# Surface Magnetism

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The temperature below which a body possesses a surface magnetic moment is calculated in terms of the surface anisotropy constants. Necessary conditions for the existence of surface magnetism are found. Allowance is made for the dependence of the magnetic moment on direction near the surface when the anisotropy axes on the surface and within the body do not coincide.

OMEL'YANCHUK and the present author[1] have predicted the possible existence of surface magnetism; we have shown that in the case when a body has negative surface magnetic energy, it should have a macroscopic magnetic moment that decreases exponentially in the interior of the sample. The temperature at which the surface magnetic moment appears is somewhat higher than the Curie temperature of the ferromagnet. In the present paper, the possible appearance of a surface magnetic moment is analyzed with allowance for the volume and surface anisotropy of the magnet.

The volume part of the magnetic free energy $F_V$ includes the exchange energy and the anisotropy energy

$$F_V = \int_0^\infty \left\{ AM^2 + BM^4 + C\left(\frac{d\mathbf{M}}{dz}\right)^2 + \beta M_y^2 \right\} dz. \tag{1}$$

The notation is standard; for concreteness we shall assume that $\beta > 0$ ($\beta \sim 1$);

$$A = \alpha(T - T_c) / T_c, \qquad \alpha > 0 \tag{2}$$

($T_c$ is the Curie temperature; B, C > 0). It is convenient to use for estimates the relation

$$C = \alpha_1 a^2, \quad \alpha, \alpha_1 \approx T_c / \mu M_0 \gg 1, \tag{3}$$

where a is the interatomic distance, $\mu$ is the Bohr magneton, and $M_0$ is the saturation magnetic moment at $T \ll T_c$. The surface energy $F_S$ will not be specified precisely for the time being. We assume merely that

$$F_s = M_s^2 f_s(\theta_s), \tag{4}$$

where $M_S$ is the magnetic moment on the boundary and $f_S$ is a function of the angle $\theta_S$ between $M_S$ and the x axis, which is directed along the magnetic moment into the interior of the sample; the magnetic moment at any section (at any value of z) is parallel to the plane of the surface. In order of magnitude, the function $f_S(\theta_S)$ is equal to

$$f_s = \tilde{\beta}(\theta_s) a. \tag{5}$$

As a rule, the surface anisotropy exceeds the volume anisotropy. This means that $|\tilde{\beta}|$ is larger and possibly even much larger than $\beta$.

We can show that under certain conditions, at temperatures close to $T_c$, the magnetic moment M = M(z) differs from zero and attenuates exponentially as $z \to \infty$. Minimizing the free energy

$$F = F_V + F_s \tag{6}$$

with respect to the magnitude and direction of the magnetic moment M with components $M_x = M\cos\theta$, $M_y = M\sin\theta$, and $M_z = 0$, we obtain a system of equations and boundary conditions

$$\left[A + C\left(\frac{d\theta}{dz}\right)^2 + \beta\sin^2\theta\right]M + 2BM^3 - C\frac{d^2M}{dz^2} = 0, \tag{7}$$

$$\beta M^2 \sin\theta\cos\theta - C\frac{d}{dz}\left(M^2\frac{d\theta}{dz}\right) = 0; \tag{8}$$

$$C\left(\frac{dM}{dz}\right)_s - M_s f_s(\theta_s) = 0, \tag{9}$$

$$C\left(\frac{d\theta}{dz}\right)_s - \frac{\partial f_s(\theta_s)}{\partial\theta_s} = 0. \tag{10}$$

We assume that the value of the magnetic moment changes over a distance $d_M$ greatly exceeding the distance $d_\theta$ over which the direction of the magnetic moment changes:

$$d_M \gg d_\theta. \tag{11}$$

We shall subsequently refine the assumption (11), but it must be borne in mind that it is not necessary for the existence of a surface solution, and serves to simplify the calculation. Owing to the condition (11) we can assume in (8) that $M^2 \equiv$ const. By the same token, the problem of determining the direction of the magnetic moment is solved independently of the calculation of M(z). From (8) at $M \equiv$ const we have

$$\left(\frac{d\theta}{dz}\right)^2 - \frac{\beta}{C}\sin^2\theta = 0,$$

Since in the interior (at $z \to \infty$) we have $\theta = 0$ and $d\theta/dz = 0$. It is easy to verify that when taking the square root it is necessary to use the minus sign:

$$d\theta / dz = -(\beta / C)^{1/2} \sin\theta \tag{12}$$

(the plus sign corresponds to the assumption that $\theta(z = \infty) = \pm\pi$; all the conclusions remain valid in this case).

