MAGNETIC ANISOTROPY OF NICKEL

E. I. KONDORSKIĬ and E. STRAUBE

Moscow State University

Submitted February 9, 1972

Zh. Eksp. Teor. Fiz. 63, 356–365 (July, 1972)

A theory of magnetic anisotropy of nickel is developed in which its band structure and shape of the Fermi surface are taken into account. It is shown that the theoretical values of the magnetic anisotropy constant at absolute zero temperature are in satisfactory agreement with the experimental value for the helium temperature range. It is shown that the main contribution to the anisotropic part of the energy (AE) is due to the Brillouin band regions which would contain degenerate or quasidegenerate states in the absence of spin-orbit interaction. It is necessary in this case that the Fermi levels be located within one or several, but not all, bands with degenerate or quasidegenerate states. The contributions to the AE from other regions of the Brillouin band are smaller by several orders of magnitude than the main contributions mentioned above.

RECENT experimental and theoretical investigations[1-3] have greatly increased and refined our knowledge of the band structure of ferromagnetic transition metals. The degree of accuracy of the band theory for nickel is such that it is possible at present to calculate quantitatively many physical quantities of this metal, including the magnetic-anisotropy constant. The first attempt to calculate the magnetic-anisotropy constant of nickel within the framework of the band model were made by Brooks[4] and Fletcher[5]. They, however, did not have at that time the necessary data on the band structure, and were forced to use an unrealistic model. In addition, Sloncewskij[6] has shown that serious errors result from the fact that the redistribution of the occupied and free states at the Fermi level as a function of the magnetization direction was neglected in[4,5]. Mori[7], in analogous calculations, took into account the real band structure of nickel, but in the calculation of the anisotropic part of the energy (AE) he disregarded the existence of degenerate states, and even noted that these states make no noticeable contribution to the AE. On the other hand, Furey[8], in an estimate of the contributions made to the AE by different regions of the Brillouin zone, reached the conclusion that contributions comparable with the experimental values can be made only by those regions in which there can be degenerate or quasidegenerate states without the spin-orbit interaction.

In the present paper we present a theory of the magnetic anisotropy of ferromagnetic metals, based on the band model, and show that the main contribution to the anisotropic part of the energy is made by electrons from those regions of the Brillouin zone in which there would be degenerate or quasidegenerate states without the spin-orbit interaction. In the first part of the article we derive formulas for the change of the ferromagnetic-crystal energy following perturbation by the spin-orbit interaction, in the second part we describe a method of calculating this energy for nickel from the known data on its band structure, and in the third part we present the results of numerical calculations of the magnetic-anisotropy constant of nickel at T = 0°K and the results of a comparison of the theoretical value with the experimental data.

1. CHANGE OF FERROMAGNETIC-CRYSTAL ENERGY FOLLOWING PERTURBATION BY SPIN-ORBIT INTERACTION

We consider a ferromagnetic crystal with a rigid crystal lattice at absolute zero temperature. The states of the electrons are determined in the Hartree-Fock approximation by the following Hamiltonian:

$$\hat{H} = \hat{H}_0 + \hat{H}_{so}; \tag{1}$$

$$\hat{H}_0 = \frac{\hat{p}^2}{2m} + V + V_{ex} + \frac{e\hbar}{2mc} g\hat{\sigma}\mathbf{H}, \tag{2}$$

$$H_{so} = \frac{\hbar}{4m^2c^2}\hat{\sigma}[\nabla V(\mathbf{r})\hat{\mathbf{p}}], \tag{3}$$

where V and V_{ex} are the Coulomb and exchange energy operators, $\hat{\sigma}$ are Pauli matrices, and H is the external magnetic field.

