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Surface magnetism of non-ideal iron borate single crystal

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Considered is the influence of crystalline structure imperfections in near-surface layer of easy-plane weak ferromagnet iron borate, $FeBO_3$, on the effects of surface magnetism observed therein. It is shown that the surface reconstruction and point defects therein change the surface magnetic properties of the crystal very considerably.

Рассмотрено влияние несовершенств кристаллической структуры приповерхностного слоя легкоплоскостного слабого ферромагнетика бората железа, $FeBO_3$, на эффекты наблюдаемого в нем поверхностного магнетизма. Показано, что реконструкция поверхности и наличие в ней точечных дефектов весьма значительно изменяют поверхностные магнитные свойства этого кристалла.

A change in surrounding symmetry of magnetic ions Fe^{3+} at the surface of easy-plane weakly ferromagnetic $FeBO_3$ crystal as compared to the volume results in an excess anisotropic magnetic energy of near-surface layers [1]. The magnetic moments of ions in the near-surface area, remaining in the basal plane, appear "fixed" in certain directions. An external magnetic field applied in the basal plane results in formation of near-surface transitional magnetic layer of domain wall type, where the magnetic moments of ions smoothly rotate from their orientation in the volume (orthogonal to the magnetic field) to the orientation at the surface [2]. Unlike usual ferromagnets, the surface magnetism in iron borate is well observable due to specific features of the crystal magnetic structure. The purpose of this work is to calculate the critical field value H_s providing the magnetization of the transition layer to the saturation in the case when the surface is reconstructed or contains point defects as vacancies of magnetic ions Fe^{3+}. Thus, we will consider the magneto-dipole contribution to the surface anisotropy energy.

A surface is a structural defect, therefore, not only magnetic but also elastic interactions must change in the near-surface area. The latter circumstance results in distortion of crystal structure in the near-surface area, i.e., partial reconstruction of surface. Since the surface anisotropy energy and especially critical field, by definition, depend heavily on the parameter of crystal lattice [1], the surface reconstruction must influence considerably these quantities. A reconstruction is connected usually with decreasing distances between near-surface atoms. To take the surface reconstruction into account in the theory of surface magnetism, let us proceed from the following simple model. The lattice parameters in a thin layer formed by a few near-surface monolayer of magnetic ions differ from parameters in the volume. These differences are equivalent to strains which would be caused by some external pressure. For simplicity, we will consider strains caused by a hypothetical hydrostatic pressure. Perhaps such a model does not answer reality completely, but it allows estimating the degree of strain influence on values of surface magnetizing fields.

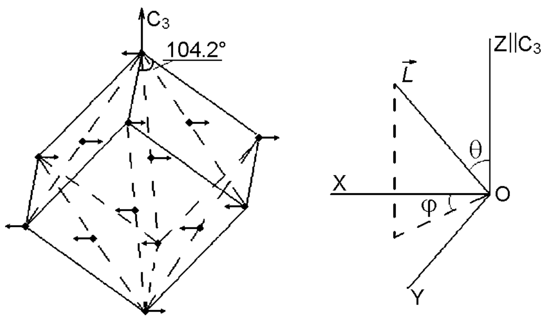

Fig. 1. Elementary rhombohedron of $FeBO_3$ crystal with (10$\bar{1}$4) type faces: in absence of external pressure, there is edge length a_r = 5.9Å; plane angle at a vertex α = 104.2°.

Since hydrostatic pressure does not change the crystal lattice symmetry, the same approach as for an ideal crystal can be applied to calculate the surface anisotropy energy under pressure [1]. Due to exchange coupling with magnetic moments in the volume, the magnetic moments of near-surface ions Fe^{3+} in an easy-plane antiferromagnetic crystal practically are essentially in the basal plane. In this case, the surface density of the surface anisotropy energy has the form

$$\sigma = a_s \sin^2\varphi + b_s \sin\varphi\cos\varphi, \qquad (1)$$

where a_s and b_s are the surface anisotropy constants; φ, azimuthal angle of antiferromagnetic vector, determined in the basal plane (Fig. 1).

Let us consider the reconstruction influence on the surface magnetism of iron borate for (10$\bar{1}$4) face on which surface anisotropy is considerable [1]. To calculate the energy density (1), the $FeBO_3$ rhombohedron with faces of (10$\bar{1}$4) type was used with the edge length of $20 \cdot a_r$, similar to that presented in Fig. 1. The Figure presents the used coordinate system as well. Here and further, the z axis coincides with the 3-fold symmetry axis of the crystal, x and y axes are in the basal plane, the x one being directed along 2-fold axis and y is in symmetry plane. The surface anisotropy energy for this face must be invariant with respect to reflection in the symmetry plane yz. This means that $b_s = 0$ in (1). The surface anisotropy characteristic to be measured is the critical magnetizing field of the transition layer in difficult direction H_s, which for face (10$\bar{1}$4) has the form [1]

$$H_s = 4a_s^2/AM. \qquad (2)$$

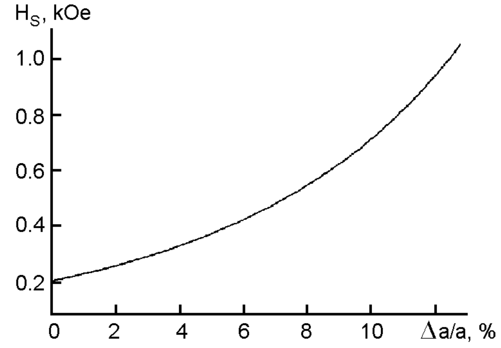

Fig. 2. Dependence of saturation field on the relative decrease of of elementary (10$\bar{1}$4) rhombohedron edge length.