From (12) and (10) we obtain an equation for the determination of $\theta_S$:

$$\sin\theta_s + \partial f_s / \partial\theta_s = 0. \tag{13}$$

Knowing $f_S(\theta_S)$ we determine $\theta_S$ and obtain from (12) the relation $\theta = \theta(z)$:

$$\operatorname{tg}\frac{\theta}{2} = \operatorname{tg}\frac{\theta_s}{2}\exp\left\{-\left(\frac{\beta}{C}\right)^{1/2} z\right\}, \tag{14}$$

from which we see that

$$d_\theta = (C / \beta)^{1/2} \approx (T_c / \mu M_0 \beta)^{1/2} a. \tag{15}$$

Equations (12) and (13) can be obtained by minimizing the functional

$$f_a=\int_0^\infty\left[C\left(\frac{d\theta}{dz}\right)^2+\beta\sin^2\theta\right]dz+f_s(\theta_s). \qquad (16)$$

Using (12), we obtain the value of $f_a$:

$$f_a=2(\beta C)^{1/2}(1-\cos\theta_s)+f_s(\theta_s)\equiv 2(\beta C)^{1/2}\varphi_a. \qquad (17)$$

We note the following: (a) $M^2 f_a$ is the anisotropy energy at $M^2\equiv$ const; (b) Eq. (13) is obtained by equating $\partial f_a/\partial\theta_S$ to zero; (c) in order for the anisotropy energy to be minimal, it is necessary to have

$$\frac{\partial^2 f_a}{\partial\theta_s^2}\equiv 2(\beta C)^{1/2}\cos\theta_s+\frac{\partial^2 f_s}{\partial\theta_s^2}>0. \qquad (18)$$

Postponing the calculation of $\theta_S$ and $f_a$, let us consider Eq. (7) with the boundary condition (9). Since $\theta=\theta(z)$ tends to zero very rapidly (over a distance $d_\theta=(C/\beta)^{1/2}$, see (15)), we can leave out the second and third terms in the square brackets for all z with the exception of $z\lesssim d_\theta$. If we integrate (7) over the interval $(0, z_0)$, $d_\theta\ll z_0\ll d_M$, assuming that $M\equiv$ const,

$$(AM+2BM^3)z_0+M\int_0^{z_0}\left[C\left(\frac{d\theta}{dz}\right)^2+\beta\sin^2\theta\right]dz$$

$$-C\left[\left(\frac{dM}{dz}\right)_{z=z_0}-\left(\frac{dM}{dz}\right)_{z=0}\right]=0$$

set the limit of the integral at $z_0=\infty$, and substitute $(dM/dz)_0$ from the boundary condition (7), then by letting $z_0\to 0$ (using the inequality $z_0\ll d_M$) we obtain the effective boundary condition

$$C(dM/dz)_S=f_aM_S \qquad (9')$$

for the simplified equation

$$[AM+2BM^3]M-C\frac{d^2M}{dz^2}=0. \qquad (7')$$

To calculate the temperature $T_S$ at which we obtain a nonzero solution of Eq. (7′) with boundary condition (9′), but one that attenuates in the interior of the sample, it is necessary, discarding the nonlinear term $2BM^3$, to analyze the solution of the linear equation

$$\frac{d^2M}{dz^2}-\frac{A}{C}M=0. \qquad (19)$$

It is clear that a damped solution can exist only at $A>0$, i.e., at $T>T_c$, when

$$M=M_S\exp\{-(A/C)^{1/2}z\}, \qquad (20)$$

and from the boundary condition (9′) we determine, taking (2) and (17) into account, the temperature $T_S$ at which the surface moment appears

$$\tau_S^{1/2}=-2\left(\frac{\beta}{\alpha}\right)^{1/2}\varphi_a(\theta_S),\quad \tau_S=\frac{T_S-T_c}{T_c}, \qquad (21)$$

or

$$\tau_S=\frac{4\beta}{\alpha}\varphi_a^2(\theta_S). \qquad (22)$$

It is seen from (21) that the necessary and sufficient condition for the existence of surface magnetism is

$$\varphi_a(\theta_S)<0. \qquad (23)$$

In other words, the surface should lower the anisotropy energy of the body, and only then can a surface magnetic state exist. We now define more precisely the condition (11). According to (20), (21), (15), and (17), it can be written in the form

$$|\varphi_a|\ll 1. \qquad (24)$$

We recall that the condition (24) is necessary only to justify the applicability of the calculation method.

Let us formulate the result: the temperature $T_S$ at which a surface magnetic moment appears is determined by formula (22), where $\varphi_a(\theta_S)$ is specified by (17) ($\varphi_a<0$); $\theta_S$ is determined from (13) under the condition (18).