We denote the eigenvalues of the operators $\hat{H}$ and $\hat{H}_0$ by $E_n(k, \alpha_i)$ and $E_n^{(0)}(k)$, respectively, where α_i are the direction cosines of the external magnetic field H relative to the basis vectors of the unit cell. Then the change $\Delta E(\alpha_i)$ of the energy of the ferromagnetic crystal following introduction of the spin-orbit interaction is

$$\Delta E(\alpha_i) = \Delta E_V(\alpha_i) + \Delta E_S(\alpha_i), \tag{4}$$

$$\Delta E_V(\alpha_i) = \frac{N}{\Omega}\sum_n \int_{\Omega_n^{(0)}} d^3k\,[E_n(k, \alpha_i) - E_n^{(0)}(k)], \tag{5}$$

$$\Delta E_S(\alpha_i) = \frac{N}{\Omega}\sum_n \int_{\Delta\Omega_n} d^3k\,\mathrm{sign}[E_F(\alpha_i) - E_n(k, \alpha_i)]E_n(k, \alpha_i); \tag{6}$$

Here N is the total number of unit cells in the crystal and Ω is the volume of the Brillouin zone. The summation is over the bands n. The integration regions $\Omega_n^{(0)}$ in expression (5) for $\Delta E_V(\alpha_i)$ (volume contribution) are determined by the inequalities $E_n^{(0)}(k) \leq E_F^{(0)}$, where $E_F^{(0)}$ is the energy corresponding to the Fermi level with the spin-orbit interaction turned off. The term $\Delta E_S(\alpha_i)$ (6) (surface contribution) in expression

(4) takes into account the redistribution of the occupied and free states following application of the spin-orbit interaction. The integration regions $\Delta\Omega_n$ are bounded by the surfaces $E_n(k, \alpha_i) = E_F(\alpha_i)$ and $E_n^{(0)}(k) = E_F^{(0)}$. The Fermi energy $E_F(\alpha_i)$ with allowance for the spin-orbit interaction is determined from the condition that the total number of occupied states be constant:

$$\sum_n \int_{\Delta\Omega_n} d^3k \,\mathrm{sign}[E_F(\alpha_i) - E_n(k, \alpha_i)] = 0. \quad (7)$$

In the derivation of expressions (5) and (6) for $\Delta E_V(\alpha_i)$ and $\Delta E_S(\alpha_i)$ we neglected the change of the operators V and V_{ex} of the Hartree-Fock Hamiltonian (2) following the change in the states of the electrons resulting from the introduction of the spin-orbit interaction. It was shown that the errors due to this neglect are small in comparison with ΔE_V and ΔE_S.

The calculation of $\Delta E_S(\alpha_i)$ (6) is made difficult by the fact that it calls for a determination of the Fermi surface $E_n(k, \alpha_i) = E_F(\alpha_i)$ following the perturbation by the spin-orbit interaction. Sloncewski[6] proposed a method convenient for the calculation of the surface contribution in the case of a weak dependence of $\Delta E_n(k, \alpha_j) = E_0(k, \alpha_i) - E_n^{(0)}(k)$ on the wave vector k. We shall henceforth be interested in the surface contribution from k-space regions in which degeneracy or quasidegeneracy exists near the Fermi level when the spin-orbit interaction is turned off, i.e.,

$$|E_{n,m}^{(0)}(k) - E_F^{(0)}| \leqslant |(\hat{H}_{so})_{mn}|, \quad (8)$$

where $(H_{SO})_{mn}$ is the matrix element of the operator $\hat{H}_{SO}$ between the eigenfunctions of the Hamiltonian $\hat{H}_0$, and in this case $\Delta E_{m,n}(k, \alpha_i)$ depends strongly on k and Sloncewskij's method can not be used.

To reduce the difficulties connected with the determination of the integration region in (6), we transform this expression as follows:

$$\Delta E_S(\alpha_i) = \Delta E_{S1}(\alpha_i) + \Delta E_{S2}(\alpha_i) = \frac{N}{\Omega}\sum_n \left(\int_{\Delta\Omega_n'} d^3k\, F(k) - \int_{\Delta\Omega_n''} d^3k\, F(k) \right), \quad (9)$$

$$F(k) = \mathrm{sign}[E_F^{(0)} - E_n(k, \alpha_i)]\,(E_n(k, \alpha_i) - E_F^{(0)}). \quad (10)$$

