



Surface magnetism of real iron borate monocrystals

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ABSTRACT

A theory of the surface magnetism of iron borate, FeBO₃, allowing for the non-ideality of the crystal structure of the near-surface layer is constructed. Since the magnetizing field of a near-surface layer appears to be inversely proportional to the tenth power of the crystal lattice parameter, the influence of the non-ideality on the surface magnetism should be substantial. The suggested models of reconstruction make it possible to describe experiments if the magnitude of the deformations is in agreement with literature data. The theoretical dependence of the value of the surface anisotropy on the concentration of point defects in a near-surface layer of the crystal is also established.

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1. Introduction

The magnetic properties in the thin near-surface layer of magnets can differ from those of the bulk. This is due to magnet's surface, being the natural defect of a structure. The magnetic effects, caused by the surface, are called surface magnetism. The influence of surface ordinarily extends on a near-surface layer, the thickness of which, determined by many factors, is varied from several atomic layers to hundred thousands of atomic layers. A symmetry change in the surroundings of magnetic ions at the surface of a crystal results in their surplus magnetic energy as compared to the ions in the bulk. Neel was the first to specify the special surface magnetic anisotropy in ferromagnets caused by such symmetry breaking [1]. However the appearance of this comparatively weak anisotropy is usually suppressed by demagnetization fields and considerable crystallographic anisotropy. By Neel's estimates, a surface anisotropy may appear only in very small ferromagnetic particles ~ 100 Å. For this reason, the special surface magnetic properties are especially influential for ultrathin films.

Iron borate, FeBO₃, belongs to a class of magnetic materials in which a surface anisotropy appears not only in films but even in the near-surface area of massive monocrystals. These are antiferromagnets with weak ferromagnetism and magnetic anisotropy of an easy-plane type. A surface anisotropy in such crystals will not be suppressed because of the smallness of the demagnetization fields, proportional to weak magnetization, and

practical absence of crystallographic anisotropy in the basal plane. Thus crystals of easy-plane weak ferromagnets are ideal models for the observation of surface anisotropy. Such anisotropy was found and investigated in isometric monocrystals of iron borate, and the theory of surface magnetism for a perfect crystal structure was developed [2]. The purpose of the present work is to assess the influence of different possible imperfections of a crystal's structure in the near-surface area on the surface magnetic anisotropy of an iron borate monocrystal. The first results of such research have been published [3].

2. Surface magnetic anisotropy and transition layer

It was experimentally found [2] that on the face (10 $\bar{1}$ 4) of an iron borate monocrystal, a uniaxial surface anisotropy exists with a very considerable critical field $H_c \approx 1$ kOe, magnetizing a near-surface magnetic layer to saturation along the hard magnetization axis ($HA \parallel 2_x$). For the faces of other crystal types, surface anisotropy with an accuracy up to values of demagnetization fields was not found. For all the types of non-basal faces of iron borate, the surface anisotropy energy, determined as a difference of energies of magnetic ions on the surface versus deep inside the crystal, was calculated in the magneto-dipolar approximation [2]. In a general case, this energy, with the account of an easy-plane crystallographic anisotropy, which does not allow the magnetic vectors to go out from a basal plane, has the form

$$\sigma_{(ijk)} = a_s \sin^2 \varphi + b_s \sin \varphi \cos \varphi. \quad (1)$$

Here φ is the azimuth angle of the antiferromagnetic (AF) vector, measured in a basal plane from the axis 2_x ; a_s , b_s the calculated

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constants of surface anisotropy. For the face (10 $\bar{1}4$) at room temperature, $a_s=0.014$ erg/cm 2 , $b_s=0$. From Eq. (1), one can see that equilibrium orientation of the AF vector in this case coincides with the axis 2_x , as in the experiment [2]. Surface anisotropy, fastening the magnetic moments, and the external magnetic field result in formation of a near-surface inhomogeneous magnetic layer of a domain-wall type, in which the magnetic moments turn smoothly from a surface deep into the crystal. The effective thickness of such a transition layer is much greater than the crystal lattice parameter, being the characteristic scale of thickness of near-surface area, in which the magnetic moments are fastened by surface anisotropy. In the case of weak ferromagnets, surface magnetism appears essentially as the transition layer.

An inhomogeneous layer appears in the magnetic field. The surplus energy related to this layer reads as [2]

$$\gamma_\varphi = \int_0^\infty \left\{ \frac{A}{2} \left(\frac{d\varphi}{dS} \right)^2 + MH_t [\sin(\beta - \varphi) + 1] \right\} dS = 4\sqrt{AMH_t} (1 - \cos\alpha_0), \quad (2)$$

where M is the spontaneous magnetization of the crystal; H_t the projection of the external magnetic field on the basal plane; S the distance from the surface of the crystal; $\alpha_0=(\pi/2 + \beta - \varphi_0)/2$; φ_0 the azimuth angle of AF vector on the surface of the crystal and β the angle between the directions of H_t and 2_x .

The equation for determination of the equilibrium angle of surface spins φ_0 , taking into account Eqs. (1) and (2), has the form [2]

$$\frac{\partial}{\partial \varphi_0} (\gamma_\varphi + \sigma) = -2\sqrt{AMH_t} \sin\alpha_0 + a_s \sin 2\varphi_0 + b_s \cos 2\varphi_0 = 0. \quad (3)$$

Eq. (3) determines, in fact, surface magnetization curves for all types of non-basal crystal faces. In looking at the face (10 $\bar{1}4$), for which surface anisotropy is large, magnetizing along HA ($\beta=0$) in the limit $H_t \rightarrow H_c$ ($\varphi_0 \rightarrow \pi/2$), Eq. (3) gives

$$H_c = \frac{4a_s^2}{(AM)}. \quad (4)$$

Thus at room temperature, we get $H_c \approx 0.2$ kOe. For the other face types, this value is much smaller, which is in agreement with the experiment and allows one to consider further only face (10 $\bar{1}4$) when studying the surface magnetism of iron borate.

