to 30% Nb remain superconducting and no appreciable reduction in T_s due to the iron was observed in the present experiments, consistent with the conclusion advanced above.

We have also plotted in Fig. 2 the susceptibility χ per gram of the Nb - Mo alloys without iron. If we assume that the susceptibility measures the density of states at the Fermi surface, we may relate an increase in the average number of electrons per atom N to an increase in the Fermi energy E_F by the relation $\Delta E_F = \mu_B{}^2 \Delta N/\chi M_0 A$, where M_0 is the mass of an atom of unit atomic weight and A is the average atomic weight. The energy scale derived in this way is shown in Fig. 2.

The sharp rise in magnetic moment per atom seen in Fig. 2 is a remarkable new phenomenon and provides some insight into the electronic structure of iron present as an impurity in the Nb - Mo crystal. A possible interpretation of the observations is the following. Each iron atom has 5 d states. Following suggestions by Mott and Stevens[9] that apply to the bcc structure, we may assume that 3 of these states of symmetry t_{2g} become part of the conduction band of the host lattice. The remaining two states of symmetry e_g we suppose to be only weakly coupled to surrounding wave functions and therefore essentially localized. For the alloys of less than 50% Mo we assume that the Fermi level lies below the e_g states and no moment is observed. Above 80% Mo we suppose that the Fermi level has crossed these states and that they are occupied by two electrons whose spins align according to Hund's rule to give the observed moment. The antiparallel spin states will be split off by exchange and correlation energy so that they lie above the Fermi surface and are unoccupied. From the energy scale in Fig. 2 we may estimate the effective width of the e_g band to be about 0.3 ev.

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EFFECT OF SPIN-ORBIT SPLITTING ON THE FERMI SURFACES OF THE HEXAGONAL-CLOSE-PACKED METALS*

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All theories of the electronic properties of metals and alloys having the hexagonal-close-packed (hcp) structure have supposed that the energy gaps vanish across the hexagonal face of the first Brillouin zone.[1,2] The simple argument based on the vanishing of the structure factor put forward first by Jones[3] was not correct for a general potential. A rigorous basis for the sticking together of the bands was provided by the symmetry properties and time-reversal arguments of Herring.[4] These were generalized to include spin-orbit coupling by Elliott for various crystal structures.[5] In particular, one sees from his results that the degeneracy is removed at the point H and along the symmetry lines S and S', but not at A and L nor along the line R (Fig. 1). The implications of Elliott's work for the electronic properties of hcp metals and alloys appear to have been overlooked. Two questions arise: How big is the splitting, and what modification of the existing theories is required?

We have extended Elliott's analysis to a general point in the plane, and have found, as expected, the degeneracy to be lifted. Near A the splitting

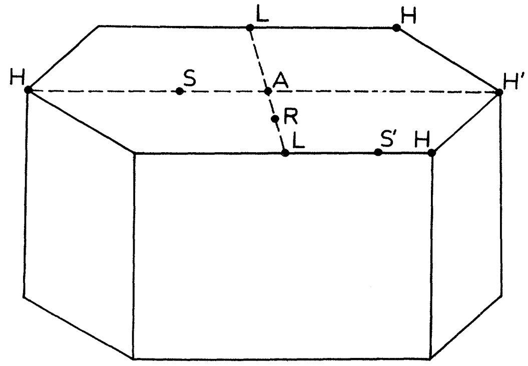

FIG. 1. The first Brillouin zone for hcp structures, showing points and lines of symmetry in the hexagonal face.

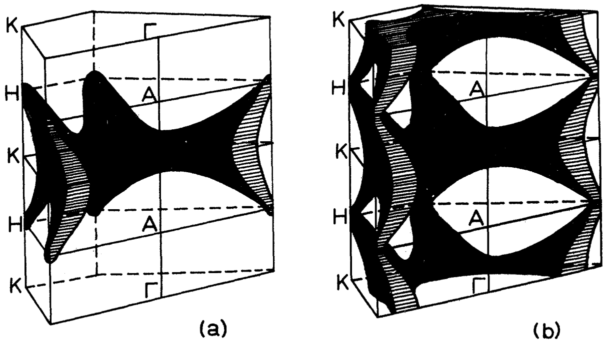

FIG. 2. The change in the connectivity properties of the Fermi surface of magnesium due to spin-orbit coupling. Diagram (a) shows the "without spin" case and (b) the surface in the second band when spin-orbit coupling is taken into account.

is very small because it is required to vanish by symmetry along the three lines R intersecting at A. The splitting increases from A along S initially as $(\Delta k)^3$ towards a maximum value for the entire plane at H.

We have calculated numerical values of the splittings at H for magnesium using the results of a previous orthogonal plane wave (OPW) calculation of the band structure.[6] A six-OPW approximation to the wave function was used; fewer OPW's would not have yielded the correct order of magnitude, more would have required an inappropriate amount of computation. The results are listed in Table I.