The integration regions $\Delta\Omega_n'$ are bounded by the surfaces $E_n^{(0)}(k) = E_F^{(0)}$ and $E_n(k, \alpha_i) = E_F^{(0)}$, which are determined by equations that do not contain the quantities $E_F(\alpha_i)$, and the region $\Delta\Omega_n''$ is bounded by the surfaces $E_n(k, \alpha_i) = E_F^{(0)}$ and $E_n(k, \alpha_i) = E_F(\alpha_i)$ (see Fig. 1). Replacement of $E_n(k, \alpha_i)$ by $E_n(k, \alpha_i) - E_F^{(0)}$ in the integrand of (10) does not change the values of the integral, by virtue of the condition (7). The contribution ΔE_{S2}, which takes into account the change of the Fermi energy, can be estimated approximately

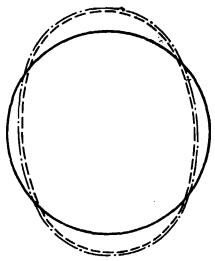

FIG. 1. Position of the Fermi surface before and after perturbation by the spin-orbit interaction: solid line–for $E_n^{(0)}(k) = E_F^{(0)}$, dashed–for $E_n(k, \alpha_i) = E_F(\alpha_i)$, dash-dot–for $E_n(k, \alpha_i) = E_F^{(0)}$.

$$\Delta E_{S2}(\alpha_i) \approx [\Delta Z(\alpha_i)]^2 / 2\nu(E_F^{(0)}), \quad (11)$$

where $\nu(E)$ is the density of states and

$$\Delta Z(\alpha_i) = \frac{N}{\Omega}\sum_n \int_{\Delta\Omega'} d^3k \,\mathrm{sign}[E_n(k, \alpha_i) - E_F^{(0)}]. \quad (12)$$

It was noted above that there are still contrasting views concerning the possibility of explaining the magnetic anisotropy observed in transition metals on the basis of the band theory. We therefore thought it useful, before performing the numerical calculations of the AE of nickel, to consider certain approximate but simple models of the band structure and estimate the orders of magnitude of the AE in these simple cases (see the Appendix). In particular, we studied a simplified band-structure model (model 3), similar to the real band structure of nickel in the region of the pockets near the point X of the Brillouin zone. In this region there are quasidegenerate states. Calculations carried out for the models in the Appendix have shown the following:

1) The contribution to the AE from the region of quasidegenerate states can, under definite conditions, be larger by one or two orders of magnitude than the contribution from the regions where there are no such states.

2) The contribution to the AE from regions in which there are degenerate or quasidegenerate states changes abruptly and can reverse sign when the character of the functions $E_m(k)$ and $E_n(k)$ changes, and depends on the proximity of the indicated regions to the Fermi level.

3) Even if the indicated regions occupy a small (0.05–0.02) part of the volume of the Brillouin cell, their contribution can be of the order of magnitude of the observed value of the AE.

4) The AE has negative values in those cases when one of the interacting bands is not filled (or is completely filled) and in this case the moduli of the electron velocities in the other band on the Fermi surface are sufficiently large. These are precisely the conditions realized in the region of the pockets near the point X of the Brillouin zone of nickel.

2. CALCULATION OF THE UNISOTROPIC PART OF THE ENERGY OF NICKEL

In the nickel band structure not perturbed by the spin-orbit interaction (see[1,2,3]) there are two types of degenerate states near the Fermi level: a) states in the vicinity of the points of tangency of the Fermi surfaces to the fourth (Fermi surface of the pockets around the point X) and fifth subbands with spin downward along the line Δ and the fifth and sixth subbands with spin downward along the line λ. The points of tangency of the Fermi surfaces correspond to doubly-degenerate subbands of symmetry Δ_5 and λ_{32}. b) The states in the vicinity of the line of the section of the surfaces of the sixth (s-like) subband with spin upward and the fifth (d-like) subband with spin downward. Such degenerate states are encountered at arbitrary points of the Brillouin zone (see Fig. 2). These states, as follows from our theory for the approximate model of the band structure, can make sufficiently large contribution to the AE. In the calculations for the real band

