MAGNETIZATION AND POLARIZATION PROFILE
IN PML-TYPE MAGNETOELECTRIC
MULTIFERROICS WITH CANTED SPIN SYSTEM

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Abstract

We calculate the profile of both magnetization and polarization of a PML-type magnetoelectric multiferroics which allow the magnetization of sub-lattices to be canted. The calculation is started by deriving the Landau energy density and followed by solving simultaneously three equilibrium equations which respect to polarization, magnetization and canting angle. It is predicted that magnetoelectricity give rise to a “bump” in polarization profile. It is also calculated that the application of a magnetic/electric field will also influence the polarization/magnetization of the material.

Keywords: multiferroics, magnetization and polarisation

Introduction

According to Schmid\textsuperscript{[1]}, materials which have ferroelectric and ferromagnet phenomena in the same phase are called “multiferroics”. In these materials, the magnetization can be manipulated by electric field, and vice versa\textsuperscript{[2]}. This phenomena can be existed, since the magnetic properties are coupled to the electric properties through a magnetoelectric interaction. The phenomena had been discussed theoretically in ferroelectric-antiferromagnet phase by Dzyaloshinskii\textsuperscript{[3]} and performed experimentally in Cr\textsubscript{2}O\textsubscript{3} by Astrov\textsuperscript{[4]}.

Theoretical studies of magnetoelectric materials are usually started by firstly deriving the energy density in Landau formalism by treating electric polarization \( P \) and magnetization \( M \) as the order parameters. This energy density consist of three parts. The first part is ferroelectric energy density with polarization \( P \) as an order parameter. The magnetic behaviour is represented by the ferromagnet energy density with magnetization \( M \) as an order parameter. The last part is magnetoelectric energy density which has both \( P \) and \( M \) as the order parameters.

The symmetry-allowed magneto-electric energy density for a ferroelectric-two sub-lattices antiferromagnetic phase, for example, can be represented as\textsuperscript{[5]}

\[
E_{NP} = \gamma P^2 (M_a \cdot M_b)
\]

(1)

where \( \gamma \) represents magnetoelectric constant, while \( M_a \) and \( M_b \) represent magnetization of sub lattices.

The more interesting model of ferro-electric-two sub-lattices antiferromagnet is represented by the
magnetoelectric energy density in the form

$$F_{NE} = (\gamma_1 L_z + \gamma_2 L_z^2)$$

which was proposed for BaMnF$_4$. Here, $\gamma_1$ and $\gamma_2$ represent the magnetoelectric constants, while $L_z$ is a component of antiferromagnetic vector. The first term on the right hand side of Eq.(2) contains the Dzyaloshinskii-Moriya (DM) interaction in the form $\mathbf{D} \cdot (\mathbf{M}_a \times \mathbf{M}_b)$. This DM interaction is responsible for the canting of sub-lattices in antiferromagnet which result in weak ferromagnetism.

In present work, using the first term on Eq.(2), we study the effect of magnetoelectric coupling through the analysis of the profile of both the polarization and the magnetization.

METHOD

In this work, we study the magneto-electric multiferroic by using the model of ferroelectric-antiferromagnet which sub-lattices are allowed to be cant. In this model, we assume that electric polarization $\mathbf{P}$ is parallel to $\hat{y}$ axis as illustrated in Fig.(1). The magnetization of sub-lattices, $\mathbf{M}_a$ and $\mathbf{M}_b$, lies in the $x$-$z$ plane and perpendicular to the electric polarization. Here, we also assume that the sub-lattice magnetization is symmetric, with $|\mathbf{M}_a| = |\mathbf{M}_b| = M_s$.

Figure 1. The configuration of canting spin system and polarization. The polarization is directed along $y$ axis, while sub lattice magnetizations are canted with canting angle $\theta$, generating weak magnetization along $x$ axis.

