Determination of level positions in the spin subbands of ferromagnetic cobalt by means of experiments involving pressure

L I. Vinokurova, A. G. Gapotchenko, E. S. Itskevich, and E. T. Kulatov
Institute of Physics of High Pressures, USSR Academy of Sciences

(Submitted 18 May 1979)
Pis'ma Zh. Eksp. Teor. Fiz. **30**, No. 1, 45–48 (5 July 1979)

The Baric derivative (BD) of the frequency a was measured in ferromagnetic GPU cobalt using the de Haas-van Alphen (dHvA) method. We show that the magnitude of the BD cross sections of the Fermi surface may be used to determine the position of levels which produce them in the ferromagnetic band structure.

PACS numbers: 71.25.Hc, 71.25.Pi

Cobalt is the least investigated of the three ferromagnetic $3d$ metals, and the number of works dealing with its electron structure is considerably smaller than those for Ni and Fe. From the experimental standpoint this is explained above all by difficulties in obtaining perfect crystals, and from the theoretical, by the complexity of its band structure. Accordingly, only comparatively recently have works appeared in which the de Haas–van Alphen (dHvA) effect was used to obtain certain extremal

 0021-3640/80/010039-04$00.60

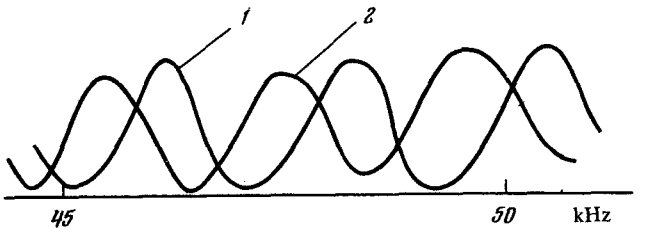

FIG. 1. Sections of the oscillation curves with phase shifted by pressure. Curve 1—pressure 1.5 kbar; curve 2—11 kbar.

cross sections of the Fermi surface (FS),[1,2] permitting verification of the few calculations of ferromagnetic GPU cobalt.[3-5]

A point common to the existing models of the cobalt band structure is the fact that Co, like Ni, is considered to be a strong ferromagnetic, i.e., in the spin-polarized bands with a large space factor (BLSF) the d-bands lie below the Fermi level and are fully filled. The FS for BLSF consists of one[4] or two[5] electron surfaces. The difference between models also pertain to whether there exists a neck at a point Γ in the Brillouin zone to which frequency β may be assigned, and whether open trajectories in the [0001] direction exist on this surface. A condition for the existence of such a neck is $E_F > E_{\Gamma_5}$.[5] In the case of a band with a smaller space factor (BSSF) the Fermi level passes through a complex system of d-levels and the FS of this spin band contains many sheets whose size and location are critical to the selection of a potential.

The paucity of experimental data (limited to certain small FS cross sections only), the deficiency of crystals that would permit observation of larger cross sections, and a considerable divergence in the band structure models all tend to stimulate the use of pressure as a parameter that may exert different effects on the FS cross sections for different models and, therefore, influence the choice of one of them.

We measured the dHvA effect under a pressure of up to 11 kbar. Pressure, was produced in a fixed-pressure chamber,[6] and the dHvA effect was measured with the aid of a modulation procedure used in the study of Ni and Fe.[7,8] Specimen were cut in the form of $1\times1\times4$ mm parallelepipeds. The internal field was estimated at 12.6 kG. Because of imperfections of our crystal ($\rho(300\text{ K})/\rho(4.2\text{ K})\approx150$) only the lower frequency α ($F_\alpha\approx1.06$ mHz) and a small number of oscillations could be observed. Hence, to achieve sufficient accuracy the BD was determined by a phase shift method used in the generation of pressure by a liquid on solid helium.

Figure 1 shows a phase shift by $\Delta\theta$ of several sections of oscillation curves relating to pressures of 1.5 and 11 kbar. BD was calculated from the formula $d\ln S/dP=(B/F)(\Delta\theta/\Delta P2\pi)$ and equalled $(-1.4\pm0.3)\times10^{-3}$ kbar^{-1}.

Calculations of BD were made[8,9] dependent on the redistribution of electrons among the bands, where the reduced magnetization M was explained within the framework of Stoner's theory as a decrease in the exchange splitting ΔE between the spin bands, i.e., it was assumed that $\delta\Delta E/\Delta E=\delta M/M$.

If, however, instead of the experimental effective mass we use in calculations the

band effective mass obtained from calculations, which is more appropriate for this model, then an evaluation based on Stoner's theory yields a value that is reduced when compared to the experimental. Therefore, it is necessary to have a formula for the BD which is free of the parameter ΔE whose relationship with M may exhibit different nature for the strong and weak ferromagnetics.[10]

Assuming that the change of the magnetic moment under pressure is determined by a flow of electrons from BLSF to BSSF which is accompanied by a volume change in parts of the FS, we get the following from simple considerations

$$\frac{d \ln S}{dP} = - \frac{m^*}{2e\hbar S} \frac{M}{N_\sigma \mu_B} \frac{d \ln M}{dP}, \tag{1}$$

where S is the area of extremal cross section, M is the atomic magnetic moment, μ_B is Bohr's magneton, N_σ is the density of states in the spin band at the Fermi level, and m^* is effective band mass.

