ESTIMATE OF THE SPIN-ORBIT PARAMETER ξ_{5d} IN METALLIC TUNGSTEN

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In the previous Letter, Walsh and Grimes[1] have presented the results of size-effect experiments on body-centered cubic tungsten which, on the basis of the Lomer model for the Fermi surface of chromium-group metals,[2,3] yield clear evidence for the presence of spin-orbit interactions in metallic tungsten. By comparing the results of nonrelativistic augmented-plane-wave energy-band calculations for tungsten with these experimental results, it has been possible to estimate the $5d$ spin-orbit parameter ξ_{5d} in tungsten to be approximately 0.03 Ry (0.4 eV). Using this value for ξ_{5d}, one can account for the disappearance of the electron lenses along the $\langle 100 \rangle$ axes in tungsten, a result which is consistent with the de Haas–van Alphen measurements of Sparlin and Marcus.[4]

It is difficult to obtain an accurate estimate of the atomic spin-orbit parameter ξ_{5d} from the measured optical spectra[5] for tungsten since intermediate, rather than Russell-Saunders, coupling is obeyed. Roughly, the possible values range from 0.02 to 0.05 Ry. Herman and Skillman[6] have calculated a first-order perturbation-theory estimate of ξ_{5d} using self-consistent Hartree-Fock-Slater atomic functions and they have obtained a value of 0.03 Ry.

The present estimate for ξ_{5d} is obtained from a simplified spin-orbit calculation involving $5d$ band states along the $\langle 100 \rangle$ or Δ direction in the Brillouin zone. The results of these calculations, as a function of ξ_{5d}, are shown in Fig. 1. In Fig. 1(a), the single and double group notation[7] for the various states is indicated, the former being included in parentheses. The state with Γ_1 symmetry corresponds to the bottom of the $6s$ conduction band; those states with $\Gamma_{25'}$, Γ_{12}, and $H_{25'}$ symmetry represent tungsten $5d$ band states. The computed Fermi energy is indicated by the broken horizontal line. Detailed comparison of the nonrelativistic Fermi surface which results from these calculations with the results of

