Fermi surface of yttrium under pressure

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The pressure-induced changes in certain cross sections of the Fermi surface of yttrium have been measured by the de Haas–Van Alphen method. The parameters of the yttrium band structure calculated from these measurements are used to discuss the helicoidal magnetic ordering of heavy rare-earth metals in connection with the Dzyaloshinskiĭ theory {Zh. Eksp. Teor. Fiz. **47**, 336 (1964) [Sov. Phys.—JETP **20**, 223 (1965)]}.

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A study of the deHaas–Van Alphen effect in yttrium under pressure can yield information on the changes in the parameters of the Fermi surface. When such a study is combined with band-structure calculations, it can lead to qualitative conclusions regarding the relationship between the electron spectrum and the parameter of the helicoidal magnetic structure in the antiferromagnetic phase of heavy rare-earth metals, e.g., terbium and dysprosium.

Dzyaloshinskiĭ has shown[1] that the stability of the spiral magnetic structure of the heavy rare-earth metals is a consequence of the approximate equality of the wave vector of the structure, **Q**, and the vector Δk between the nearly parallel regions of different parts of the Fermi surface in the paramagnetic phase or other topological features of the Fermi surface. Other workers have shown[2–5] that the band-calculation prediction of the quantity Δk_{LM}, which connects the parallel parts of the electron and hole parts of the Fermi surface along the line LM (Fig. 1a), agrees well with the value found experimentally for the vector **Q** of heavy rare-earth metals by neutron diffraction.[6]

The paramagnetic phase of the heavy rare-earth metals is a high-temperature phase, so that this feature of the paramagnetic Fermi surface cannot be studied experimentally (by using the de Haas–Van Alphen effect, for example). Yttrium, a 4*d* metal, has the same structure of valence *sd* bands as the heavy rare-earth metals, whose Fermi surfaces are accordingly called "yttrium-like." Information on the Fermi surface of yttrium under pressure, the acquisition of data on $\Delta k_{LM}(p)$, and a comparison with the corresponding dependence of the vector $\mathbf{Q}(p)$ of magnetically ordered heavy rare-earth metals present a unique possibility for using pressure as a tool for studying the correlations between **Q** and Δk.

In this letter we are reporting measurements of the de Haas–Van Alphen effect over the pressure interval from 0 to 11 kbar for a yttrium crystal ($\rho_{300}/\rho_{4.2} = 460$) in magnetic fields oriented along the [001] axis and in the basis plane. Large-amplitude

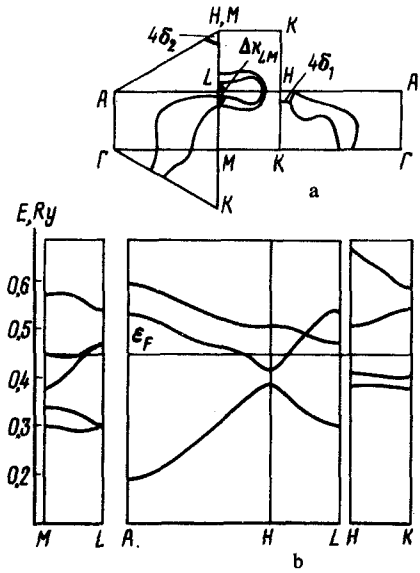

FIG. 1. Fermi surface of yttrium at standard pressure (1a) from Ref. 3. Shown here are the $4\delta_1$ and $4\delta_2$ cross sections, observed in the present experiments, and the quantity Δk_{LM} (see the text proper). The energy bands of *hcp* yttrium were calculated by the model-Hamiltonian method along certain high-symmetry directions for standard pressure (1b).

oscillations with beats have been observed by a modulation method[7] in magnetic fields up to 80 kOe at $T = 1.5$ K (Fig. 2). The zero-pressure de Haas–Van Alphen frequencies and also the relative amplitudes agree with the results of Ref. 8, where extensive de Haas–Van Alphen measurements were carried out for a yttrium single crystal with $\rho_{300}/\rho_{4.2} = 700$ at $T = 0.45$ K. Mattocks and Young[8] observed 12 de Haas–Van Alphen frequencies, corresponding to nearly all parts of the Fermi surface.

We adopted the following procedure[8] for identifying the frequencies detected in the present experiments: 1—The fundamental frequency $F(4\delta_1)$, with a high amplitude, arises from the minimal, nearly circular cross section of the complicated electron Fermi surface of the fourth band near the H point in the Brillouin zone (Fig. 1a) and has the value 3.25 MG; 2—the frequency $F(4\sigma_2) = 3.9$ MG is found from the beats and is attributed to that cross section of the same surface which lies directly in the *AHL* plane (Fig. 1a). The baric derivaties for these parts of the Fermi surface were calculated by the method of least squares and found to be in agreement at the values

$$d\ln F(4\delta_{1,2})/dp = (5.7 \pm 0.3)\cdot 10^{-3}\ \text{kbar}^{-1}.$$

We were not able to see oscillations with the field in the basis plane, even at a zero pressure.

