Experimental Evidence for the X2 Hole Pocket in the Fermi Surface of Ni from Magnetic Crystalline Anisotropy

Gersdorf, R.

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in the understanding of adsorption on semiconducting surfaces in general. We plan to discuss our methods and findings at length in a forthcoming publication.

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Experimental Evidence for the $X_{2\downarrow}$ Hole Pocket in the Fermi Surface of Ni from Magnetic Crystalline Anisotropy

R. Gersdorf

Natuurkundig Laboratorium der Universiteit van Amsterdam, Amsterdam, The Netherlands

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The anomalous behavior of the magnetic crystalline anisotropy in Ni metal at 4 K can be interpreted by the passage of the top of the $X_{2\downarrow}$ sub-band through the Fermi energy, when the magnetization direction is changed. The number of holes in the corresponding hole pocket varies between 0 and 1.4×10^{-5} holes/atom. Fair agreement between theory and measurements is obtained.

It is known[1,2] that the magnetic crystalline anisotropy in Ni metal at low temperature cannot be described with only a few anisotropy constants, as is the case with most other magnetic metals and alloys. Aubert *et al.*[2] recently published very accurate measurements of the torque due to this anisotropy as a function of the crystallographic direction of the magnetization, which show significant Fourier components at least up to degree 34.

On analyzing these results we observed a small anomaly in the torque as a function of the magnetization direction if this direction has an angle of about 18° with the nearest cubical axis. This anomaly has been observed earlier by Franse,[1] who tentatively associated it with the movement of the top of a band through the Fermi level. Furthermore, we found that the Fourier components of degree 12 and higher can be interpreted as due to an anomalous contribution, which is zero unless the magnetization direction lies within 18° of the nearest cubical axis. The measured torque can be decomposed into a regular torque, which is described with four conventional anisotropy constants, plus a much smaller anomalous contribution, as shown in Fig. 1.

We suggest that the latter contribution is due to a movement through the Fermi-energy level of the top of the $X_{2\downarrow}$ band. Band calculations position this band near the Fermi level; an old semiempirical calculation by Zornberg[3] places it at the Fermi energy within the attained accuracy of 0.002 Ry (30 meV). In more recent self-consistent calculations, Wang and Callaway[4] find the top of the $X_{2\downarrow}$ band about 0.03 Ry (0.4 eV) above the Fermi level. The partial inclusion of electron correlations reduces[4] this difference to 0.002 Ry; these authors suggest that, with another correction, the top of this band may be pushed down below the Fermi energy.

Because of spin-orbit coupling, all energy bands shift slightly if the magnetization direction is varied; Wang and Callaway[5] computed that the top of the $X_{2\downarrow}$ band at the point in reciprocal

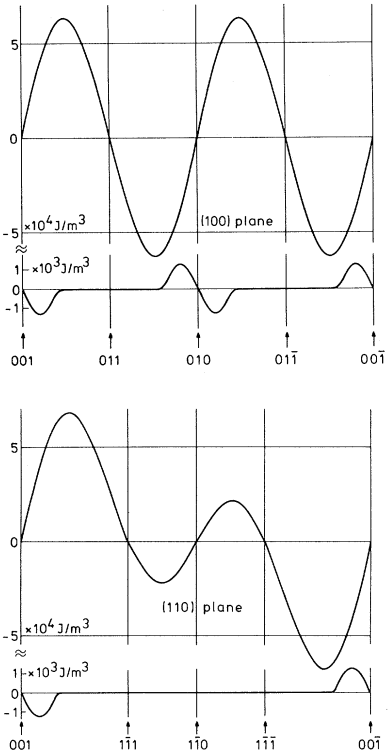

FIG. 1. Magnetic anisotropy torque of Ni at 4 K in two crystallographic planes, decomposed into a regular part, which can be described with four constants, plus a anomalous part. Note that the amplitude of the anomalous torque is only 2% of the amplitude of the regular torque.

space, denoted by $X(0,0,1)$, shifts downward by 0.0017 Ry (23 meV) if the magnetization direction is rotated from the [0,0,1] to the [1,0,0] direction. {It is clear that $X(0,0,1)$ and $X(1,0,0)$ are no longer equivalent if spin-orbit coupling is taken into account and the magnetization lies in the [0,0,1] direction.} A similar shift of the $X_{5\downarrow}$ band has been found by an analysis of de Haas-van Alphen data.[6]

We can interpret the anisotropy measurements now by assuming that the top of the $X_{2\downarrow}$ band at $X(0,0,1)$ lies slightly above the Fermi energy, at a direction of the magnetization along the [0,0,1] axis, but that it shifts down when the magnetization is rotated, and that it lies exactly at the Fermi energy if the magnetization is rotated 18° away from [0,0,1]; see Fig. 2. (Due to cubic symmetry, the energy change should be the same up to second order in the angle if the magnetization rotates away from [0,0,1] in any plane containing this direction.) This causes a

