Band structure of bcc cobalt

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A self-consistent density-functional band-structure calculation using linear combinations of Gaussian orbitals for bcc cobalt has been performed. Also determined were the Fermi surface and x-ray form factors to make possible comparison with measurements on a film of bcc cobalt on chromium recently prepared by Walmsley *et al.* of Stanford University. The calculation was performed for several lattice parameters, including the experimental value $a=2.77$ Å.

I. INTRODUCTION

This calculation of the band structure of bcc cobalt was motivated by recent experiments by a group at Stanford University who succeeded in growing a film of bcc cobalt on a chromium substrate.[1] The film has been shown to be ferromagnetic. Although its magnetic moment is not yet known precisely, preliminary measurements indicate that the moment is close to its hcp value. Up to now Fe and Ni are the only ferromagnetic transition metals for which accurate band structures have been obtained by the density-functional method[2,3] for the normal lattice structure and which can be compared with experiment. Self-consistent calculations for the hcp phase of bulk cobalt are more difficult and have not yet been reported. There are, however, calculations for cobalt in the fcc structure.[4,5] Fe and Ni differ in several aspects, two of which are relevant here: The ratio of moments obtained from the Curie-Weiss law (p_c) and from the saturation magnetization (p_s) is close to 1 for Fe ($p_c/p_s=1.03$) and 1.46 for Ni.[6] In Ni the majority-spin d bands are fully occupied whereas the iron d bands are not. Photoemission measurements of the bandwidth and the exchange splitting give values that agree with the calculated values for Fe but not for Ni.[7] It is far from clear what the reason for these discrepancies is and so one would like to have another system where one could compare calculated results with experiments. It is the purpose of this calculation to make this kind of comparison possible.

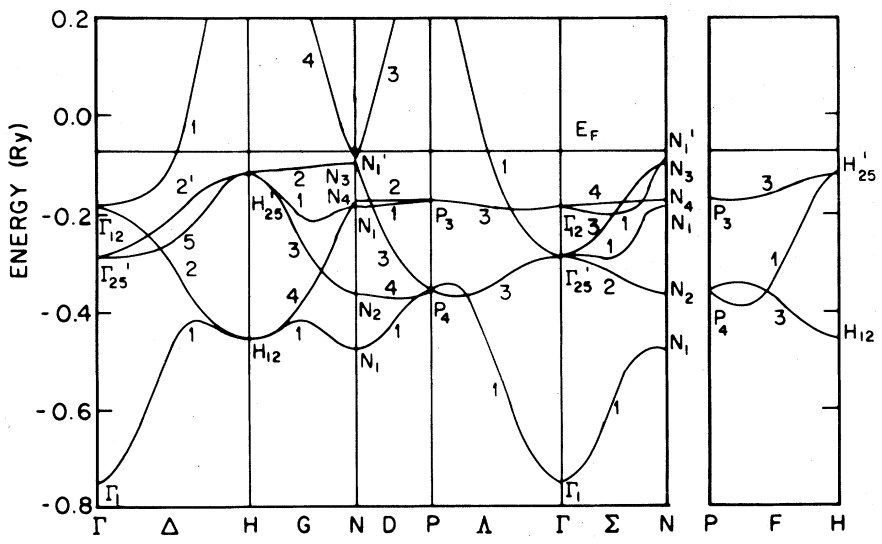

FIG. 1. Energy bands in ferromagnetic bcc cobalt along some lines of high symmetry for majority spin.

TABLE I. Representative energies (in rydbergs).

Band	$\Gamma_\uparrow$	$\Gamma_\downarrow$	$P_\uparrow$	$P_\downarrow$	$H_\uparrow$	$H_\downarrow$	$N_\uparrow$	$N_\downarrow$
1	−0.7492 (1)	−0.7427 (1)	−0.3550 (4)	−0.2790 (4)	−0.4543 (12)	−0.3615 (12)	−0.4743 (1)	−0.4074 (1)
2	−0.2854 (25′)	−0.1832 (25′)	−0.3550 (4)	−0.2790 (4)	−0.4543 (12)	−0.3615 (12)	−0.3613 (2)	−0.2684 (2)
3	−0.2854 (25′)	−0.1832 (25′)	−0.3550 (4)	−0.2790 (4)	−0.1105 (25′)	+0.0076 (25′)	−0.1840 (1)	−0.0715 (1′)
4	−0.2854 (25′)	−0.1832 (25′)	−0.1694 (3)	−0.0340 (3)	−0.1105 (25′)	+0.0076 (25′)	−0.1716 (4)	−0.0584 (1)
5	−0.1844 (12)	−0.0520 (12)	−0.1694 (3)	−0.0340 (3)	−0.1105 (25′)	+0.0076 (25′)	−0.0911 (3)	−0.0366 (4)
6	−0.1844 (12)	−0.0520 (12)	+0.5343 (3)	+0.5823 (3)	+0.6462 (15)	+0.6381 (15)	−0.0777 (1′)	+0.0288 (3)

