BAND STRUCTURE AND FERMI SURFACE OF ZINC AND CADMIUM*

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We report here the results of band-structure calculations for the hexagonal-close-packed metals Zn and Cd based on an empirical non-local pseudopotential scheme which includes spin-orbit effects. The results agree to within a few percent with all reported extremal cross-sectional areas of the Fermi surface as measured by the de Haas–van Alphen effect,[1-8] are consistent with all other reported measurements of the Fermi surface properties,[9] and give the correct compensation of electrons and holes in the bands to an accuracy of 3×10^{-4}

electrons per atom in Cd (or equivalently 0.7% of the total number of electron or hole states) and 1.2×10^{-3} electrons per atom in Zn (2.5% of the number of states).

The band structure was calculated by solving numerically a complex secular equation of order n ($18 \le n \le 32$), the value of n being chosen to satisfy the star-of-k group symmetry of each of the six major symmetry points and used in the region of the Brillouin zone immediately surrounding these points. The matrix elements of the Hamiltonian are specified by

$$\langle \vec{k}'s' | \mathcal{H} | \vec{k}s \rangle = (\hbar^2 k^2/2m)\delta_{\vec{k}\vec{k}'}\delta_{ss'} + \delta_{\vec{k}-\vec{k}',\vec{G}}\,S(\vec{G})\{U_L(\vec{G})\delta_{ss'} + V_N(\vec{k}\vec{k}')\delta_{ss'} + W_{SO}(\vec{k}s,\vec{k}'s')\}, \qquad (1)$$

where s, s' denote spin indices, $\vec{G}$ is any nonzero reciprocal lattice vector denoted in hexagonal notation by $(h, k, \overline{h+k}, l)$, $S(\vec{G})$ is the structure factor

$$S(\vec{G}) = \cos 2\pi \{\tfrac{1}{6}(h + 2k) + \tfrac{1}{4}l\}, \qquad (2)$$

and U_L, V_N, and W_{SO} correspond to the local potential, the nonlocal potential and the spin-orbit interaction, respectively. Only four local coefficients were taken to be nonzero, corresponding to $\langle 0002 \rangle$, $\langle 10\bar{1}0 \rangle$, $\langle 10\bar{1}1 \rangle$, and $\langle 10\bar{1}2 \rangle$ type reciprocal lattice vectors. The values used for these in the calculations are listed in Table I. The nonlocal potential operator V_N is expressed in the form

$$V_N = \sum_{ti} v(t) |t, R_i\rangle\langle t, R_i|, \qquad (3)$$

where the index t runs over the s, p, and d states of the last occupied shell in the Zn or Cd cores and the functions $|t, R_i\rangle$ are the Hartree-Fock-Slater atomic functions[10] centered at the atomic sites R_i. The coefficients $v(t)$ are also shown in Table I. The spin-orbit term was expressed in the form

$$W_{SO}(\vec{k}s, \vec{k}'s') = i[\lambda_p + \lambda_d(\vec{k}\cdot\vec{k}')]\vec{k}'\times\vec{k}\cdot\vec{\sigma}_{ss'}, \qquad (4)$$

where $\vec{\sigma}_{ss'}$ are the ss' components of the Pauli matrices; the coefficients λ_p and λ_d are listed in Table I together with the values of the respective Fermi energies and the total num-

ber of carriers in the first and second band (holes) and third band (electrons) as obtained by numerical integration.

The band structures resulting from these parameters are displayed in Figs. 1 and 2. As can be easily seen, they are different from previously reported band calculations[11,12] in several respects. This difference results essentially from the fact that the dominant contribution to the pseudopotential arises primarily from the outer d shells of the respective ion cores. This portion of the potential dominates the character of the bands around Γ, L, K, and H. In both metals the third-band lens centered at Γ appears to be nearly free-electron like; this results from the fact that Γ_3^+ remains nearly unaffected by the d-like character of the potential. In both metals, the third and fourth bands centered at L are raised well above the Fermi level.

We have made a detailed comparison between the theoretical de Haas–van Alphen frequencies, as calculated by numerical integration of extremal cross-sectional areas of the Fermi surface, and the experimental values of Stark et al.[6-8] It includes normal orbits as well as orbits due to magnetic breakdown[13,14] between bands 1 and 2 as well as between bands 2 and 3. If the error in the calculations is expressed as ΔE_F, the necessary shift in the Fermi energy to bring the theoretically calculated fre-

Table I. Parameters of the band-structure calculations.

