.

In Zn, analysis is more difficult because x and Δ occur only as a weak modulation on a strong carrier—the arm periods. It was possible to obtain an unambiguous value for the Δ points out to a θ of 6°. However, there is no way of distinguishing from our data whether x lies below the arm period as shown in Fig. 1(a) or an equivalent distance above. The lower value was selected to be consistent with the relative sizes of the spin-orbit splitting in Zn and Cd (reference 1) and with the effect of this splitting on the difference in cross section of arm junction and cap surface as explained below. For θ greater than 7°, beating among the three arm periods makes detection of the Δ oscillation difficult due to its decreasing amplitude and to the presence of a comparable arm period. Therefore, the angular extent of the Δ period is not sharply determined. Near $\theta = 15°$, where the Δ period might beat distinctly with the arm periods, a careful search yielded no sign of its presence up to 23 kilogauss nor did any unexplained periods appear at larger θ.

The arm data in Zn agree with the few periods observed by Verkin and Dmitrenko,[2] while those in Cd fit very well with the work of Berlincourt,[3] but no mention of the x and Δ periods appears in either paper. We feel that the identification of Δ's as cap surface periods and x's as arm junction periods is correct because the other periods observed in Zn and Cd agree with the general form of portions of the Fermi surface predicted by the single orthogonalized plane wave construction,[4] and because this construction requires arm junctions and cap surfaces in the single zone scheme.

The presence of the spin-orbit energy gap decreases the cross section of the cap surface and increases that of the arm junction from the common value that these cross sections would have in

