



# ANTIFERROMAGNETIC AND ELECTRIC DOMAINS IN MULTIFERROIC $\text{BiFeO}_3$

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## Motivation

Recently, oxide multiferroics have attracted much attention due to their large magnetoelectric effect which allows tuning of magnetic properties with electric field and vice versa. These materials have opportunities for potential applications in information storage, spintronics and sensors. Other potential applications include multiple-state memory devices with dual magnetic and electric control.

One of most promising from its application point of view is multiferroic  $\text{BiFeO}_3$ , which shows both ferroelectric ( $T_C=1143\text{K}$ ) and antiferromagnetic ( $T_N=643\text{ K}$ ) ordering at room temperature. For the technical application of  $\text{BiFeO}_3$  it is important to know its domain structure. Antiferromagnetic order makes the description of the domain structure in this material more difficult. It is caused by the fact that the antiferromagnetic domains nature isn't entirely known. Because of the net magnetization absence in antiferromagnetic materials there are no sources of the long-range demagnetization forces, which in ferromagnets cause the domain structure formation.

In the present paper we study the competition between antiferromagnetic and electric domain in  $\text{BiFeO}_3$  crystal. Our model is based on the assumptions about magnetoelastic nature of antiferromagnetic domains and on the presence of so called "destressing" energy in samples of finite sizes, which is similar to the demagnetization energy in ferromagnets.

## Model

The crystal structure of bismuth ferrite is characterized by a rhombohedrally distorted perovskite unit cell (Fig. 1).

$\text{BiFeO}_3$  shows complicated spatially modulated magnetic structure with a large period, incommensurate with the lattice parameter. The magnetic moments of iron ions retain their local mutually antiferromagnetic G-type orientation and rotate along the propagation direction of the modulated wave in the plane perpendicular to the hexagonal basal plane (Fig. 2).

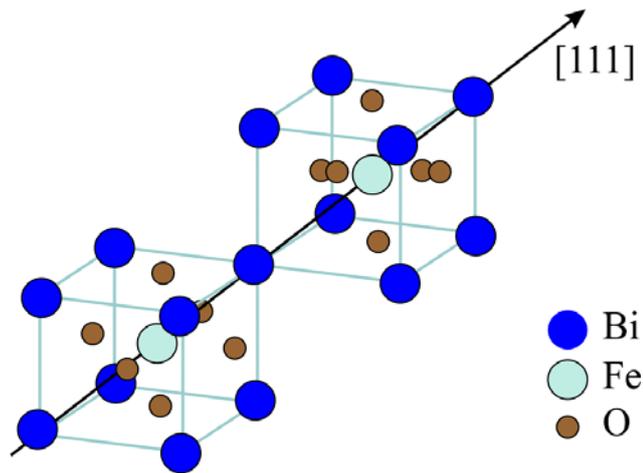


Fig.1 Structure of the  $\text{BiFeO}_3$  unit cell.

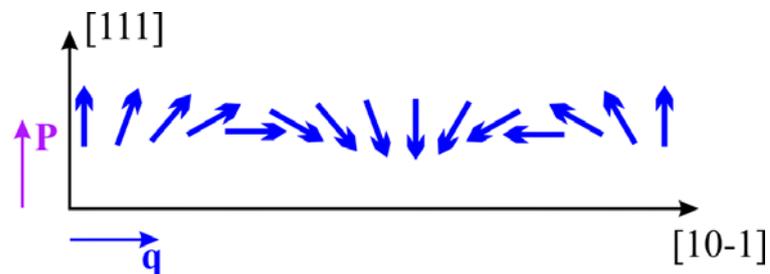


Fig. 2 Ferroelectric and antiferromagnetic structure of  $\text{BiFeO}_3$ . The spontaneous polarization  $P$  is along the  $[111]$  direction and the spiral magnet propagation defined by the wavevector  $\mathbf{q}$  is along the  $[10-1]$  direction. These two directions define the cycloidal plane where the spin rotation occurs. [1]