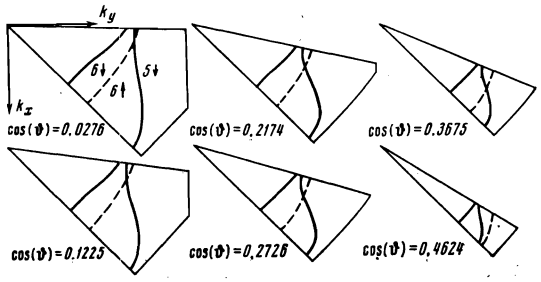

FIG. 2. The intersection of the Fermi surfaces with the cones ϑ = const in 1/48 of the Brillouin zone, with $k_z \leqslant k_x \leqslant k_y$. The polar axis is the k_z axis.

structure of nickel, we did not confine ourselves to calculation of the contributions made to the AE only by the regions indicated above. For comparison, we calculated also the contributions from regions in which there are no degenerate or quasidegenerate states.

To perform the numerical integrations in (5), (9), and (12) it is necessary to have information on the order of magnitude and on the character of the k-dependence of the contributions made to the AE by the degenerate states listed above. Thus, for the case of degeneracy of type (b) we introduced the spherical coordinates k_r, ϑ, and φ with origin at the point Γ and with polar axis along the (001) axis of the Brillouin zone, and wrote down the equation $k_r = k_{FS}(\vartheta, \varphi)$ of the Fermi surface of the s-like subband unperturbed by the spin-orbit interaction, as well as the equations $k_r = k_{FS}$ and $\varphi' = \varphi_0(\vartheta)$ which define the line of intersection of this surface with the Fermi surface of the d-like subband. We introduced the variables $k' = k_r - k_{FS}$ and $\varphi' = \varphi - \varphi_0$, which are small near the indicated intersection line, and expanded in the vicinity of this line the unperturbed values of the energies $\epsilon_{s,d} = E^{(0)}_{s,d} - E^{(0)}_F$ in powers of k' and φ' up to first-order terms. Next, we obtained by the standard method formulas for the values of the energies $\epsilon_\pm$ following perturbation of the energies $\epsilon_{s,d}$ by the spin-orbit interaction. These formulas determined the dependence of $\epsilon_\pm$ on k', φ', and on the matrix element V_{sd} of the operator $\hat{H}_{SO}$ between the states under consideration. Finally, after substituting $\epsilon_{s,d}$ and $\epsilon_\pm$ in (5) and (9) and integrating with respect to k', we obtained expressions for the contributions $\Delta E_V(\alpha_i)$ and $\Delta E_{S1}(\alpha_i)$, which characterize the dependence of these contributions on V_{sd}. It was shown that these expressions take the form

$$\Delta E_V(\alpha_i) = -\Delta E_{sd}(\alpha_i) = \iint d\vartheta\, d\varphi' F(\vartheta, \varphi', |V_{sd}|) \qquad (13)$$

with the same integrand F for ΔE_V and ΔE_{S1}. It follows therefore that in this approximation the volume and the surface contributions are equal in magnitude and opposite in sign for each value of ϑ and φ. The separate volume and surface contributions are approximately 1.5 times larger than the value of $\Delta E(\alpha_i)$ corresponding to the observed anisotropy constant K_1 of nickel. Allowance for higher orders in the expansions of $\epsilon_{s,d}$ and elimination of other approximations used in the derivation of expression (13) did not lead to the appearance of increments lower than fourth order in $|V_{sd}|$. After substituting $\epsilon_{s,d}$ and $\epsilon_\pm$ in (11) and (12) and integrating, we obtained for $\Delta Z(\alpha_i)$ the isotropic and anisotropic contributions proportional to $|V_{sd}|^2$ and $|V_{sd}|^4$, respectively. Then, according to (11), $\Delta E_{S2} \sim |V_{sd}|^6$, just as when perturbation theory is used for nondegenerate initial states. It follows therefore that $\Delta E_{S2}(\alpha_i)$ is always small in comparison with $\Delta E_V(\alpha_i)$ and $\Delta E_{S1}(\alpha_i)$.