Here A is the exchange parameter for transition layer; M, the spontaneous magnetization of the crystal. The variables characterizing a surface anisotropy and being determined in the magneto-dipole approximation, are found to be in a strong dependence on the edge length of the elementary rhombohedron a_r (Fig. 1): $a_s \sim a_r^{-5}$; $H_s \sim a_r^{-10}$. When calculating these characteristics, the change of the elementary rhombohedron parameters of (a_r and α) was determined using the strain values caused by hypothetical hydrostatic pressure:

$$u_{ij} = -S_{ijkl}\delta_{kl} \cdot p_h, \qquad (3)$$

where $i,j,k,l = x,y,z$ (see Fig. 1); u_{ij} are components of strain tensor; S_{ijkl}, components of compliance tensor; δ_{kl}, δ-function; p_h, the hydrostatic pressure. Taking into account the symmetry, we get from here the expressions connecting the diagonal components of the strain tensor:

$$u_{xx} = u_{yy},\ u_{zz} = \qquad (4)$$
$$= [(2S_{13} + S_{33})/(S_{11} + S_{12} + S_{13})]u_{xx}.$$

Here S is compliance presented in a matrix form and determined using elastic constants [3].

Using the correlations (4), dependence of the saturation field H_s on the relative length decrease of elementary rhombohedron edge $\Delta a_r/a_r$ was calculated at room temperature. The corresponding curve is presented in Fig. 2. It is seen that the experimental value of the saturation field $H_s \approx 1$ kOe at this temperature can be due to straining of near-surface layer by about 12 %. We have calculated also the magnetization curves for near-surface layer [2] at

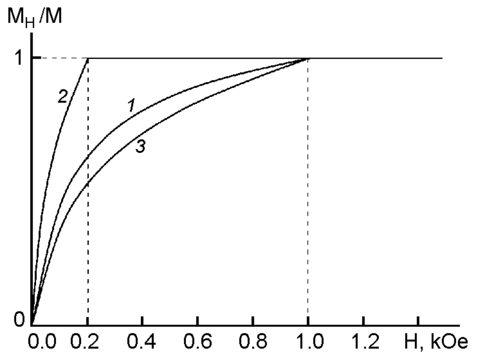

Fig. 3. Magnetization curves for surface: experimental (*1*) [1]; calculated for a crystal with the unstrained surface (*2*); calculated taking into account the surface reconstruction (*3*).

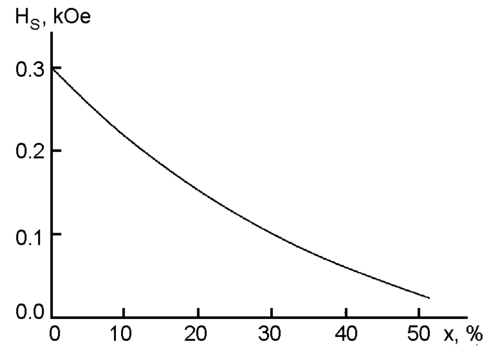

Fig. 4. Calculated dependence of saturation field on the concentration of defects.

T = 300 K for an ideal crystal and crystal with the reconstructed surface with the saturation field coincident with the experimental H_s value. These curves are presented in Fig. 3. The experimental magnetization curve is here presented as well [1].

It is well known that a near-surface area of a crystal may be more defective than its volume [4]. We have studied the influence of the near-surface layer defect structure on surface magnetism. As defects, the vacancies of magnetic ions were considered. Fig. 4 shows the calculated dependence of the magneto-dipole saturation field H_s on the concentration of vacancies at $T = 0$ K. Vacancies are assumed to be randomly distributed in the near-surface area of the crystal. As expected, the increase of vacancy concentration causes a decrease of the saturation field H_s.

Thus, the calculation has shown a strong dependence of magneto-dipole contribution to the surface anisotropy energy and critical field on the lattice strain degree and concentration of magnetic ion vacancies in the near-surface area of iron borate single crystal. The results of calculation will not change, if the admixture of diamagnetic ions in the near-surface area of grate Fe^{3+} will be considered instead of vacancies. Thus, the purposeful formation of the mentioned defects enables to control the surface anisotropy to some extent.

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Поверхневий магнетизм неідеального монокристала борату заліза

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Розглянуто вплив недосконалості кристалічної структури приповерхневого шару легкоплощинного слабкого феромагнетика борату заліза $FeBO_3$ на ефекти поверхневого магнетизму, що спостерігається у ньому. Показано, що реконструкція поверхні і наявність в ній точкових дефектів значно змінюють поверхневі магнітні властивості цього кристала.