Effect of pressure on the Fermi surface of antiferromagnetic chromium

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Pressure-induced variation of the cross sections of the Fermi surface of antiferromagnetic chromium is measured by using the de Haas-van Alphen method. A strong dependence of the wave vector of the spin-density wave on pressure is obtained.

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The Fermi surface (FS) of antiferromagnetic (AFM) chromium has a very complex shape principally because of incommensurability of the wave vector $\mathbf{Q}$ of the unattenuated spin-density wave (SDW) and the periodicity of the crystal lattice: $\mathbf{Q} = (2\pi/a_0)\ (1 - \delta_0,0,0)\ \delta_0 \approx 0.05$, SDW is associated with the magnetic ordering.[1] This incommensurability greatly complicates the FS of AFM chromium, which is usually described by "superimposing" the calculated FS of the high-temperature paramagnetic phase of chromium (see, for example, Ref. 2). This picture permits to interpret to some extent the measured frequencies of the de Haas–van Alphen effect (dHvA).[2,3]

To construct a dHvA model of AFM chromium, it is necessary to study its dependence on the interatomic distance, especially since the corresponding calculated data are available. Kulikov[2] calculated certain baric coefficients (BC) for the FS of chromium.

We investigated the dHvA effect in AFM chromium at a pressure of up to 11 kbar. It should be pointed out that conversion to the AFM phase in the absence of an external magnetic field, as was the case in this experiment, produces a polydomain structure with a different Q orientation. The compression was achieved by using a fixed-pressure chamber.[4] The dHvA oscillations were measured by using a modulation method in the magnetic fields up to 80 kOe at $T = 1.5$ K. The direction of the magnetic field H during the measurements was parallel to the crystallographic axis $\langle 100 \rangle$.

Two dHvA frequencies were observed at the normal pressure, whose values and amplitudes are in agreement with the results of Ref. 5 in which the measurements were conducted in the magnetic field without cooling. These frequencies, which coincide with those of Ref. 3, are identified as follows: 1) frequency $F_\zeta = 4.25$ MHz is due to the cross section ζ, which is produced as a result of intersection of the second-order paramagnetic ellipsoids (Fig. 1a) and 2) the frequency $F_\nu = 12.5$ MHz, is called the ν frequency. We assume that the latter cross section is produced as a result of first-order intersection (Fig. 1b).

Figure 2 shows the results of the analysis of the experimental material. The calcu-

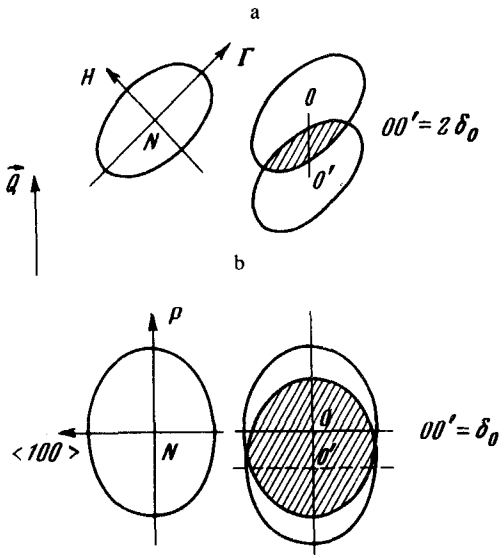

FIG. 1. (a)—Formation of the ζ-orbit as a result of intersection of the second-order paramagetic ellipsoids, (b)—formation of the ν orbit as a result of intersection of the first-order paramagnetic ellipsoids.

lated BC for these sections of the FS ($d \ln S / d \ln V$) are given in Table I. The indicated error is equal to the magnitude of the dispersion.