Similar results were obtained in case (a), for which we introduced cylindrical coordinates with a polar axis coinciding with the high-symmetry line.

We now proceed to describe the numerical methods of calculating the integrals (5) and (9), developed with allowance for the results obtained by investigating the two-band model. The most important of these results is the conclusion that, in the linear approximation in k' and φ', the absolute values of the volume and surface contributions are separately equal for each point φ and ϑ. Therefore appreciable fractions of these contributions are separately cancelled out for each group of limiting points with coordinates φ and ϑ, making it possible to reduce the number of limiting points and choose them in most rational fashion.

We introduce suitable systems of curvilinear coordinates (μ, ν, ω) which make it possible to describe the equal energy surfaces $E^{(0)}_n(k) = E^{(0)}_F$ and $E_n(k, \alpha_i) = E^{(0)}_F$ in the form $\omega_n = \omega_n(\mu, \nu)$. These coordinate systems are chosen such that $\omega_n = \omega_n(\mu, \nu)$ are single-valued functions that are as smooth as possible. We then have for the integrals of the type (5) and (9)

$$I = \int d^3k\, f(k) = \iint d\mu\, d\nu \sum_n \int_{\omega_n^{(1)}(\mu,\nu)}^{\omega_n^{(2)}(\mu,\nu)} d\omega \left| \frac{\partial(k_x, k_y, k_z)}{\partial(\mu, \nu, \omega)} \right|_j g(\mu, \nu, \omega). \qquad (14)$$

In each subinterval $\omega_n^{(1)}(\mu, \nu) \leq \omega \leq \omega_n^{(2)}(\mu, \nu)$ we integrated numerically using Simpson's rule with five limiting points in the case of the volume contribution, and with three limiting points in the case of the surface contribution. The regions of integration with respect to μ and ν were broken up into subintervals, in each of which numerical integration was performed by the Gauss rule with three limiting points. The Fermi surface of the fifth and sixth subbands with downward spin, with the exception of the neck region near the point L, and of the sixth subband with spin upward, can be represented in the form $k_{Fn} = k_{Fn}(\vartheta, \varphi)$ with the aid of the spherical coordinates k_r, ϑ, and φ with origin at the point Γ. The Fermi surface of the pockets is described accordingly with the aid of spherical coordinates with origin at the point X. The neck of the Fermi surface of the sixth subband is separately described in similar fashion. A more detailed description of the employed numerical methods will be given in a separate article.

The initial energy spectrum of the electrons, unperturbed by the spin-orbit interaction, was chosen to be the band structure calculated by Connolly[2] by the APW method, and used, following him, the band-structure interpolation scheme proposed in[9]. The values of the parameters $E_{x^2-y^2, x^2-y^2}(1, 1, 0)$ and $E_{3z^2-r^2, 3z^2-r^2}(1, 1, 0)$ for the subbands with downward spin were modified somewhat in comparison with those given in Table III of Connolly's paper[2]. This was done to improve the agreement with the experi-

mental data obtained by different authors in investigations of the de Haas-van Alphen effect, and particularly to eliminate the pockets of the third subband with spin downward in the vicinities of the point X.

The allowance for the spin-orbit interaction was modified somewhat in comparison with the work of Hodges et al.[9]. To be able to reduce the order of the secular equation for the eigenvalues $E_n(k, \alpha_i)$ the eigenfunctions of the Hamiltonian $\hat{H}(1)$ were expanded not in the basis functions of the interpolation scheme, but in the eigenfunctions of the operator $H_0(2)$. We took into account not only the matrix elements of the operator H_{so} between d-like functions, but also the matrix elements between plane waves and plane waves and d-like functions. The employed approximation correspond to neglect of the matrix elements between the orthogonalized plane waves (OPW) and OPW and d-like functions, as justified by Mueller et al.[10]. To obtain the spin-orbit coupling we used the value $\zeta_{so} = 7.5 \times 10^{-3}$ Ry, which was determined by Hodges et al.[11]

We characterize the AE by means of the energy difference ΔE_{an} per unit cell between the magnetization directions [111] and [100]:

$$\Delta E_{an} = N^{-1}[\Delta E(111) - \Delta E(100)].$$

With such a choice, the number of non-equivalent parts, equal in volume to $1/48$ of the Brillouin zone, is decreased to seven (cf., e.g.,[12,13]).

