# Influence of pressure on the de Haas–van Alphen effect and exchange splitting in iron

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(Submitted 5 July 1978)
Pis'ma Zh. Eksp. Teor. Fiz. **28**, No. 5, 280–283 (5 September 1978)

The effect of pressure on the oscillation frequencies is measured; the change in the positions of the energy band and the change of the magnetization are calculated.

PACS numbers: 71.25.Hc, 75.30.Et, 75.30.Cr, 75.50.Bb

A number of thorough experimental studies have identified the main parts of the Fermi surface (FS) of ferromagnetic iron.[1,3] The principal method of determining the FS is the de Haas–van Alphen (dHvA) effect. These studies have confirmed the main results of the spectrum calculations made by Wood[4] and Wakoh and Yamashita[5] as refined by Gold and co-workers.[1]

In the band with the lower occupation ("down" spin), the terms $\Delta'_2$, $\Delta_5$, and $\Delta_2$, which intersect somewhat below the Fermi level (Fig. 1) form the "jack" part of the FS, in the six "necks" of which, on the $\Gamma H$ axes of the Brillouin zone, are located the "lenses" (see Fig. 6 of Ref. 1) formed by the terms $\Delta_2$ and $\Delta'_2$ and separated by spin-orbit interaction from the neck. According to the data of Ref. 1, the lens is almost a sphere, with less than 8% deviation from sphericity. The dHvA oscillations for the lens are relatively easy to measure, and its structure has been well investigated. In addition, the very nature of the lens makes its value sensitive to the position of the Fermi level.

Lozanrich and Gold[6] attempted to investigate the temperature dependence of the cross-section area of the lens in the region 1–4 K, for the purpose of relating it to the change in the exchange ferromagnetic splitting $\Delta_0$. However, the relative change in the frequency of the dHvA oscillations between 1 and 4 K turned out to be very small ($\Delta F/F = 10^{-5}$, i.e., within the limits of the measurement error).

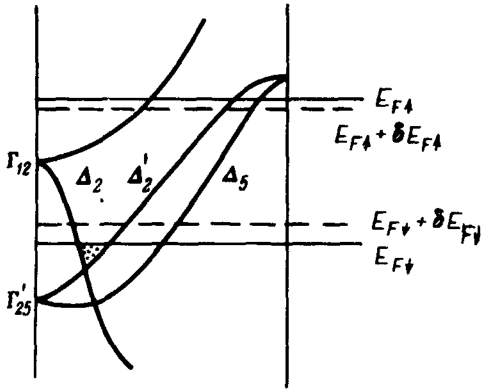

FIG. 1. Part of the band spectrum of iron along the $\Gamma H$ direction. When the ferromagnetic splitting changes, the "lens" cross section area changes.

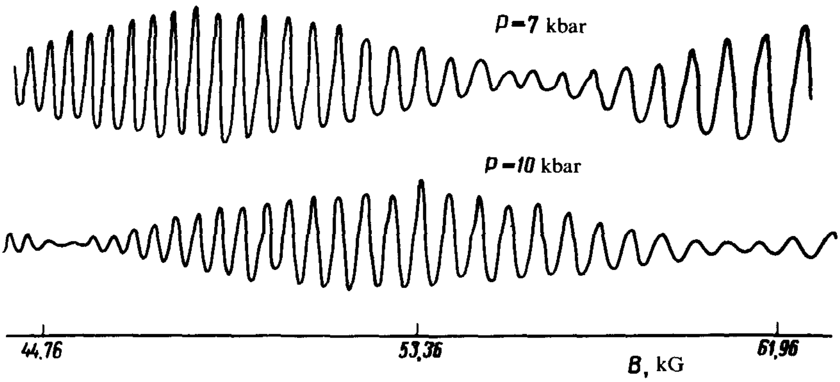

FIG. 2. Form of the oscillation curves at H‖[110]. A shift of the beat node is observed under the influence of the pressure, as well as a decrease of the number of oscillations between the nodes and the antinode with increasing pressure.

We have investigated the influence of pressure up to 11 kbar on the cross section of the lens at a magnetic-field direction along the crystallographic axes [100], [110], [111]. We measured the dHvA oscillation frequencies in the field interval up to 80 kOe for two spherical iron single crystals. The compression was produced with the aid of a fixed-pressure chamber.[7]

At H‖[100] and [110], owing to some nonsphericity of the lens, there are two cross sections of nearly equal areas, which produce beats of the oscillation curves; an example is shown in Fig. 2. The results of the analysis of the experimental data are shown in Fig. 3, which gives also the $F(P)$ dependences for magnetic-field directions along the indicated crystallographic axes. Using least squares, we calculated the values of $d\ln S/dP$; the error is equal to the variance. $d\ln S[100]/dP=(0.85\pm 0.20)\times 10^{-2}$ kbar$^{-1}$, $d\ln S[111]/dP=(0.80\pm 0.05)\times 10^{-2}$, and $d\ln S[110]/dP=(0.90\pm 0.10)\times 10^{-2}$. The reason for the larger error at H‖[100] is the admixture of oscillations from the neck of the jack. Although the results hint at a tendency of the lens to become elongated, we assume that, within the limits of errors, the pressure does not change the degree of its isotropy. The isotropy of the lens and of the angular dependence of $d\ln S/dP$ allows us to assume that the pressure does not alter the effective mass ($m^*_{P=0}=0.71m_0$)[11], i.e., the slope of the dispersion curves making up the lens relative to the $\Gamma H$ axis.