From the temperature dependence of the amplitude of the frequency $4\delta_1$, measured over the same pressure interval, we calculated the effective masses $m^*(4\delta_1)$,

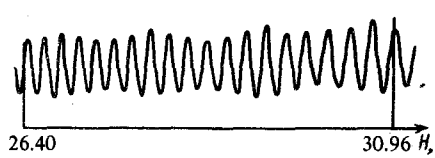

FIG. 2. de Haas–Van Alphen oscillations in yttrium for H [001], $T = 1.5$ K, and $P = 10.2$ kbar. The fundamental harmonic is related to the $4\delta_1$ cross section. The beats arise because of an admixture of the frequency associated with the $4\delta_2$ cross section, which lies near $F(4\delta_1)$.

which turned out to be $(0.37 \pm 0.03) \cdot m_0$ at a zero pressure and to be independent of the pressure, within the experimental errors, i.e., $d \ln m^*(4\delta_1)/dp = 0$. From the magnetic-field dependence of the amplitude of the de Haas–Van Alphen oscillations at a constant $T = 1.5$ K we can determine the Dingle temperature T^D and its baric derivative for the $4\delta_1$ cross section:

$$T^D = (1.0 \pm 0.2)\ \text{K} \quad \text{and} \quad \frac{d \ln T^D(4\delta_1)}{dp} = 0.$$

We should point out that T^D remains constant when the pressure is removed.

The $4\delta_1$ and $4\delta_2$ cross sections have large baric derivatives. Even if we discard the value $2/3 \cdot K_T = 1.673 \cdot 10^{-3}$ kbar^{-1} [the compressibility is $K_T = (2.51 \pm 0.1) \cdot 10^{-3}$ kbar^{-1}; Ref. 9], which is related to a simple scale increase of the Fermi surface under pressure, we are left with a value of 4×10^{-3} kbar^{-1} which is due entirely to a change in the crystal potential upon the compression of the lattice.

We have used these experimental results in an effort to determine the pressure-induced change Δk_{LM} at the LM symmetry line. For this purpose we carried out a self-consistent calculation of the yttrium band structure at 168 points at 1/24 of the irreducible part of the Brillouin zone at a zero pressure, using the model-Hamiltonian method of Ref. 10. The Fermi energy ϵ_F was found from the state-density curve; it corresponds to a filling of the conduction band to 3 electrons/atom. The state density at the Fermi level turns out to be 27 electrons/(atom·Rydberg).

Figure 1b shows the band structure of *hcp* yttrium along certain high-symmetry directions—those of most interest for a comparison with experiment. At standard pressure, the calculated cross-sectional area $S^T(4\delta_2)$ is 10.6 MG [$S^{\text{exp}}(4\delta_2) = 4$MG], and we find $\Delta k_{LM} = 0.58\pi/c$, in satisfactory agreement with the wave vector measured in Ref. 6 for the helicoidal spin wave, $\mathbf{Q} = 0.54\pi/c$, for a magnetically ordered alloy of Y with Gd.

Although the change in the potential caused by the pressure makes an extremely important contribution to the baric derivatives for the $4\delta_1$ and $4\delta_2$ cross sections, the experimentally established independence of the effective mass of this zone from the pressure near the H point, i.e., the consistency of its shape, means that we can use the rigid-zone approximation to calculate the shift of the Fermi level under pressure from the experimental value of the baric derivative of the $4\delta_2$ cross section, using

$$d \ln S^{\text{expt}}/dp = \frac{d \ln S^T}{d\epsilon_F} \frac{d\epsilon_F}{dp} \qquad (d\epsilon_F/dp > 0).$$

Working in this manner, we found that compression reduces Δk_{LM} to $0.36\pi/c$ at 30 kbar and that the baric derivative of this vector is $d \ln \Delta k_{LM}/dp = -13 \times 10^{-3}$ kbar^{-1}.

Fleming and Liu[11] have reported a theoretical study of the effect of pressure on the parameters of a simple-spiral magnetic order in terbium and dysprosium. They worked from a calculation of the paramagnetic zone structures at standard pressure and at a high pressure (20 kbar). They found $(d \ln \mathbf{Q}/dp)_{\text{theor}} = -10 \times 10^{-3}$ kbar^{-1} for terbium and dysprosium. The experimental value of $d \ln \mathbf{Q}/dp$ for terbium is

-18×10^{-3} kbar^{-1} (Ref. 12). These results agree satisfactorily with the value found by us for $d \ln \Delta k_{LM}/dp$.

Yet further confirmation of the decrease in **Q** during compression comes from data on the alloying of a few atomic percent of light rare-earth metals (praseodymium and neodymium) with terbium (the ratio c/a is increased as a result of this alloying, in a manner reminiscent of the compression of the pure metal).[13]

In summary, we have observed a definite correlation between the pressure dependence of the quantity Δk_{LM}, which related the corresponding parts of the Fermi surface of yttrium, and the pressure dependence of the wave vector of the helicoidal magnetic structure, **Q**, for yttrium-like heavy rare-earth metals, in accordance with the theory of Ref. 1.

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