| Crystal structure parameters | | $U_L(G)$ Local pseudopotential | | | | $v(t)$ Nonlocal pseudopotential | | | λ_t Spin-orbit parameters | | Fermi energy | Calculated electron states | Calculated hole states |
| | | | | | | | | | | | | per atom | per atom |
a (Å)	c (Å)	(0002) (Ry)	$(10\bar{1}0)$ (Ry)	$(10\bar{1}1)$ (Ry)	$(10\bar{1}2)$ (Ry)	$v(s)$ (Ry)	$v(p)$ (Ry)	$v(d)$ (Ry)	p	d	(Ry)		
Zn 2.6596	4.8618	+0.0040	+0.0150	+0.0345	+0.0200	0	0	3.15	0.0050	0	0.8005	0.0450	0.0462
Cd 2.9684	5.5261	−0.0170	+0.0235	+0.0290	+0.0300	0	0.38	1.78	0.0105	0	0.651	0.0482	0.0485

quency into exact agreement with experiment, it turns out that the maximum error is of the order of 1.4×10^{-3} Ry in Zn and 6×10^{-4} Ry in Cd. The agreement between theory and experiment and the internal consistency of the calculation can be considered excellent.

An attempt was made to fit the experimental data for both metals using a purely local pseudopotential approximation. The best fit that could be achieved in either case resulted in average errors that were about an order of magnitude larger than those discussed above.

The following conclusions can be drawn from an analysis of the parameters and the results:

(1) Contrary to the case of Mg,[15] previously studied in similar detail, no sensible agreement between theory and experiment can be achieved by using only a local pseudopotential, i.e., by choosing all $v(t) = 0$.

(2) There is a strong repulsive d-like interaction in both Zn and Cd due to the $3d$ and $4d$ core states, respectively; the energy of these states lies very close to and below the conduction band and causes the strong overcancellation of the Coulomb potential. The d-like potential is the dominant term in the pseudopotential which, on the other hand, shows the customary good cancellation for p-like and s-like states.

(3) There are definitely no electron states in the third and fourth bands around the point L in the Brillouin zone; the so-called "butterflies" and "stars" which appeared in previous calculations as well as in the interpretation of various experiments do not exist and the frequencies and orbits previously assigned to them are due to other sheets of the Fermi surface.

(4) In zinc the oblique-arm structure,[1] which has been observed many times experimentally, is due, as first predicted by Harrison,[11] to magnetic breakdown between the first- and second-band hole surfaces.

(5) The magnetic breakdown effects in the galvanomagnetic properties of Zn for fields close to the [0001] axis are limited in their angular range only by geometrical features of the Fermi surface,[16] mostly the diameter of the horizontal arm of the "monster," and not by a rapidly varying energy gap between the second-band "monster" and the third-band "needle."