3. RESULTS

We have considered first the Brillouin-zone region adjacent to the line of high symmetry Σ and bounded in $1/48$ of the Brillouin zone with $k_Z \leq k_X \leq k_i$ by the surfaces $\cos\vartheta = 0.3675$ and $k_X = 0.22k_Y + 1.3k_Z$. The volume of this region is approximately 40% of the volume of the Brillouin zone, and no degenerate or quasidegenerate states are encountered in it near the Fermi surface. In the secular equation for $E_n(k, \alpha_i)$ we took into account the first six subband for each spin direction. The numerical integration was performed on the basis of 135 limiting points for the volume contribution and 81 points for the surface contributions. The values of the volume and surface contributions turned out to be smaller than the experimental values by more than two orders of magnitude. This result shows convincingly that only the presence of degenerate states near the Fermi level can cause the observed value of the AE of nickel.

In calculating the volume contribution from the regions contained inside the pockets present near the point X of the zone, we chose 90 limiting points, and in the calculation of the surface contribution of these pockets we chose 54 limiting points. We obtained the following values of the contributions:

$$(\Delta E_v)_{an} = -2.075 \cdot 10^{-7} \text{ Ry / un. cell} \quad (15)$$

$$(\Delta E_s)_{an} = 1.398 \cdot 10^{-7} \text{ Ry / un. cell} \quad (16)$$

The large contribution from a relatively small value of the zone is due principally to the interaction of the third and fourth subbands with downward spin, the energy difference between which near the Fermi surface of the pockets is equal in order of magnitude to the spin-orbit coupling constant. In the remaining volume of the Brillouin zone, one encounters the already considered degeneracy of the fifth subband with downward spin and the sixth subband with upward spin, and also small energy differences between the fourth, fifth, and sixth subbands with downward spins. Bearing in mind the strong dependence of the contributions of these regions on k, we chose a sufficiently large number of limiting points, namely 945 and 567 points to calculate the volume and surface contributions respectively. We obtained the following values for the contributions of the indicated regions:

$$(\Delta E_v)_{an} = 6.19 \cdot 10^{-7} \text{ Ry / un. cell} \quad (17)$$

$$(\Delta E_s)_{an} = -6.47 \cdot 10^{-7} \text{ Ry / un. cell} \quad (18)$$

Summing (15)–(18) we obtain for the contribution of the entire Brillouin zone

$$\Delta E_{an} = -0.95 \cdot 10^{-7} \text{ Ry / un. cell} \quad (19)$$

The experimental value of ΔE_{an}, determined by Fronse[14] is -1.99×10^{-7} Ry/unit cell. The agreements between the experimental and theoretical values should be regarded as satisfactory, since the possible errors in the estimate of the spin-orbit coupling constant ζ_{so} are relatively large. Thus, according to Zornberg[1], ζ_{so} can range from 6.4×10^{-3} to 9.5×10^{-3} Ry.

We can draw the following conclusions from our results: The band model makes it possible to explain the observed magnetic anisotropy of nickel at R = 0°K. The decisive contributions to the AE are made by those regions of the Brillouin zone, in which one encounters quasidegenerate states near the Fermi level, and this level lies inside some of the quasidegenerate bands. An example is the quasidegeneracy of the third and fourth band with downward spin near the Fermi surface of the pockets. In this case the band of the fourth subband contains the Fermi level, and the band of the third subband lies below this level and is completely filled.