We used the obtained experimental data on the BC of AFM chromium and the results of calculation of the paramagnetic band structure performed in Ref. 2, in order

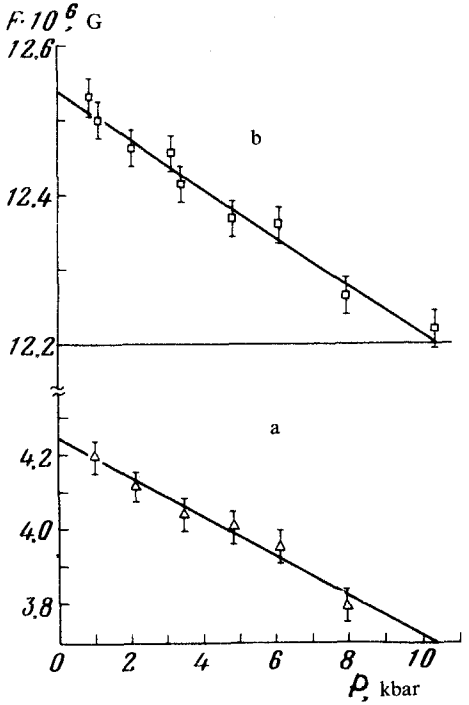

FIG. 2. Dependence of dHvA frequency (F) on pressure: a—for the ζ cross section; b—for the ν cross section.

	Frequency ζ	Frequency ν
$d\ln S/d\ln V$	26 ± 4	5.22 ± 0.3
$d\ln S_0/d\ln V$	− 1.6	− 2.9
$d\ln S/d\ln \delta/a$	− 1.62	− 0.51
$d\ln(\delta/a)/d\ln V$	− 17.8 ± 2.5	− 17.4 ± 0.6
$\frac{d\ln\left(Q\frac{a}{2\pi}\right)}{dp}\times 10^3$ kbar^{-1}	− 0.46 ± 0.08	− 0.45 ± 0.02

to explain such large BC for a metal with a very small compressibility and to confirm the aforementioned identification of the orbits.

First, we note that the BC of the cross sections of the paramagnetic ellipsoids S_0, which were obtained in the band calculation,[2] are not large and their sign is different from that of the BC of the AFM cross sections. These values of the cross sections in Figs. 1a and 1b are given in Table I. The BC for S_0 show that the ellipsoids increase under pressure. They are close to the BC in similar parts of the FS of molybdenum. Figures 1a and 1b show that only an increase of δ_0 in this case, may lead to the measured sign of the BC. Moreover, it should be emphasized that separation of the ellipsoid centers has a greater effect on the intersection cross section for the orbit ζ, where there are elliptic cross sections and a second-order intersection, than for the orbit ν, where the ellipsoid cross sections are almost circular and intersect in the first order. The BC measured experimentally behave this way.

To estimate the necessary variation of the **Q** vector, we used a simple geometric model,[6] which connects the volumetric variations of δ and of the cross sections of the AFM and paramagnetic chromium:

$$\frac{d\ln\frac{\delta}{a}}{d\ln V}=\frac{\frac{d\ln S}{d\ln V}-\frac{d\ln S_0}{d\ln V}\left(1-\frac{1}{2}\frac{d\ln S}{d\ln \delta/a}\right)}{\frac{d\ln S}{d\ln\frac{\delta}{a}}}, \tag{1}$$

$$\frac{d\ln\left(Q\frac{a}{2\pi}\right)}{dp}=-\frac{\delta_0}{1-\delta_0}\left(\frac{d\ln\frac{\delta}{a}}{dp}+\frac{d\ln a}{dp}\right). \tag{2}$$

The cross-sectional areas vary with varying δ, i.e., $d\ln(\delta/a)$, where the ζ-orbits were taken from Ref. 6 in which the influence of uniaxial deformations on the dHvA effect was studied, and for the ν orbit we shall calculate them, assuming that the corresponding cross section is approximately circular.

Subtituting in Eq. (1) the experimental and calculated values for $d\ln S/d\ln V$ and $d\ln S_0/d\ln V$, we obtain the volumetric variation of δ, which cannot be regarded small (see Table I) compared to the results of Ref. 6, where a negligible variation of δ due to uniaxial deformations was shown. Using Eq. (2) we calculated the pressure-induced variation of the vector Q. This value is very close to that obtained in a direct neutron-diffraction experiment—0.5×10^{-3} kbar^{-1}.[7] It is also fairly close to the value obtained in Ref. 2 from a "first-principle" calculation of the band structure.

Thus, the large and negative BC of the FS cross sections of AFM chromium are attributable to a large pressure dependence of the wave vector of the SDW. This effect reduces sharply the Néel temperature under pressure.[8]

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