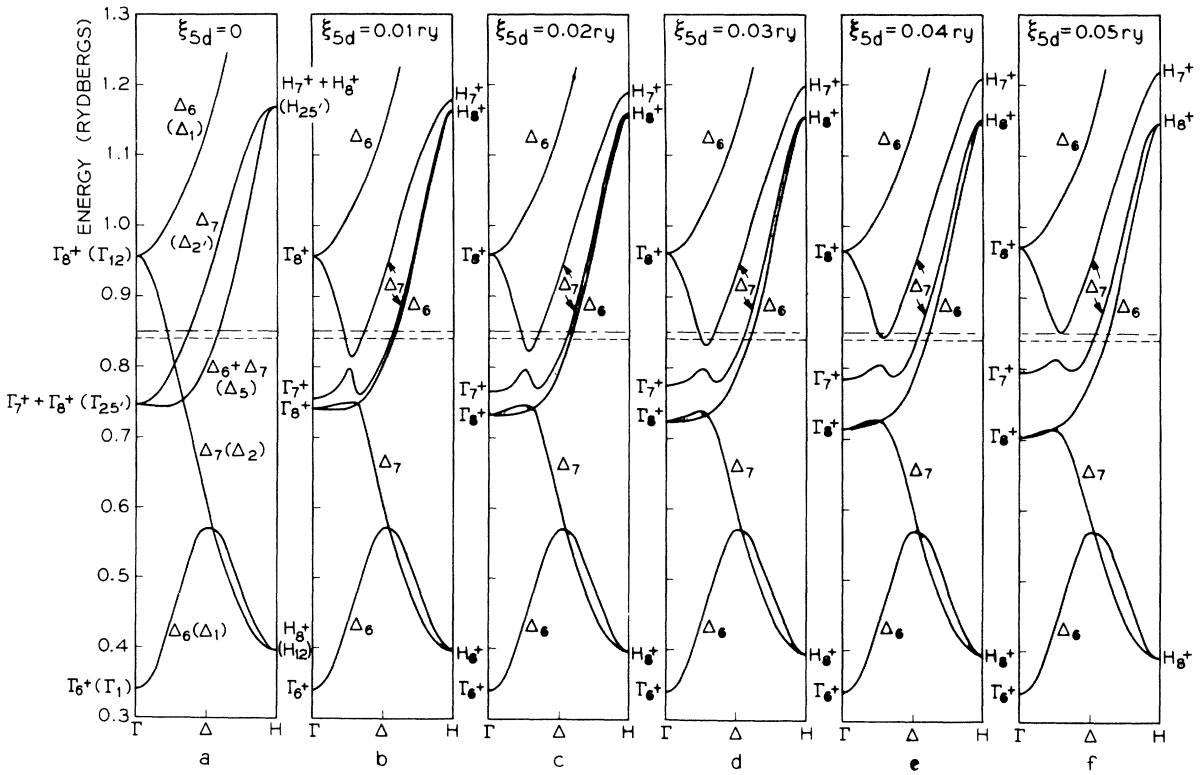

FIG. 1. Results of a simplified spin-orbit calculation along the $\langle 100 \rangle$ or Δ direction for body-centered cubic tungsten as a function of the spin-orbit parameter ξ_{5d}.

de Haas–van Alphen measurements by Sparlin[8] indicates that the s-d energy separation shown in Fig. 1(a) is approximately 0.1 Ry too small. Thus, the state with Γ_1 symmetry should have an energy of approximately 0.24 Ry instead of 0.34 Ry, the $5d$ states remaining fixed. It is estimated that this modification will lower the Fermi energy in the $5d$ bands by about 0.01 Ry. This is indicated by the dashed horizontal line.

The introduction of spin-orbit interactions results in a splitting of the Δ_5 degeneracy and removal of the Δ_7 crossings. To obtain a semiquantitative estimate of these effects, it is convenient to adopt a simplified model regarding the wave functions for these states. We assume that the wave functions for the energy band states with Δ_2-, Δ_2'-, and Δ_5-type symmetry are purely $5d$-like in character. If it is further assumed that these $5d$ functions all have the same radial function $P_{5d}(r)$, then the spin-orbit effects can be described in terms of a single spin-orbit parameter ξ_{5d}. Although it is well known that the d radial functions vary throughout the d bands,[9] it should be a good approximation to assume a fixed radial function in the vicinity of the Fermi energy.

In Fig. 1, the interaction of the three states with Δ_7 symmetry has been studied as a function of ξ_{5d} along the Δ direction. Neglecting off-diagonal matrix elements, it is found that the Δ_5 state is split by $\pm\frac{1}{2}\xi_{5d}$, the Δ_7 and Δ_6 states having the higher and lower energies, respectively. Including the effects of off-diagonal spin-orbit matrix elements between the three Δ_7-type states requires the solution of a three-by-three secular determinant; the results are shown in Figs. 1(b) through 1(f) for ξ_{5d} ranging from 0.01 to 0.05 Ry. In these calculations, the off-diagonal matrix elements between the three Δ_6-type states have been neglected. In the vicinity of the Fermi energy, the effects of the lower and upper Δ_6 states on the central one should be small and cancel to a first approximation.

From the experimental observation by Walsh and Grimes that the spin-orbit splitting between the electron "jack" at Γ and the hole octahedron at H is 5% of the Γ-H distance, we can estimate from Fig. 1 that the spin-orbit parameter ξ_{5d} at the Fermi surface in metallic tungsten is approximately 0.03 Ry. One interesting consequence of a spin-orbit parameter ξ_{5d} equal to approximately 0.03 Ry concerns the existence of electron lenses within the necks joining the electron octahedron at Γ with the balls along Δ. Sparlin and Marcus have not observed de Haas–van Alphen periods in tungsten which can be associated with these lenses.[4] Neglecting the spin-orbit interaction, the presence of necks implies the existence of lenses since the two surfaces must touch in the {100} and {110} planes.[3] Since the lenses are a result of the highest Δ_7 state passing through the Fermi energy, the present calculations suggest that the lenses will disappear in tungsten when ξ_{5d} is between 0.03 and 0.04 Ry. Thus, within the accuracy of the present calculation, the lenses in tungsten are either very small or nonexistent.

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