Thermodynamical potential of the sample includes the potentials of electric and magnetic subsystems. The total expression for the free-energy density has the form

$$F = F_m + F_{me} + F_{an} + F_e + F_L, \quad (1)$$

where  $F_m$  is the magnetic energy in the external magnetic field  $\mathbf{H}$

$$F_m = \frac{\mathbf{M}^2}{2\chi_{\perp}} + \frac{b\mathbf{l}^2}{2} - \mathbf{H}\mathbf{M}, \quad (2)$$

$\mathbf{l} = \mathbf{L}/L$  is the unit antiferromagnetic vector.  $\chi_{\perp}$  is the magnetic susceptibility in the direction perpendicular to the antiferromagnetic vector.

$F_{me}$  is the magnetoelectric interaction energy

$$F_{me} = -D \cdot (\mathbf{P}[\mathbf{M} \cdot \mathbf{l}]), \quad (3)$$

where  $\mathbf{P}$  is electric polarization,  $D$  is coefficient of homogeneous magnetoelectric interaction. This interaction causes the weak ferromagnetism to appear.

$F_e$  is the energy density of electrical subsystem in the external electric field

$$F_e = \frac{a_2}{2} P_{zo}^2 - \mathbf{P}\mathbf{E}. \quad (4)$$

Anisotropy energy can be written as

$$F_{an} = -\frac{K_6}{6} (l_+^6 + l_-^6), \text{ where } l_{\pm} = l_x \pm il_y. \quad (5)$$

The last term in (1) -  $F_L$  is Lifshitz invariant. It corresponds to the inhomogeneous magnetoelectric interaction. This interaction leads to the space-modulated spin structure appearance.

$$F_L = \alpha P_{zo} \left( l_x \nabla_x l_z + l_y \nabla_y l_z - l_z \nabla_x l_x - l_z \nabla_y l_y \right) \quad (6)$$

where  $\alpha$  is the coefficient of the magnetoelectric origin [2]. Here we suppose that  $\mathbf{E} \parallel \mathbf{Z}$  and  $P=(0,0,P_{zo})$  and here we use the orthogonal coordinate system in which the  $\mathbf{Z}$  axis is along [111] direction, axes  $\mathbf{X}$  and  $\mathbf{Y}$  are in the (111) plane, where  $\mathbf{X} \parallel [10-1]$ .

To take into account the crystal form, the **destressing energy** [3]

$$\begin{aligned}
 F_{des} = & \frac{1}{2} \left( K_{11} \langle l_x^2 \rangle^2 + K_{22} \langle l_y^2 \rangle^2 + K_{33} \langle l_z^2 \rangle^2 + \right. \\
 & + 2K_{12} \langle l_x^2 \rangle \langle l_y^2 \rangle + 2K_{13} \langle l_x^2 \rangle \langle l_z^2 \rangle + 2K_{23} \langle l_y^2 \rangle \langle l_z^2 \rangle + \\
 & \left. + 4K_{44} \langle l_y l_z \rangle^2 + 4K_{55} \langle l_x l_z \rangle^2 + 4K_{66} \langle l_x l_y \rangle^2 \right)
 \end{aligned} \tag{7}$$

and depolarization energy

$$F_{dep} = \frac{1}{2} N_3 \langle P_{zo} \rangle^2 \tag{8}$$

should be added into the free energy density expression.

There  $K_{ij}$  are the shape depended coefficients of destressing,  $N_3$  is the depolarization coefficient. The angle bracket means averaging by volume of the crystal. The equations (7), (8) are written for the case of ellipsoid of rotation.

## Results

In the equilibrium state, in case of absence of any external fields, and strong own anisotropy ( $K_6 \gg D^2 \chi_{\perp} P_z$ ), the 6 domain types with 3 different directions of the cycloid wavevector ( $\mathbf{q}_1, \mathbf{q}_2, \mathbf{q}_3$  Fig. 3) and 2 polarization directions ( $\mathbf{P} \uparrow \uparrow \mathbf{Z}$  and  $\mathbf{P} \uparrow \downarrow \mathbf{Z}, \mathbf{Z} \uparrow \uparrow [111]$ ) are possible.