As we know, $d \ln M/dP = -3.1\times10^{-4}$ kbar^{-1}.[12] The values of N_σ for BSSF and BLSF are 15.3 and 1.9 electrons/(atom-Rydberg).[4a] The band mass m^* calculated from the experimental $M^* = 0.11\, M_0$;[2] moreover for the BSSF the many-particle mass increase constant λ was calculated to be 0.45 which agrees with other values.[5] The negative sign of the experimental baric derivative means that, according to Eq. (1), the given surface is a hole type in BSSF and electron type in BLSF. The value of BD(α) calculated for the measured frequency α is -11.3×10^{-3} kbar^{-1} for BLSF and -1.4×10^{-3} kbar^{-1} for BSSF. The estimated value of BD(α) for BSSF is in good agreement with our experimental data and it confirms the generally-accepted opinion that the cross section α is located in this band.

The foregoing method of evaluating BD was also used for another frequency F_β ($\sim$3.53 mHz) which is heretofore unique, whose BD was measured to be -2.2×10^{-3} kbar^{-1}.[11] Reference 12 gives reasons according towhich the cross section β should be referred to the hole surface in BSSF.

The question concerning contributions of different origins to the total BD of FS cross sections of a ferromagnetic was discussed:[9] contributions dependent on the magnetic overflow and those associated with changes in the crystal potential. The first can be calculated by means of Eq. (1) or a similar formula as was done in Ref. 8, and the second is determined from the experimental data on a "modular" metal. Taking into account the topological equivalence of GPU and G lattices, the same potential portion of BD may be taken for the proposed neck β in the BLSF of Co as for a copper neck which is $+1.8\times10^{-3}$ kbar^{-1}. The BD(β) calculated from Eq. (1) is -3.6×10^{-3} kbar^{-1} for BLSF and -0.4×10^{-3} kbar^{-1} for BSSF. The value of m^* was $0.1m_0$.[5] The resultant BD(β) is -1.8×10^{-3} kbar^{-1} for BLSF and $+1.3\times10^{-3}$ kbar^{-1} for BSSF.

Thus, the experimental values of baric derivatives of FS cross sections lead to the conclusion that the cross section α belongs to the hole surface and may be found in the BSSF, while the cross section β belongs to the electron surface in the BLSF and,

therefore, the condition $E_F > E_{\Gamma_5}$ is satisfied in the band structure of Co, and the BLSF surface contains open trajectories along [0001].

[1]J.R. Anderson, J.J. Hudak, and D.R. Stone, AIP Cond. Proc. **10**, 46 (1973); I. Rosenman and F. Battalan, Phys. Rev. **B5**, 1340 (1972).

[2]K. Maczawa, M. Takahashi, and Y. Saito, J. Phys. Soc. Japan **45**, 869 (1978).

[3]S. Wakoh and J. Yamashita, ibid. **28**, 1951 (1970); S. Ishide, ibid. **33**, 369 (1972).

[4]C.M. Singal and T.P. Das, Phys. Rev. **B16**, 5068 (1977); J.D. Connoly, Intern. J. Quantum Chem. **IIs**, 257 (1968).

[5]F. Battalan, I. Rosenman, and C.B. Sommers, Phys. Rev. **B11**, 545 (1975).

[6]E.S. Itskevich, Prib. Tekhn. Eksp. No. 4, 148 (1963) [Instrum. Exp. Tech. USSR].

[7]L.I. Vinokurova, A.G. Gapotchenko, and E.S. Itskevich, Pis'ma Zh. Eksp. Teor. Fiz. **26**, 443 (1977) [JETP Lett. **26**, 317 (1977)].

[8]L.I. Vinokurova, A.G. Gapotchneko, and E.S. Itskevich, ibid. **28**, 280 (1978) [ibid. **28**, 256 (1978)].

[9]L.I. Vinokurova, A.G. Gapotchenko, E.S. Itskevich, E.T. Kulatov, and N.I. Kulikov, Zh. Eksp. Teor. Fiz. **76**, 1644 (1979) (in print) [Sov. Phys. JETP 834, (1979)].

[10]K.J. Duff and T.P. Das, Phys. Rev. **B3**, 192 (1971).

[11]J.R. Anderson, T.T. Hudak, D.R. Stone, and J.E. Schirber, Proc. Intern. Conf. Manget., ICM-73 M. **III**, 344 (1974).

[12]J.R. Anderson, High-Pressure and Low-Temperature Physics, C.W. Chu and Wollam, Eds., Plenum Publishing (1978).