3. Surface reconstruction

Elastic interactions, in addition to magnetic interactions, also change in the near-surface area. This must result in distortion of the crystal's structure in a near-surface area, which is a partial reconstruction of the surface that must cause an additional change of magnetic energy in the near-surface layer. Discrepan-

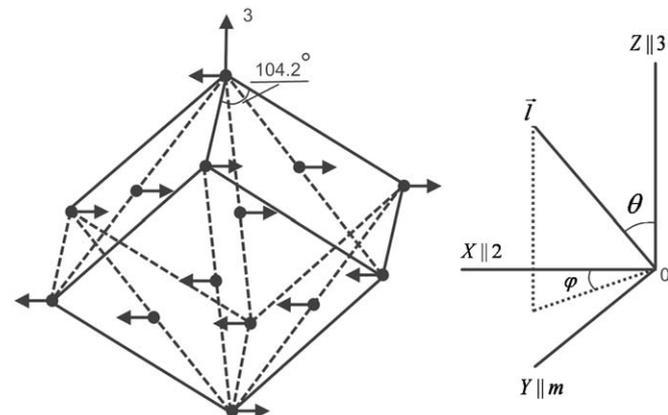


Fig. 1. Rhombohedron of FeBO $_3$ crystal with the faces (10 $\bar{1}4$).

cies between theoretical and experimental values of the field H_c for the face (10 $\bar{1}4$) can be attributed to the displacement of Fe $^{3+}$ ions on the surface from their crystallographic positions. The calculated constant of surface anisotropy a_s is inversely proportional to the fifth degree of the crystal lattice parameter a_r , which means: $H_c \sim a_s^2 \sim a_r^{-10}$. Thus the field H_c may be very sensitive to variation of a_r in a thin (few atomic layers) near-surface layer.

Now we will consider the influence of the reconstruction on the surface magnetism of iron borate for the face (10 $\bar{1}4$). In the magneto-dipolar approximation, taking into account the reconstruction, we will calculate the energy of surface anisotropy and the critical field for this face. The reconstruction is connected with the change of the distances between near-surface atoms. Thus the atoms can be displaced both normally and tangentially to the surface [4]. The distances between the atoms can both decrease and increase. Because it is unknown how quickly the lattice of iron borate relaxes deep within the crystal, we will first analyze the two limiting variants of reconstruction. In the first case, let us assume that only the surface layer of Fe $^{3+}$ ions is displaced and that this displacement takes place along the rhombohedron (10 $\bar{1}4$) edge (Fig. 1), not parallel to the face of the crystal. In the second limiting case, we assume that several near-surface atomic layers are displaced, so that the distances between them change identically.

Calculated within the framework of the two described limiting cases, Fig. 2 depicts the dependence of the surface anisotropy constant a_s on relative change of length in the direction of deformation of elementary rhombohedron edge $\Delta a_r/a_r(\%)$: the line 1 represents the first case, the line 2 represents the second case. Fig. 3 shows the dependences of $H_c(\Delta a_r/a_r)$ obtained for these two cases (lines 1 and 2, correspondingly).

We also considered the intermediate case, where each subsequent layer of Fe $^{3+}$ ions is displaced by half of the displacement of the previous layer. The corresponding curves $a_s(\Delta a_r/a_r)$ and $H_c(\Delta a_r/a_r)$ are presented in Figs. 2 and 3 (line 3).

In all the considered cases, the value a_s increases without a change in its sign, if the distances between the near-surface layers of Fe $^{3+}$ ions increase (Fig. 2). At convergence of these layers, the constant a_s diminishes to zero and then, changing a sign, grows by its module. The last circumstance testifies to re-orientation of the axes of easy magnetization (EA) and HA that does not correspond

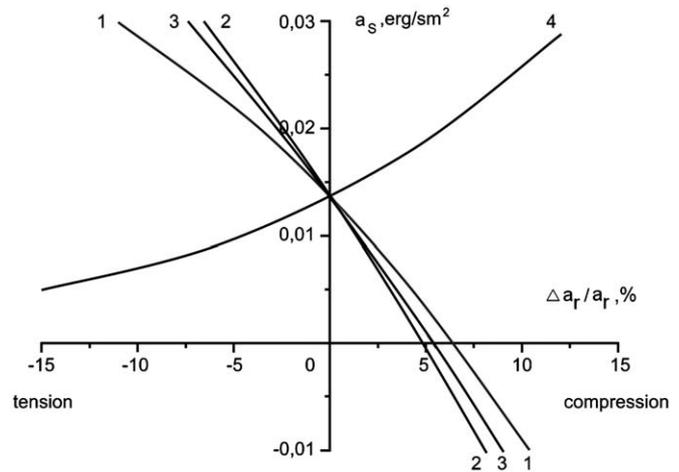


Fig. 2. The dependence of the surface (10 $\bar{1}4$) anisotropy constant on relative change of length of the elementary rhombohedron edge for the following cases: the displacement of one surface layer of Fe $^{3+}$ ions (line 1); the displacement of a several near-surface atomic Fe $^{3+}$ layers, so that the distances between them change identically (line 2); the displacement of each subsequent Fe $^{3+}$ layer by the half of the displacement of the previous layer (line 3); the displacement under hydrostatical pressure (line 4) $T=300$ K.

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