APPENDIX

We have considered the following 2-band structure models:

1. Two remote bands 1 and 2, when there are no degenerate levels and the band energy difference is

$$|E_2(k) - E_1(k)| \gg |H_{so}|_{12}. \quad (A.1)$$

2. Two bands with degenerate levels lying on a symmetry axis.

3. Two bands with almost spherical Fermi surfaces and with degenerate levels lying on the almost spherical surface $k \approx k_{12}$, such that

$$|E(k_{12}) - E_F^{(0)}| \approx |H_{so}|_{12}, \qquad k_{12} > k_{F1} > k_{F2}, \quad (A.2)$$

where k_{F1} and k_{F2} are the Fermi radii of the first and second bands, not perturbed by spin-orbit interaction. One of the bands, e.g., the second, is weakly filled or is not filled at all, i.e.,

$$\varkappa_2 = k_{F_2}/k_{F_1} \ll 1, \quad (A.3)$$

and in addition the following inequalities hold.

$$[E_F^{(0)} - E_1(0)]^2 \gg |H_{so}|_{12}^2. \quad (A.4)$$

The band energies unperturbed by the spin-orbit inter-

action are conveniently expressed in this model in the following approximate form:

$$\varepsilon_1^{(0)} = -\Delta_1\left[1-\frac{1+a\varkappa^2}{1+a}\varkappa^2\right], \quad \varepsilon_2^{(0)} = -\Delta_2\left[1-\frac{\mu\Delta_1}{(1+a)\Delta_2}\varkappa^2\right], \quad \text{(A.5)}$$

where $\varkappa = k/k_{F_1}$ and $\epsilon(k) = E(k) - E_F^{(0)}$ are the coordinates and Δ_1 and Δ_2 are the absolute values of $\epsilon_1^{(0)}$ and $\epsilon_2^{(0)}$ at the bottom of the band, and $\mu = m_1^*/m_2^*$ is the ratio of the effective masses of the electrons of the first and second bands. The dimensionless parameter a describes the deviation of the $\epsilon_1^{(0)}(\varkappa)$ dependence from quadratic in the region of large $\varkappa$.

In the case of carriers of the hole type, the model 3 can be regarded as a roughly approximate description of the band structure of nickel in the region of the "pockets" around the point X of the Brillouin zone.

4. A model differing from model 3 in that both bands are approximately equally filled. Then the conditions (A.2) and (A.4) are satisfied, and the condition (A.3) is replaced by

$$\varkappa_2 \leqslant 1. \quad \text{(A.6)}$$

5. Two bands, one having spherical and the other cylindrical Fermi surfaces, with a condition analogous to (A.2) satisfied in the region of the degenerate states. In this case the energies $\epsilon_1^{(0)}$ and $\epsilon_2^{(2)}$ were assumed in the form

$$\varepsilon_1^{(0)} = -\Delta_1(1-\varkappa^2), \quad \varepsilon_2^{(0)} = -\Delta_2\left[1-\frac{\mu\Delta_1}{\Delta_2}(\varkappa_x^2+\varkappa_y^2)\right]. \quad \text{(A.7)}$$

Model 1 was considered by Brooks[4] and Fletcher[5] without allowance for the surface contribution. If we take into consideration the surface contribution, the calculation for nickel (cf., e.g.,[8]) leads to a value $\Delta E_{an} \approx -10^{-9}$ Ry/unit cell, which is smaller by two orders of magnitude than the observed quantity. In the case of model 2, as shown by Sloncewskij[6], the sum of the volume and surface contributions is also smaller by one or two orders of magnitude than the value of ΔE_{an} observed for nickel, in spite of the presence of degenerate states. We were the first to consider models 3--5. For these models we calculated $(\Delta E_V)_{an}$ and $(\Delta E_S)_{an}$ using formulas (5) and (9) of the present article and obtained relations between the quantity ΔE_{an}, which characterizes the magnetic anisotropy, and the parameters of the band structure described by the given model, such as $\beta = \zeta_{so}/\Delta_1 r$, a, μ, and others. These calculations and their results will be presented in greater detail in a separate article. For our problem, greatest interest attaches in the results obtained with the aid of model 3.

