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Abstract

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N. A. POTAPKOV

MAGNETIC ANISOTROPY OF UNIAXIAL FERROMAGNETS

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For the theory of ferromagnetism, it is of interest to obtain the dependence of magnetic anisotropy on the spin-orbital and spin-spin interaction of the electrons of unfilled d-shells. It is more convenient to choose the Hamiltonian of the system in the second-quantization representation, since this simplifies the determination of the eigenvalues of the energy. The expression for the Hamiltonian of a uniaxial ferromagnet was obtained in work ([1]).

$$\mathcal{H} = -\mu \sum H S_f - \frac{1}{2} \sum I(f_1, f_2) S_{f_1} S_{f_2} - \frac{1}{2} \sum \delta I(f_1, f_2) S^z_{f_1} S^z_{f_2} - \sum B(f, m) S^2_f; \quad (1)$$

$$B(f, m) = B \left\{ m - \frac{B}{2} \left[\frac{(2-m)(3+m)}{E_{m+1} - E_m} - \frac{(2+m)(3-m)}{E_{m-1} - E_m} \right] \right\}. \quad (2)$$

Here μ is the Bohr magneton; f is the lattice-site vector; S are spin operators; I is the exchange electrostatic interaction; δI is the magnetic interaction; B is the matrix element of the energy of the spin-orbital interaction; m is the orbital quantum number; E_m is the energy of a d-electron with orbital moment m. A more detailed characterization of the quantities used is given in work ([1]).

The energy levels E_m, which in the isolated atom are degenerate, are split under the action of the crystal field. In the crystal of cobalt, to which our calculations will apply, the energy levels are distributed as follows:

$$E_{\pm 2} < E_{\pm 1} < E_0. \quad (3)$$

It may be assumed that the states with $m = \pm 2$ contain four electrons, and those with $m = \pm 1$, three electrons. Then the magnetic properties will be determined by d-electrons with uncompensated spin, which are in states with $m = 1$ or -1. The distribution of orbital moments over the crystal lattice can be obtained from an estimate of the minimum of the energy of interaction between orbital moments. For cobalt, a layered distribution of orbital moments proves energetically favorable, when the orbital moments in the basal plane are parallel, and for neighboring planes antiparallel. Thus, the crystal lattice of cobalt may be represented in the form of two sublattices g and h, for which $m_g = 1$, $m_h = -1$.

In calculating the free energy we shall restrict ourselves to the region of low temperatures. In this approximation the spin operators may be represented in terms of Bose operators of "creation" and "annihilation"

$$S_f^x = (b_f^+ + b_f)\cos\vartheta + (1 - 2n_f)\sin\vartheta,$$

$$S_f^y = i(b_f^+ - b_f), \tag{4}$$

$$S_f^z = -(b_f^+ + b_f)\sin\vartheta + (1 - 2n_f)\cos\vartheta.$$

Here ϑ is the angle between the symmetry axis of the crystal and the magnetization vector.

The Hamiltonian of the system, to within quadratic terms, takes the form

the following form:

$$\mathcal{H} = E_0 + \sum D_f\left(b_f^+ + b_f\right) + \sum A_f b_f^+ b_f + \sum R(f_1, f_2) b_{f_1}^+ b_{f_2} + \frac{1}{2}\sum S(f_1, f_2)\left(b_{f_1}^+ b_{f_2}^+ + b_{f_1} b_{f_2}\right), \tag{5}$$

where the following notation has been introduced

$$E_0 = -\left[\frac{1}{2}\bar{I} + \frac{1}{2}\delta\bar{I}\cos^2\vartheta + \mu\left(H^z\cos\vartheta + H^x\sin\vartheta\right)\right]N - \sum B(f,m)\cos\vartheta; \tag{6}$$

$$D_f = \mu H^z\sin\vartheta - \mu H^x\cos\vartheta + \delta\bar{I}\sin\vartheta\cos\vartheta + B(f,m)\sin\vartheta \tag{7}$$

$$A_f = 2\left[\bar{I} + \mu\left(H^z\cos\vartheta + H^x\sin\vartheta\right) + \delta\bar{I}\cos^2\vartheta + B(f,m)\cos\vartheta\right]; \tag{8}$$

$$R(f_1, f_2) = -\left[2I(f_1, f_2) + \delta I(f_1, f_2)\sin^2\vartheta\right]; \tag{9}$$

$$S(f_1, f_2) = -\delta I(f_1, f_2)\sin^2\vartheta; \tag{10}$$

$$\bar{I} = \sum I(h), \qquad \delta\bar{I} = \sum \delta I(h). \tag{11}$$

The Hamiltonian of the system (5) can be brought to the form

$$\mathscr{H} = E_0 + \Delta E_0 + \sum E_k \xi_k^+ \xi_k \tag{12}$$

by means of a canonical transformation of the operators. In this case, as is not difficult to verify, the last term of the Hamiltonian gives a contribution of higher order than the other terms. We shall therefore omit it in the subsequent calculations. To reduce the Hamiltonian (5) to diagonal form, we introduce the transformation

$$b_f = \alpha_f + \sum u_{fk} \xi_k, \tag{13}$$

where the α_f are c-numbers, and the operators ξ_k satisfy the commutation relations

$$\xi_k \xi_{k'}^+ - \xi_{k'}^+ \xi_k = \delta_{k,k'}, \tag{14}$$

and the normalization conditions for the coefficients $u_{f,k}$ are

$$\sum u_{f,k} u_{f,k'}^* = \delta_{k,k'}, \qquad \sum u_{f,k} u_{f',k}^* = \delta_{f,f'}. \tag{15}$$