(6) The inclusion of spin-orbit effects in the calculation is of great importance in understand-
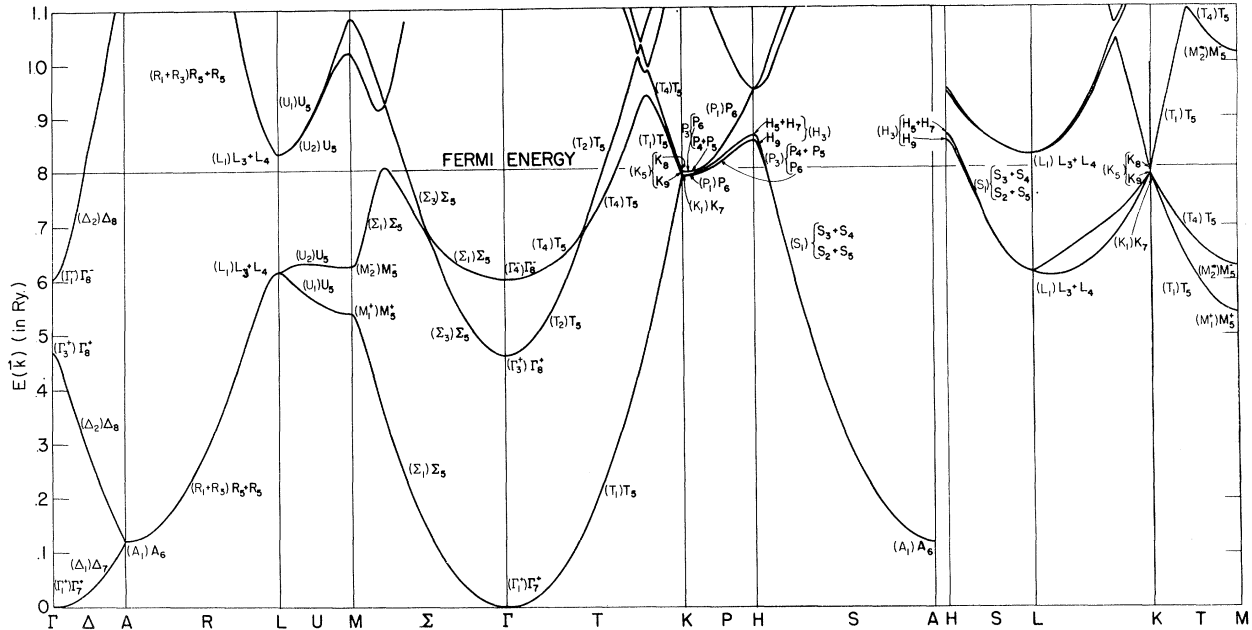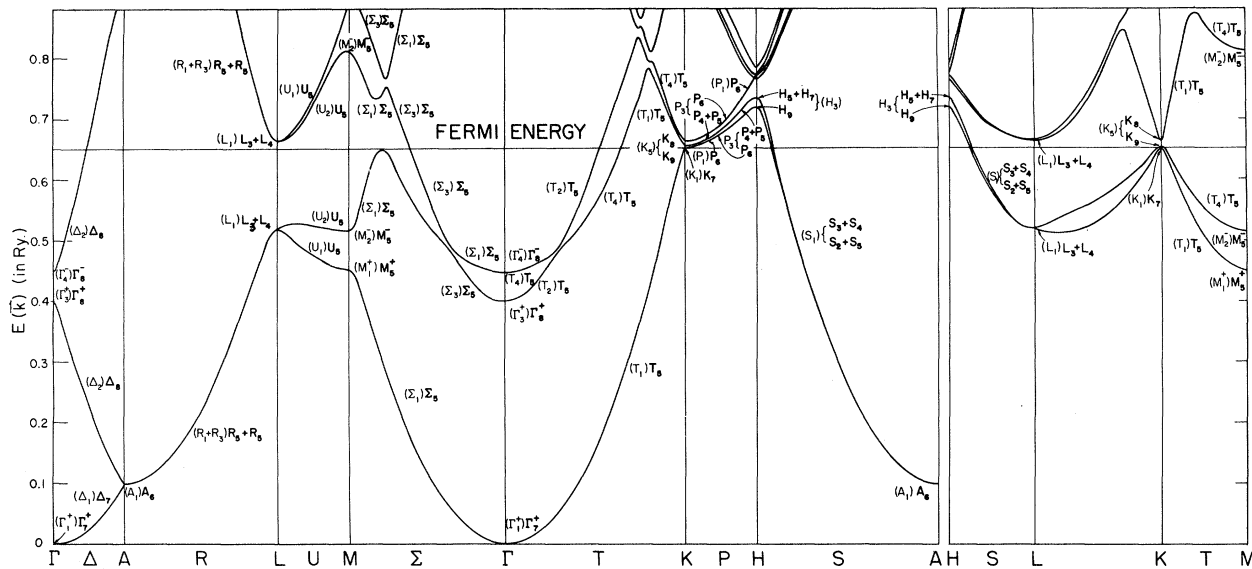
FIG. 1. Band structure of Zn.

FIG. 2. Band structure of Cd.

ing the band structure in the vicinity of the K-H line in the Brillouin zone as well as the magnetic breakdown effects; this has been previously recognized[17] but it is still surprising to see that at K the spin-orbit splitting of the K_5 level is greater than the K_1-K_5 splitting due to the crystal potential.

(7) The adequacy of the spin-orbit Hamiltonian[18] of formula (4) was demonstrated in a practical way in this calculation. In Cd, λ_p was chosen so as to give the necessary splitting

at H which accounts for the difference in frequency between the cap and the junction for fields parallel to the c axis. That value gave very good agreement between theory and experiment for all orbits which depend critically on the splitting of the level K_5. Such a test could not be performed in Zn because of the lack of an experimental value for the cap orbit.

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LEVELS EXCITED IN ^{206}Pb WITH BOTH TWO-NEUTRON STRIPPING AND PICKUP REACTIONS*

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Single-nucleon stripping and pickup reactions to the same final nucleus have long been used to gain information about the amplitudes of a few configurations in the wave functions of each final state. Now that reliable two-nucleon stripping calculations[1,2] are available, it is possible to test both the phases and amplitudes of many configurations in a proposed wave function for the final nucleus. To demonstrate this technique, a high-resolution study of levels in ^{206}Pb excited in the (t,p) and (p,t) reactions is reported here. The observed cross sections are compared with the predictions of two-nucleon stripping calculations using the wave functions calculated for ^{206}Pb by True and Ford,[3] by Miranda,[2] and by Broglia and Riedel.[2]

The experimental data were obtained using a magnetic spectrograph of the Elbek design in conjunction with 20-MeV triton and 22-MeV proton beams from the Los Alamos tandem Van de Graaff facility. The energy resolution of the experiments was 0.06%, or 10 keV for the tritons and 19 keV for the protons. Exposures were made at spectrograph angles of 20°, 35°, and 65° and the results were averaged to decrease the effects of angular variations in the magnitudes of the relative cross sections. Absolute cross sections were not measured, and for purposes of comparison the ground-state yields of the two reactions were normalized to each other after the angular averaging. The result of this procedure produces a rough estimate of the relative total cross sections to the various observed levels. The energy assignments from the two reactions agree within ±3 keV and are listed in Table I.