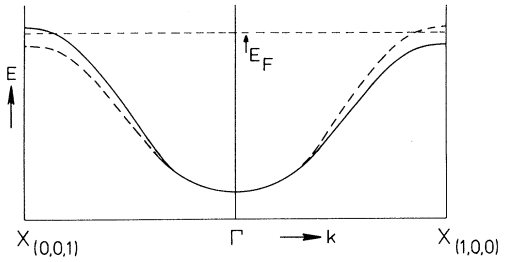

FIG. 2. Schematic representation of the $X_{2\downarrow}$ subband in Ni, as dependent on the direction of the magnetization. Solid line, M along [0,0,1]; dashed line, M along [1,0,0].

negative contribution to the total energy of the crystal, due to redistribution of electrons from the top of the $X_{2\downarrow}$ band to other parts of the Fermi surface, as long as the magnetization direction lies within 18° from a cubical axis. If the top of the band lies an energy ϵ above the Fermi level, the energy amounts to

$$E = \frac{-1}{15\pi^2}\left(\frac{2m^*}{\hbar^2}\right)^{3/2}\epsilon^{5/2}. \tag{1}$$

Denoting the angle between the magnetization direction and the nearest cubical axis by φ, we may assume that for small φ the energy ϵ depends quadratically on φ so that $\epsilon = C(\varphi_0^2 - \varphi^2)$ if φ_0 is the value of φ for which the top of the band lies exactly at the Fermi energy (φ_0 is about 0.3 rad). On substituting this expression in (1) we get for the energy E and the torque $L = -\partial E/\partial\varphi$, as functions of φ,

$$\begin{aligned} &E = -B(\varphi_0^2 - \varphi^2)^{5/2}, \quad L = -5B(\varphi_0^2 - \varphi^2)^{3/2}\varphi, && \text{if } \varphi < \varphi_0; \\ &E = 0 \text{ and } L = 0, && \text{if } \varphi \geq \varphi_0. \end{aligned} \tag{2}$$

B is a constant, equal to $(C^{5/2}/15\pi^2)(2m^*/\hbar^2)^{3/2}$.

If we fit the measured anisotropy torque with a regular function, containing four conventional anisotropy constants, plus an anomalous function we get fair agreement between the experimental data and the fitting function. The agreement was improved somewhat by broadening the above function a little near the anomaly; this is probably related to the difference between a real Ni crystal and an ideal, perfect crystal at 0 K.

We obtained the following values for the four regular anisotropy constants $K_1, \ldots, K_4$, defined in the usual way, and the two anomalous constants B and φ_0, relating to Ni at a temperature

of 4.2 K in a field of 19 179 Oe:

$K_1 = -129\,675 \pm 20$ J/m^3,

$K_2 = 47\,060 \pm 450$ J/m^3,

$K_3 = 13\,240 \pm 80$ J/m^3,

$K_4 = -10\,100 \pm 1200$ J/m^3,

$B = 105\,700 \pm 1000$ J/m^3,

$\varphi_0 = 0.307 \pm 0.002$ rad.

Assuming that this anomalous part is indeed caused by the shift of the top of the $X_{2\downarrow}$ band, we can now calculate some parameters of this band. Taking m^* equal to $197m_0$,[5] we get $C = 5.92 \times 10^{-21}$ J = 37 meV. The maximum height of the top of the $X_{2\downarrow}$ band above the Fermi energy is therefore $\epsilon_m = C\varphi_0^2 = 5.58 \times 10^{-22}$ J = 3.5 meV. Extrapolating the relation $\epsilon = C(\varphi_0^2 - \varphi^2)$ to $\epsilon = \frac{1}{2}C(\cos 2\varphi - \cos 2\varphi_0)$, which has the required symmetry, we find an experimental difference between $X_{2\downarrow}(0,0,1)$ and $X_{2\downarrow}(1,0,0)$ of value $C = 37$ meV. Because of uncertainties in this extraplation and in the numerical band calculations, we think the agreement with the calculated value[5] of 23 meV is satisfactory.

We find therefore that $X_{2\downarrow}(0,0,1)$ lies 3.5 meV above the Fermi energy, and that $X_{2\downarrow}(1,0,0)$ lies about 33.5 meV below the Fermi energy (magnetization is along $[0,0,1]$).

The maximum number of holes in the $X_{2\downarrow}$ pocket is now

$$N_m = (6\pi^2)^{-1}(2m^*\epsilon_m/\hbar^2)^{3/2} = 1.3 \times 10^{24} \text{ holes/m}^3$$
$$= 1.4 \times 10^{-5} \text{ holes/atom.}$$

If we assume this hole pocket is spherical (because of symmetry, it should be an ellipsoid of revolution; band calculations indicate it is nearly spherical), we can estimate the maximum de Haas–van Alphen frequency connected with this hole:

$$F_{\text{dHvA}} = m^*\epsilon_m/\hbar e = 59 \text{ T } (= 590\,000 \text{ G}).$$

This de Haas–van Alphen frequency, which has never been found experimentally, should be observable in a nearly perfect crystal, only if the field is along a $[0,0,1]$ axis.

At temperatures above liquid-helium temperature, ϵ_m becomes comparable to or smaller than kT; it is therefore understandable that the anomalous contribution to the anisotropy is observable at low temperature only.

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