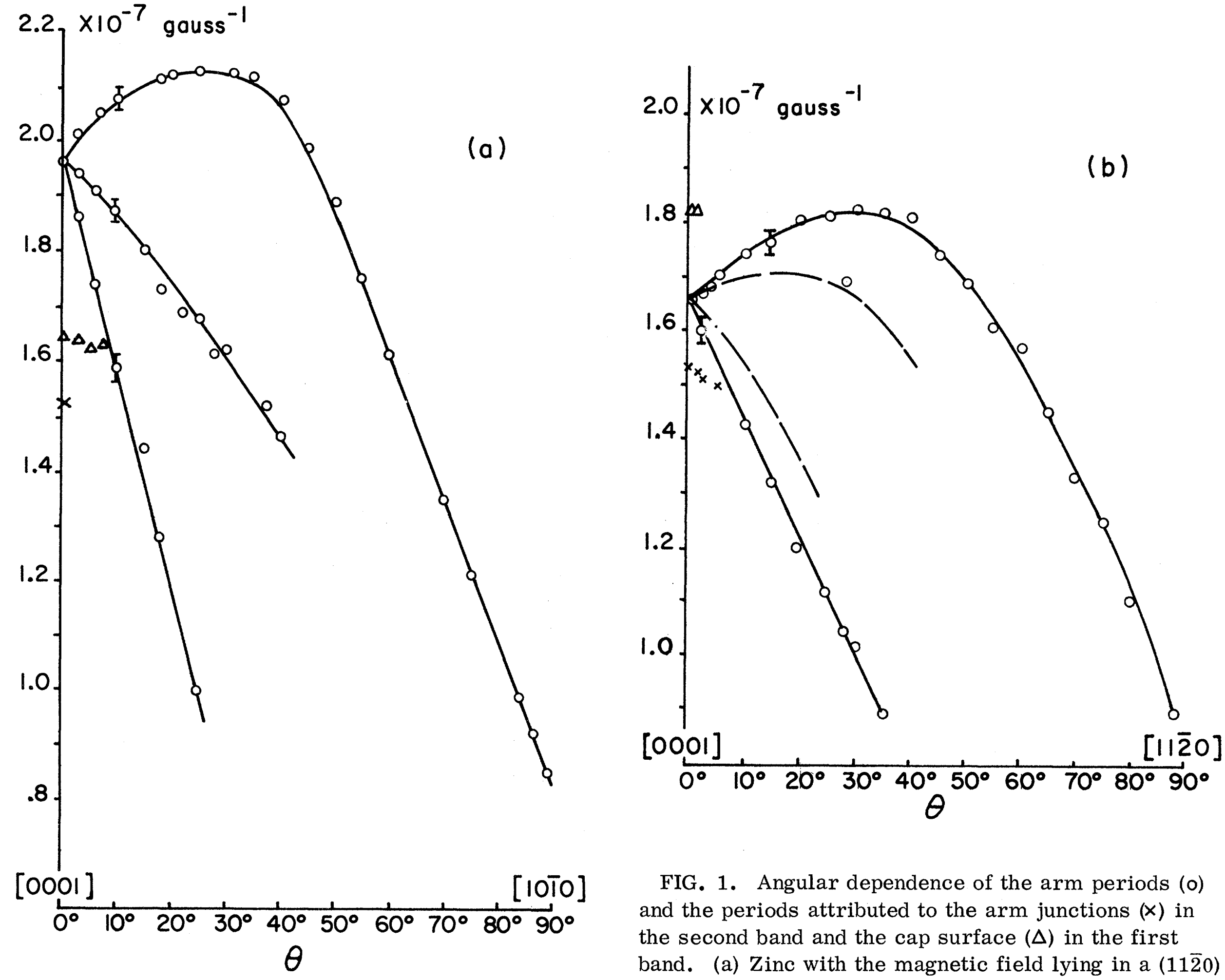

FIG. 1. Angular dependence of the arm periods (o) and the periods attributed to the arm junctions (×) in the second band and the cap surface (Δ) in the first band. (a) Zinc with the magnetic field lying in a (11$\bar{2}$0) plane (in reciprocal space). (b) Cadmium with the magnetic field lying in a (10$\bar{1}$0) plane (in reciprocal space). The dashed lines are drawn for the other arm periods expected using cross sections described by the full line.

the limit of a vanishing gap. If we use the nearly free electron approximation to estimate the influence of the size of the energy gap on the difference between cap surface and arm junction at the Brillouin zone face, the periods of Fig. 1 for magnetic field along the hexagonal axis yield a ratio of the spin-orbit energy gap in Cd to that in Zn of 2.2. This value is in reasonably good agreement with the estimate of 3 given in reference 1. The alternative possible assignment for the x period in Zn, discussed above, leads to an energy gap in Zn greater than that in Cd, an unlikely situation.

Our observation of periods due to the cap surface and arm junctions in Zn in magnetic fields as high as 23 kilogauss seems at first glance surprising in view of the possibility, first pointed out by Cohen and Falicov,[5] of "magnetic breakdown" of the spin-orbit energy gap. Blount[6] has shown that the relevant parameter determining breakdown is $\hbar\omega_c E_F/E_g^2$; i.e., when this quantity is much greater than one, the semiclassical electron orbits are determined by ignoring the energy gap in question. (Here ω_c is the cyclotron frequency, E_g is the energy gap, and E_F is the Fermi energy.) Using Cohen and Falicov's value for E_g in Zn,[1] we obtain for a field of 23 kilogauss a value for the above parameter that is of the order of one. Thus one would expect behavior characteristic of a transition region with additional scattering processes which would seriously decrease the amplitude of de Haas–van Alphen oscillations.

However, the criterion for breakdown should depend upon the inclination of the semiclassical orbit relative to the Brillouin zone plane under consideration. Intuitively, it would seem that if the electron's orbit cuts the Brillouin zone plane at a steep angle, then the probability for "jumping the gap" ought to be higher than if the electron moves parallel to the zone plane. This result is borne out by detailed calculations; in fact, when the electron moves parallel to the zone plane, magnetic breakdown is completely inhibited. Thus, the spin-orbit energy gap across the hexagonal zone face in such metals should be seen, even at high fields, when the magnetic field is directed along the hexagonal axis of the crystal.

We have calculated the transition probability for scattering out of a semiclassical orbit as a result of the perturbation: $V = V_0 \cos(\vec{K}, \vec{r})$. According to nearly free electron theory, $E_g = 2V_0$. The method used is an alternative one to Blount's and is one suggested by Cohen.[7] We start with the transition probability per unit time due to scattering:

$$w = (2\pi/\hbar)\langle \sum_{k'} |V_{kk'}|^2 \delta(E_{k'} - E_k)\rangle_k, \qquad (1)$$

where $\langle \ \rangle_k$ indicates an average over the orbit out of which the electron is being scattered. When the plane of the electron's orbit makes a small dihedral angle θ with the Brillouin zone plane, we obtain for the transition probability per cyclotron period:

$$w/\omega_c = E_g^{\,2}/32\hbar\omega_c \theta E_F \sin^2\phi, \qquad (2)$$

where ϕ is the polar angle of the electron's orbit (measured with respect to the magnetic field). When the orbit cuts the Brillouin zone plane at right angles, the calculation of w/ω_c may also be effected easily; the result for this case differs from (2) primarily through the deletion of the factor θ. By a WKB argument Blount[6] has shown that when $w/\omega_c \gg 1$, the probability for electron tunneling is $\exp(-\pi w/8\omega_c)$. Combining Eq. (2) with Blount's exponential factor and the E_g of reference 1 suggests that the effects of spin-orbit coupling should be observable within an angular range of about 6° from the hexagonal axis in zinc.

One would expect the arm junction period to exist over only a limited angular region due to the disappearance of an extremal cross section for this region of the Fermi surface, but the cap surface period should be present (barring magnetic breakdown) over the entire range of θ. We have observed the cap surface period for θ as large as 6° in Zn and 1° in Cd, and the arm junction period for θ as large as 1° in Zn and 10° in Cd. It is obvious from this that our data to date can cast little light on the question of the quantitative correctness of the present theory of magnetic breakdown.

We have been unable so far to observe cap surface and arm junction periods in magnesium.

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