We can now define the dependence of the surface energy on the angle $\theta_S$.

Let

$$F_S=\beta_{ik}M_i^SM_k^S,\quad i,k=x,y. \qquad (25)$$

The symmetrical matrix $\beta_{ik}=a\tilde\beta_{ik}$ (the direction of its principal axes relative to the crystallographic axes of the crystal and the values of the diagonal elements $\beta_1$ and $\beta_2$) determine completely the surface properties of the magnetic material. If we denote by $\psi$ the angle between the first axis of the matrix $\beta_{ik}$ and the x axis, then the surface energy is written in the form

$$F_S=M_S^2[\beta_1\cos^2(\theta_S+\psi)+\beta_2\sin^2(\theta_S+\psi)]. \qquad (26)$$

We then obtain from (4) and (17)

$$\varphi_a=q_1\cos^2(\theta_S+\psi)+q_2\sin^2(\theta_S+\psi)+1-\cos\theta_S, \qquad (27)$$

where

$$q_j=\beta_j/2(\beta C)^{1/2}=\tilde\beta_j/2(\beta\alpha_1)^{1/2}\quad (j=1,2) \qquad (28)$$

are dimensionless quantities that determine, together with the angle $\psi$, the properties of the surface.

We note that in accordance with (5) and (3) the quantities $|q_j|$ are, as a rule, small, since the denominator contains the exchange constant $\alpha_1$. It is possible, however, that in some exceptional cases $|q_j|$ reaches the value $\sim 1$. We shall first assume that $|q_j|\ll 1$ and solve approximately Eq. (13), which in this case takes the form

$$\sin\theta_S=(q_1-q_2)\sin 2(\theta_S+\psi). \qquad (29)$$

In the approximation linear in $q_j$ we have

$$\theta_S\approx(q_1-q_2)\sin 2\psi,\quad \varphi_a\approx q_1\cos^2\psi+q_2\sin^2\psi. \qquad (30)$$

Finally,

$$\tau_S\approx(\tilde\beta_1\cos^2\psi+\tilde\beta_2\sin^2\psi)^2/\alpha\alpha_1. \qquad (31)$$

We recall once more the condition (23):

$$\tilde\beta_1\cos^2\psi+\tilde\beta_2\sin^2\psi<0.$$

In conclusion, let us consider the special case which admits of an exact solution (without assuming that $|q_j|$ is small). Let $\psi=\pi/2$, $\tilde\beta_2=0$, and $\tilde\beta_1<0$ (on the surface, the magnetic moment has an energywise favored direction along the y axis; we recall that the x axis coincides with the direction of the magnetic moment in the interior of the magnet). In this case

$$\begin{aligned}\varphi_a&=1-\cos\theta_S-|q_1|\sin^2\theta_S,\\ \frac{\partial\varphi_a}{\partial\theta_S}&\equiv\sin\theta_S-2|q_1|\sin\theta_S\cos\theta_S=0,\\ \frac{\partial^2\varphi_a}{\partial\theta_S^2}&\equiv\cos\theta_S-2|q_1|\cos 2\theta_S>0.\end{aligned} \qquad (32)$$

Consequently the stable solution ($\partial^2\varphi_a/\partial\theta_S^2>0$) is

$$\sin\theta_s = 0 \ \text{for} \ |q_1| \leqslant 1/2, \qquad (33)$$
$$\cos\theta_s = 1/2|q_1| \ \text{for} \ |q_1| \geqslant 1/2;$$

$$\varphi_a = \begin{cases} 0 \ \text{for} \ |q_1| \leqslant 1/2, \\ |q_1|^{-1}(|q_1| - 1/2)^2 \ \text{for} \ |q_1| \geqslant 1/2. \end{cases} \qquad (34)$$

Hence

$$\tau_s \approx 4\frac{[|\bar{\beta}_1| - (\beta\alpha_1)^{1/2}]^2}{\alpha\alpha}, \ |\bar{\beta}_1| \geqslant (\beta\alpha_1)^{1/2}, \ \bar{\beta}_1 < 0. \qquad (35)$$

In the derivations of the formulas we did not take into account the dependence of the anisotropy constants on the temperature. It is easy to show that in those cases when the surface-anisotropy constants are small in comparison with the exchange constant $\alpha$, allowance for the temperature dependence of $\beta_i$ produces practically no change in the results, since the temperature $T_S$ is close to the Curie temperature $T_c$ (no surface magnetic state is produced at the temperature at which the surface anisotropy reverses sign).

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[1]M. I. Kaganov and A. M. Omel'yanchuk, Zh. Eksp. Teor. Fiz. **61**, 1679 (1971) [Sov. Phys. JETP **34**, 895 (1972)].

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