If the exchange splitting in the ferromagnetic state is the same for each point of the Brillouin zone, then a band structure can be represented with two individual Fermi levels—for the electron spin up (↑) and down (↓), and $\Delta_0=E_{F\uparrow}-E_{F\downarrow}$.

The obtained data can be related to the changes of the relative positions of the Fermi levels and of the dispersion curves that make up the lens, and can be compared with the effect of the pressure on the magnetization. The relative change $\sigma\Delta/\Delta_0$ of the exchange splitting with decreasing distance between the atoms can be connected with the change of the FS and, according to Stoner's theory, with the magnetization change $\delta M/M$. Simple calculations (see, e.g.,[6]) yield the connection between the relative change of the lens cross sections (assuming the lens to be isotropic) and the splitting. Then $d\ln\Delta_0/dP=-4.8\times 10^{-2}$ kbar and $d\ln S/dP=-3.8\times 10^{-4}$ kbar$^{-1}$. Kondorskiĭ

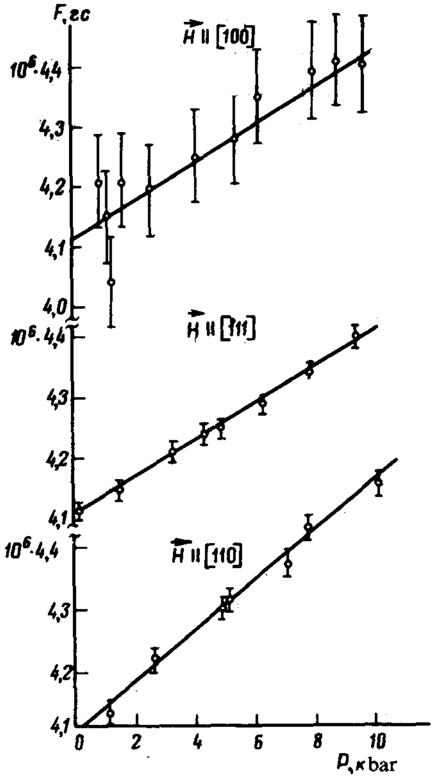

FIG. 3. Plots of $F(P)$ at different orientations of the magnetic field.

and Sedov have measured the atomic magnetic moment of iron under pressure and at $T = 4.2$ K they obtained $d\ln M/dP = K_\sigma = d\ln\Delta/dP = -3.1\times10^{-4}$ kbar$^{-1}$,[8] in satisfactory agreement with our data.

The absolute displacements of the levels $E_{F\downarrow}$ and $E_{F\uparrow}$ can be calculated by assuming that

$$d\ln E_{F\downarrow}/dP = d\ln S/dP \quad (d\ln m^*/dP = 0): \quad \delta E_{F\downarrow} = -\frac{N_\uparrow}{N_\uparrow + N_\downarrow}\delta\Delta, \quad \delta E_{F\uparrow} = \frac{N_\downarrow}{N_\uparrow + N_\downarrow}\delta\Delta,$$

where $\delta\Delta$ is determined from the formula

$$\frac{\delta E}{F} = -\frac{m^*}{e\hbar F}\frac{N_\uparrow}{N_\uparrow + N_\downarrow}\delta\Delta,$$

and $N_\uparrow$ and $N_\downarrow$ are the densities of states in the corresponding spin bands on the Fermi surface. Substituting the required quantities, we obtained (at $P = 1$ kbar): $\delta E_{F\uparrow} = -2.3\times10^{-4}$ eV, $\delta E_{F\downarrow} = 5.3\times10^{-4}$ eV, $\delta\Delta = \delta E_{F\uparrow} - \delta E_{F\downarrow} = -7.6$

$\times 10^{-4}$ eV. In addition, assuming parabolicity of that part of the spectrum which makes up the lens, we can estimate the distance $E'_{\downarrow}$ to the bottom of the band (points of intersection of the dispersion curves): $E'_{\downarrow} = \delta E_{F\downarrow}/(\delta F/F) = 9.5\times 10^{-2}$ eV.

It is interesting to note that whereas the baric coefficients of the magnetization of iron and nickel are close ($-3.1$ and $-2.9\times 10^{-4}$ kbar$^{-1}$, respectively),[8] the same coefficients differ by more than one order of magnitude for the measured sections of the Fermi surface ($\sim 8\times 10^{-3}$ kbar$^{-1}$ for the lens in iron, as against $\sim 1\times 10^{-4}$ for the hole pocket in $X_5$ of nickel).[9,10] This difference is due, to a considerable degree, to the difference between the state densities of the quasiparticles at the Fermi level. For iron $N_{\uparrow} = 5$, $N_{\downarrow} = 1.5$[11] and for nickel $N_{\uparrow} = 2.4$, $N_{\downarrow} = 21.1$[12] (all $N$ are in units of electron/(atom-Rydberg), and the factors $N_{\uparrow}/(N_{\uparrow} + N_{\downarrow})$ are equal to 0.7 and 0.1, respectively.

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