To determine the eigenvalues of the energy E_k and the correction to the ground-state energy ΔE_0, we obtain the equations

$$E_k u_{f,k} = A_f u_{f,k} + \sum R(f,f') u_{f',k}; \tag{16}$$

$$\Delta E_0 = \sum A_f \alpha_f^* \alpha_f + \sum R(f_1,f_2) \alpha_{f_1}^* \alpha_{f_2}; \tag{17}$$

$$D_f + A_f \alpha_f + \sum R(f,f') \alpha_{f'}^* = 0. \tag{18}$$

In solving the equations we use the representation of the crystal lattice in the form of two sublattices g and h. The quantities $B(f,m)$ for the different sublattices will be related by

$$B(g,1) = -B(h,-1). \tag{19}$$

After splitting into sublattices, using (19), the equations (16)–(18) can be reduced to a system of equations whose coefficients depend only on the difference of the coordinates of the lattice sites. From the solution of this system we obtain expressions for ΔE_0 and E_k, which, in the nearest-neighbor approximation, we write as

$$\Delta E_0 = -\frac{NB^2 \sin^2 \vartheta}{4I}, \tag{20}$$

$$E_{1,2}(q) = 2\mu\left(H^z \cos\vartheta + H^x \sin\vartheta\right) + 2\bar{I} + 2\delta\bar{I}\cos^2\vartheta \mp \left[2I(q) + \delta I(q)\sin^2\vartheta\right] \mp \frac{B^2\cos^2\vartheta}{I(q)}; \tag{21}$$

here

$$I(q) = \frac{1}{N}\sum_h I(gh)e^{i(g-h,q)}, \qquad \delta I(q) = \frac{1}{N}\sum_h \delta I(gh)e^{i(g-h,q)}. \tag{22}$$

For the free energy of the system we obtain the expression

$$F = E_0 + \Delta E_0 + kT\sum \ln\left(1 - e^{-E_{1,q}/kT}\right) + kT\sum \ln\left(1 - e^{-E_{2,q}/kT}\right). \tag{23}$$

Let us note that the second sum in (23) depends exponentially on the temperature $[\exp(-\bar{I}/kT)]$ and, in the temperature range under consideration, gives a substantially smaller contribution than the first sum. The first sum in (23) can be represented in the form

$$kT\sum \ln\left(1 - e^{-E_{1,q}/kT}\right) = -kT\sum_{n=1}^{\infty} n^{-5/2}e^{-nL'/kT}\beta'^{\,3/2}, \tag{24}$$

where

$$L' = 2\mu\left(H^z\cos\vartheta + H^x\sin\vartheta\right) + \delta I\left(2\cos^2\vartheta - \sin^2\vartheta\right) - \frac{B^2\cos^2\vartheta}{\bar{I}}; \tag{25}$$

$$\beta' = \frac{3kT}{2\pi I'\nu}, \qquad \nu = \frac{v^{2/3}}{\delta^2}, \qquad I' = 2\bar{I} + \delta\bar{I}\sin^2\vartheta, \qquad v = \frac{V}{N}; \tag{26}$$

δ is the distance between nearest neighbors.

The free energy of the system can be represented in the form

$$F = F_0 + F_A, \tag{27}$$

where F_0 is the isotropic part and F_A the anisotropic part of the free energy. To this end we expand F in powers of $\sin^2\vartheta$. Restricting ourselves to the first term of the expansion, we obtain for F_A the expression

$$F_A = K_1 \sin^2\vartheta; \tag{28}$$

K_1, the first anisotropy constant, has the form

$$K_1 = \frac{1}{2}\delta\bar{I}\left(1 - 6Z_{3/2}(L)\beta^{3/2}\right) - \frac{B^2}{4\bar{I}}\left[1 - 4Z_{3/2}(L)\beta^{3/2}\right], \tag{29}$$

where

$$\beta = \frac{3kT}{4\bar{I}\pi v}, \qquad Z_j(L) = \sum_{n=1}^{\infty} n^{-j} e^{-nL/kT}; \tag{30}$$

$$L = 2\mu H^z + 2\delta\bar{I} - \frac{B^2}{\bar{I}}. \tag{31}$$

The equilibrium direction of the magnetization vector (the angle ϑ_0) is determined from the condition of minimum free energy, and at low temperatures from the minimum of E_0. Let us give some of the cases considered:

I. $H^x = 0, \quad H^z = H$:

a) $\delta\bar{I} + \mu H > \dfrac{B^2}{2\bar{I}}, \quad \sin\vartheta_0 = 0;$

b) $\delta\bar{I} + \mu H < \dfrac{B^2}{2\bar{I}}, \quad \cos\vartheta_0 = \dfrac{\mu H}{B^2/2\bar{I} - \delta\bar{I}}.$

II. $H^x = H, \quad H^z = 0$:

a) $\mu H + \dfrac{B^2}{2\bar{I}} > \delta\bar{I}, \quad \cos\vartheta_0 = 0;$

b) $\mu H + \dfrac{B^2}{2\bar{I}} < \delta\bar{I}, \quad \sin\vartheta_0 = \dfrac{\mu H}{\delta\bar{I} - B^2/2\bar{I}}.$

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Note: Figure translations are in progress. See original paper for figures.