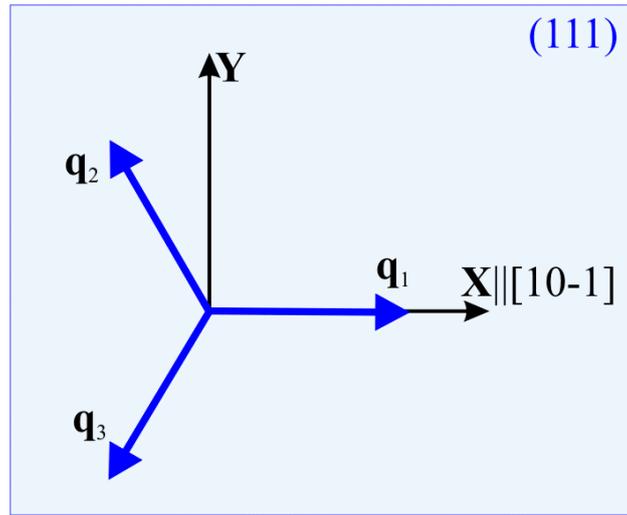


Fig. 3. The possible directions of the magnetic cycloid wavevector.

For simplicity we examine the case of three domain types:

1 type — polarization is  $\mathbf{P} \uparrow \uparrow \mathbf{Z}$ , the cycloid wavevector direction —  $\mathbf{q}_1$ ,

2 type — polarization is  $\mathbf{P} \uparrow \downarrow \mathbf{Z}$ , the cycloid wavevector direction —  $\mathbf{q}_2$ ,

3 type — polarization is  $\mathbf{P} \uparrow \downarrow \mathbf{Z}$ , the cycloid wavevector direction —  $\mathbf{q}_3$ .

In this case the magnetic field  $\mathbf{H}$  applied along axis **Y** increases the part of domains of first type (with polarization  $\mathbf{P} \uparrow \uparrow \mathbf{Z}$ ) and decreases the parts of domains of second and third types (with polarization  $\mathbf{P} \uparrow \downarrow \mathbf{Z}$ ). Thus, we can manage the electric domains by means of external magnetic field. And vice versa the electric field  $\mathbf{E}$  applied antiparallel to axis **Z** decreases the part of domains of

first type and increases the parts of domains of second and third types. This fact makes it possible to control the magnetic domains by means of electric field.

Moreover, in case of three domain types, the macroscopic polarization depends on the external magnetic field and the shape depended coefficients of destressing:

$$\langle P_z \rangle = P_{z0} \frac{4\chi_{\perp} H_y^2 + \frac{64}{3} P_{z0} E_z + 16\left(\frac{4}{3} \alpha q - \chi_{\perp} D^2 P_{z0}\right) P_{z0} + 3K_{22} - 5K_{11} + 2K_{12} - 4(K_{13} - K_{23})}{3(K_{11} + K_{22} - 2K_{12}) + \frac{64}{3} N_3 P_{z0}^2}$$

In the case of six domain types, there is no direct possibility to manage electrical domains by the magnetic field and vice versa, but there is possibility to obtain predominance of one type of domains above five others by means of electric and magnetic fields.

### Conclusions:

In certain conditions the electric and the antiferromagnetic domains in the BiFeO<sub>3</sub> sample are strongly interrelated. This fact makes it possible to control the electric polarization by means of magnetic field.

### Literature

- [1] M. Cazayous, Y. Gallais, A. Sacuto arXiv:0712.3044v1 (2007)
- [2] A. M. Kadomtseva, A. K. Zvezdin, Yu. F. Popov, A. P. Pyatacov and G. P. Vorob'ev JETP LETTERS **571-581**, 79 (2004)
- [3] H. Gomonay, V. Loktev Physics of the Solid State. **1755-1760**, 47 (2005)