From the detailed wave functions one would have anticipated the splitting to be small for H_3, and for H_1 and H_2 to be somewhat greater than half the spin-orbit-coupling parameter for a $3p$ electron in atomic Mg (5×10^{-3} ev from the term values[7] of the configuration $3s3p\ {}^3P_J$). Both are found to be the case. Approximately the same ratios of splittings in the crystal to atomic spin-orbit-coupling parameter should hold for the other hcp metals: Be, Zn, Cd, and Tl. For these metals, therefore, the spin-orbit splittings are 0.05, 9.5, 28, and 129 times as large as the corresponding splittings for Mg.

Table I. The energies at H in magnesium.

Without spin		With spin	
Level	Energy (ev)	Levels	Splitting (ev)
H_2	9.33	H_4+H_6 H_8	2.83×10^{-3}
H_1	9.63	H_8 H_9	2.86×10^{-3}
H_3	12.22	H_5+H_7 H_9	3.1×10^{-5}

Fermi level at about $E_F = 9.25$ ev.

No major changes of existing alloy theories are required because the spin-orbit splitting vanishes at the center of the hexagonal face and is very small in a sizable region around the center. However, the topological features of the Fermi surfaces of the pure metals are fundamentally changed, and the double zone scheme ordinarily used in their representation is no longer valid. Without spin-orbit coupling, that piece of the Fermi surface corresponding to holes in the first and second bands in Mg[6] and Zn[2] is multiply connected with infinite extent normal to the c axis but not parallel to it [Fig. 2(a)]. With such a Fermi surface the observed lack of saturation of the magnetoresistance for fields normal to the c axis[8,9] could not be understood. The spin-orbit splitting, however, separates the small pockets of holes in the first band from the region of holes in the second and causes the latter to extend infinitely along the c axis [Fig. 2(b)]. This explains the observed magnetoresistance, because now open orbits exist for all directions of magnetic field normal to the hexad axis.

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VOIGT EFFECT IN SEMICONDUCTORS

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Double refraction of an electromagnetic wave passing through an isotropic substance under the influence of a static magnetic field in a direction normal to the direction of propagation is known as the Voigt effect.[1] We take as the equation of motion for an electron in the conduction band,

$$\frac{d^2\vec{r}}{dt^2} + (1/\tau)\frac{d\vec{r}}{dt} = -(e/m^*)\left(\vec{E} + \frac{d\vec{r}}{dt}\times\vec{H}\right), \quad (1)$$

where $\vec{r}$ is the displacement vector of the electron, τ is the mean collision time of the electron, $\vec{E}$ is the incident radiation field, $\vec{H}$ is the external magnetic field, and m^* is the effective mass of the electron.

A straightforward classical calculation using Maxwell's equations yields, using unrationalized cgs units,

$$2n_\perp^2 = \epsilon - 4\pi\sigma_0\tau/\beta[(\alpha/\beta)^2 + \omega^2\tau^2] + \left\{\left(\epsilon - \frac{4\pi\sigma_0\tau}{\beta[(\alpha/\beta)^2+\omega^2\tau^2]}\right)^2 + \frac{16\pi^2\sigma_0^2\alpha^2}{\omega^2\beta^4[(\alpha/\beta)^2+\omega^2\tau^2]^2}\right\}^{1/2}, \quad (2a)$$

$$2K_\perp^2 = -\epsilon + 4\pi\sigma_0\tau/\beta[(\alpha/\beta)^2 + \omega^2\tau^2] + \left\{\left(\epsilon - \frac{4\pi\sigma_0\tau}{\beta[(\alpha/\beta)^2+\omega^2\tau^2]}\right)^2 + \frac{16\pi^2\sigma_0^2\alpha^2}{\omega^2\beta^4[(\alpha/\beta)^2+\omega^2\tau^2]^2}\right\}^{1/2}, \quad (2b)$$

where the magnetic permeability has been assumed equal to one, $n_\perp$ is the index of refraction for radiation with electric vector normal to both the magnetic field and the direction of propagation, $K_\perp$ is the extinction coefficient in the normal direction, and

$$\alpha = 1 + \{\omega^2\omega_c^2\tau^2/[\omega^2 + (\omega^2 - \omega_p^2)^2\tau^2]\},$$

$$\beta = 1 - \{\omega_c^2(\omega^2 - \omega_p^2)\tau^2/[\omega^2 + (\omega^2 - \omega_p^2)^2\tau^2]\},$$

$$\sigma_0 = Ne^2\tau/m^*, \ \omega_c = eH/m^*c, \ \omega_p^2 = 4\pi Ne^2/m^*\epsilon,$$

with N equal to the free electron concentration.

For radiation with electric vector parallel to the magnetic field, the index of refraction, $n_\parallel$, and the extinction coefficient, $K_\parallel$, follow immediately from Eqs. (2) by setting $\alpha = \beta = 1$.

The phase shift between components parallel and normal to the magnetic field when incident radiation of wavelength λ traverses a substance of thickness d in a direction normal to the magnetic field is

$$\delta = 2\pi d(n_\parallel - n_\perp)/\lambda. \quad (3)$$

This phase shift takes a particularly simple form