II. BAND STRUCTURE

The technique of calculation used here is essentially the same as in earlier band-structure calculations for transition metals.[2,3] A contracted orbital basis of eight s-type, five p-type, and four d-type Gaussian orbitals was used applying the guidelines of Bagayoko.[8] The orbital exponents were obtained from the atomic wave functions of Wachters.[9] The initial charge density was a superposition of neutral-atom charge densities also generated from Wachter's[9] wave function with a configuration $3d^8 4s^1$. We did calculations for the following lattice constants: 5.0, 5.2346 (the experimental value), 5.3099 (corresponding to the same atomic volume as hcp cobalt), and 5.4456 a.u. (the chromium value). Only the 5.2346-a.u. results are given. The exchange-correlation potential used was an improved von Barth–Hedin-type potential developed by Rajagopal.[10] The bands are plotted in Figs. 1 and 2 and representative energy differences are given in Table I. An interesting feature of the band structure is that it is quite different for up and down spin. This applies especially for point N in the Brillouin zone; not only is the order of representations different for up and down spin, but they also make contact to different branches: $N_4^\uparrow$ connects to the lower G_4 branch (as in the case of Fe), whereas $N_4^\downarrow$ connects to the upper G_4 branch (as in paramagnetic chromium[11]). Similar observations are valid for N_1' which also, as N_3, has different D_3 connections for up and down spin (unlike both Fe and Cr). As to orderings and connections the minority-spin band is exactly like paramagnetic chromium. The basic reason for this is that the d states are pushed upward a large amount by the large exchange splitting whereas N_1' (a p state) is more or less fixed, which enforces switching branches to avoid crossing of the two G_4 and D_3 branches.

The total bandwidth ($E_{H_{15}^\downarrow} - E_{\Gamma_1^\downarrow}$) is 19.13 eV, the occupied-band width ($E_F - E_{\Gamma_1^\downarrow}$) is 9.26 eV, the d-

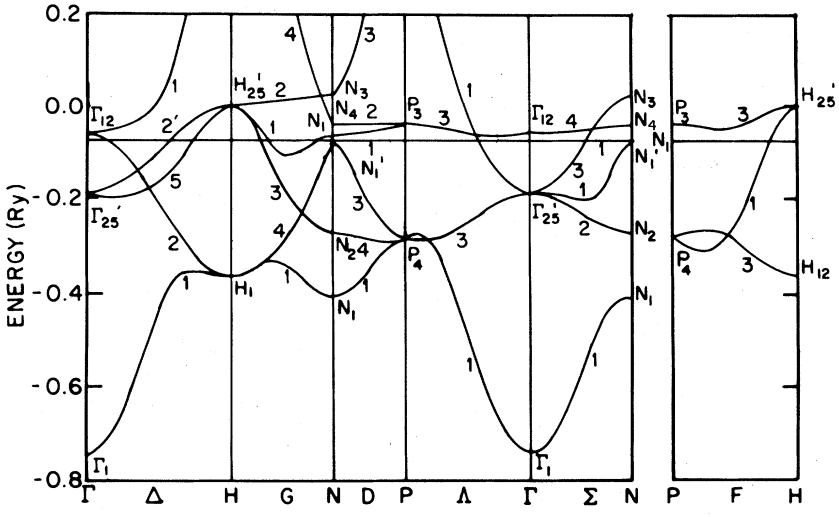

FIG. 2. Same as Fig. 1 for minority spin.

TABLE II. Band parameters for bcc and fcc Co (fcc values are from Ref. 11).

	Δ_{char}	E_F-$E_{\Gamma_1^\uparrow}$	$N_\sigma(E_F)$ (states/Ry)			μ
bcc	1.836 eV	0.6809 Ry	↑:2.079	↓:23.023	tot:25.101	$1.646\mu_B$
fcc	1.72 eV	0.662 Ry			16.87	$1.56\mu_B$

TABLE III. Charge and spin form factors.

Wave vector $(a/2\pi)k$	Charge	Spin
000	27.000	1.000
110	19.047	0.676
200	15.669	0.453
211	13.517	0.288
220	11.956	0.196
310	10.757	0.160
222	9.910	0.082
321	9.213	0.063
400	8.628	0.081
330	8.234	0.025
411	8.208	0.048
420	7.860	0.026
332	7.585	−0.007
422	7.321	−0.004
431	7.103	−0.009
510	7.070	0.022
521	6.728	−0.001
440	6.591	−0.018
433	6.463	−0.029
530	6.446	−0.013
442	6.333	−0.027
600	6.295	0.012
532	6.210	−0.022
611	6.185	0.004
620	6.081	−0.002
541	5.997	−0.022
622	5.888	−0.011
631	5.796	−0.013
444	5.722	−0.031
543	5.631	−0.027
550	5.626	−0.021
710	5.602	0.004
640	5.537	−0.017
552	5.460	−0.023
633	5.457	−0.020
721	5.441	−0.003
642	5.376	−0.019
730	5.286	−0.007
651	5.142	−0.017
732	5.136	−0.011