The table lists the values of ΔE_{an} calculated from formulas (4), (5), and (9) at the parameter values $4\pi k_{F_1}^3/3\Omega = 0.05$, $\beta = \zeta_{so}/\Delta_1 = 0.1$, $\mu = 0.2$ and at different values of the parameters $\varkappa_2$ and a (see formulas (A.3) and (A.5)). The choice of the presented value of β, which is 2.5–3 times smaller than the ratio $\zeta_{so}/(E - E_F)$ at the point X for nickel, was dictated by the need to satisfy the condition (A.4). The calculated values of ΔE_{an} should therefore turn out and did turn out smaller than the value $\Delta E_{an} = -1.99 \times 10^{-9}$ Ry/unit cell observed for nickel. We see from the table that ΔE_{an} depends strongly on the parameters that characterize the dispersion law. Thus, for a

Values of Ae calculated for the band structure corresponding to model 3 from formulas (4), (5), and (9)*

$\varkappa_2$	a	ΔE_{an}, Ry/unit cell		
		$(\Delta E_V)_{an}\cdot 10^7$	$(\Delta E_S)_{an}\cdot 10^7$	$\Delta E_{an}\cdot 10^7$
0	0	−22,3	23,8	1.5
0	1	−29,25	28.5	−0.75
0,31	1	−28,4	28.9	0,5

*The values of the parameters in the calculations are $4\pi k_{F1}^3/3\,\Omega = 0.05$, $\zeta_{so}/\Delta_1 = 0.1$, $\mu = 0.2$.

quadratic dispersion law (a = 0), the anisotropic constant is positive in the model under consideration ($\Delta E_{an} > 0$), but with increasing a, i.e., with increasing angle of inclination of the curve $\epsilon_1^{(0)}(\varkappa)$ near the Fermi level, ΔE_{an} decreases rapidly and reverses sign; the anisotropic constant becomes negative. Thus, one of the conditions necessary to obtain a negative anisotropic constant in the model under consideration is a sufficiently large slope of the $\epsilon_1^{(0)}(\varkappa)$ curve at $\varkappa = 1$, which obviously correspond to sufficiently large absolute values of the electron velocities at the Fermi level. We note that the dispersion curves for nickel in the region of the pockets near the point X, as shown by Zornberg[1], cross the Fermi level precisely at a large angle, which is a consequence of the interaction of the d-like band with the vertex at the point x_5 with the s-like band with vertex at the point X_4'. It is seen furthermore from the table that an increase of $\varkappa_2$ with a fixed value of a leads to a decrease in the absolute value of ΔE_{an} and to a reversal of its sign. The value of $\varkappa_2$ depends on the position of the Fermi level and increases with decreasing electron concentration. Thus, with decreasing electron concentration, when iron or cobalt is added to the nickel, the anisotropy constant should decrease, as confirmed by experiment. It is possible that the reason for the zero values of the anisotropy constant and of the high magnetic permeability of permalloy is connected with a similar change of the band structure in the region of the pockets around the point X.

[1] E. I. Zornberg, Phys. Rev. B1, 244 (1970).
[2] J. W. D. Connolly, ibid. 159, 415 (1967).
[3] S. Wakoh and J. Yamashita, J. Phys. Soc. Japan 19, 1342 (1964).
[4] H. Brooks, Phys. Rev. 58, 909 (1940).
[5] G. C. Fletcher, Proc. Phys. Soc. (London) A67, 505 (1954).
[6] J. C. Sloncewskij, J. Phys. Soc. Japan, 17, Suppl. B-1, 34 (1962).
[7] N. Mori, ibid. 27, 307 (1969).
[8] W. N. Furey, Thesis, Harvard University, Cambridge, 1967.
[9] L. Hodges, H. Ehrenreich, and N. D. Land, Phys. Rev. 152, 505 (1966).

[10] F. M. Mueller, A. J. Freeman, J. O. Dimmock, and A. M. Furdyna, ibid. B1, 4617 (1970).
[11] L. Hodges, D. R. Stone, and A. V. Gold, Phys. Rev. Lett. 9, 655 (1967).
[12] L. M. Falicov and J. Ruvalds, Phys. Rev. 172, 498 (1968).
[13] A. P. Cracknell, J. Phys. C (Solid State Phys.) 2, 1425 (1969).
[14] J. J. M. Fronse, On the Magnetic Anisotropy Energy and Magnetostriction of Ni and Fe, Amsterdam, 1969.

Translated by J. G. Adashko
37