band width ($E_{N_3^\downarrow}-E_{N_1^\uparrow}$) is 6.48 eV, and the occupied d-band width ($E_F-E_{N_1^\uparrow}$) is 5.52 eV. The characteristic exchange splitting, the magneton number, the Fermi energy, and the density of states at the Fermi level are given in Table II. Also given in this table are the values for fcc cobalt.[4,5] It becomes clear from that comparison that, unlike fcc and bcc Fe, there is not much difference between fcc and bcc cobalt. This is also true in comparing the overall band structure of fcc and bcc cobalt as well as the density of states which is plotted for bcc cobalt in Fig. 3. In these general terms both forms of cobalt are similar to Ni, with which they share the property that the majority-spin d bands are fully occupied. It may also be taken from the table that the calculated exchange splitting is more than twice as large as the experimental value 0.85 eV (which, however, is measured in the hcp phase). Since it is unlikely that a structural change from hcp to either bcc or fcc can have such a drastic effect on the exchange splitting, i.e., the magnetic moment probably changes only slightly, bcc cobalt seems to be like fcc Ni in having an exchange splitting that is much

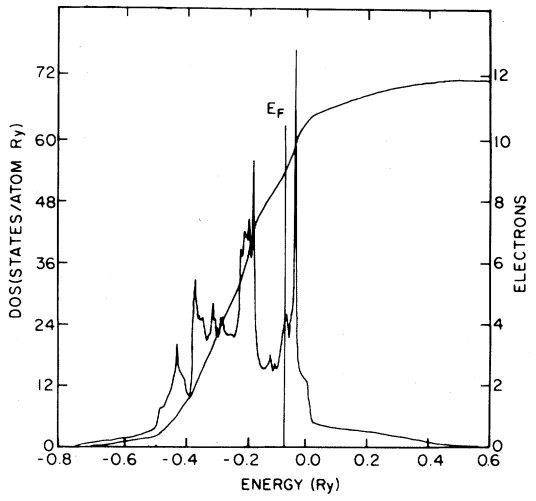

FIG. 3. Density of states including both majority and minority spins.

TABLE IV. Fermi-surface dimensions (in units of $2\pi/a$).

hole at H	0.26(ΓH), 0.13(ΓN)
jack at Γ	0.565(ΓH), 0.54(ΓN)
ball along ΓN	0.18(ΓN), 0.10($\perp\Gamma N$)
ball along HN	0.37(HN), 0.18($\perp HN$)

TABLE V. Magnetic moments for different lattice parameters.

a (a.u.)	m (μ_B)
5.00	1.545
5.2346	1.646
5.3099	1.678
5.4456	1.736

smaller than the one calculated by density-functional theory. We also determined the charge and spin form factors listed in Table III.

III. FERMI SURFACE

For the reason mentioned above the majority-spin surface is trivial, except for a small hole around N_1' whereas the minority-spin Fermi surface has interesting features. Although the general form of the minority-spin band is the same as that of the (paramagnetic) chromium band the Fermi surface is quite different. The reason for this is that the Fermi energy lies higher relative to the d band in Co$\downarrow$ than in Cr. This means, in general terms, that electron jacks expand at the expense of holes. In particular, the N hole vanishes and the H hole decreases. Because the bottom part of one Σ_1 and the G_1 branch intersect the Fermi energy, one has additional balls in the ΓN and HN directions (with one more electron than its neighborhood). Also the double jacks in ΓH increase substantially as does the small Cr ball which engulfs a large part of the surface in the (001) cross section and makes contact with the G_1 and Σ_1 balls. Also enlarged is the Γ diamond in the (001) cross section. Some dimensions of the Fermi surface are given in Table IV.

IV. CONCLUSION

The band structure of bcc cobalt has been determined by a self-consistent band calculation using the linear combination of Gaussian orbitals method within the density-functional approach in order to enable comparison to possible future experiments on bcc cobalt films on Cr. It was shown that the down- and up-spin bands are quite different, the majority-spin band being similar to Fe, the minority-spin band being of the same form as the paramagnetic chromium band. Further, bcc cobalt is similar in many respects to fcc cobalt and nickel having, for instance, fully occupied majority-spin bands. Co is only like itself in regard to the Fermi surface. Varying the lattice constant did not strongly affect the band structure so there is no indication of two stable states with very different magnetic moments as is claimed to be the case for fcc cobalt and fcc iron.[4] The magnetic moment as a function of lattice parameter in particular did not vary much as can be seen from Table V. It can be fit, approximately, by a straight line. For that reason the bands and corresponding data for lattice parameters other than the experimental value were not given here. It will be interesting to see to what degree future experiments will agree with our calculations.

ACKNOWLEDGMENT

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