The ferroelectric energy density represent this model is:

$$F_p = \frac{1}{2} \beta_1 P_x^2 + \frac{1}{2} \beta_2 P_y^2 + \frac{1}{4} \xi_1 (P_y^2 + P_x^2)$$
$$+ \frac{1}{16} \beta_3 (P_y^4 + P_x^4) - P_y P_x$$

(3)

where $\beta_1$ and $\beta_2$ represent dielectric stiffness along spontaneous polarisation, while $\xi_1$ and $\xi_2$ are dielectric stiffness constants perpendicular to the spontaneous polarisation. The external magnetic is represented by $E_y$.

The ferromagnetic energy density is described as an addition of exchange energy, anisotropy energy and Zeeman energy as

$$F_M = \lambda M_s^2 \cdot \mathbf{M}_a \cdot \mathbf{M}_b - \frac{K}{2} \left[ (\mathbf{M}_a \cdot \hat{z})^2 + (\mathbf{M}_b \cdot \hat{z})^2 \right]$$
$$- \left( \mathbf{M}_a + \mathbf{M}_b \right) \cdot E_x$$

(4)
Here, $\lambda$, $K$ and $H_0$ represent a strength of the exchange interaction, an anisotropy constant and an external field.

Since the sub-lattice magnetization and the component of antiferromagnetic vector $\mathbf{Z}$ can be described by the canting angle $\mathbf{\theta}$, then the magnetoelectric energy density can be written as

$$F_{\text{ME}} = 2\alpha R_\perp M_\perp^2 \sin \mathbf{\theta}.$$  \hfill (5)

Where $\alpha$ represents the magnetoelectric strength.

The next step is to minimize the energy density Eq.(3)-(5) which respect to polarization, sub-lattice magnetization and canting angle. This yield three equations which describe three equilibrium condition. The profile of magnetization, polarization and canting angle can obtained by solving these three equilibrium equations simultaneously.

**Results and Discussion**

Minimizing the ferroelectric and the magnetoelectric energy density respect to the $y$ component of polarization, $P_y$, yield

$$\frac{\partial (F_E + F_{\text{ME}})}{\partial P_y} = 0,$$

yield

$$\beta_s P_y + \beta_y P_y^2 = 2\alpha R_\perp M_\perp^2 \sin 2\mathbf{\theta} - 4\alpha R_\perp M_\perp^2 \cos 2\mathbf{\theta} - E = 0.$$  \hfill (6)

Instead of minimizing ferromagnetic and the magnetoelectric density respect to sub-lattice magnetization, we use the Brillouin function to describe the equilibrium condition of sub-lattice magnetization. Hence, the average magnetization of sub-lattices can be written as

$$M_s = M_s(0) \Theta_s(\lambda).$$  \hfill (7)

with

$$\Theta_s = \frac{2S + 1}{2S} \coth \left[ \frac{(2S + 1)\lambda}{2S} \right] - \frac{1}{2S} \coth \left( \frac{\lambda}{2S} \right).$$ \hfill (8)

In the Eq.(9) above, $S, \mu_B$ and $k_B$ represent spin, Bohr magneton and Boltzmann constant.

The equilibrium condition respect to canting angle can be obtained by minimizing the sum of ferromagnet energy density and magnetoelectric energy density respect to canting angle:

$$\frac{\partial (F_E + F_{\text{ME}})}{\partial \mathbf{\theta}} = 0,$$

result in

$$H^f \cos \mathbf{\theta} - \frac{1}{2} K M_s \sin^2 \mathbf{\theta} + 2\alpha R_\perp M_s^3 \cos \mathbf{\theta} + 2\alpha R_\perp M_s^3 \sin 2\mathbf{\theta} - E = 0.$$  \hfill (10)

Then, the value of polarization, magnetization and canting angle can be obtained at certain temperature by solving equations (6), (7) and (10) simultaneously. Firstly, we set the external field is zero. The numerical result is illustrated in Fig.(2).
Figure 2. The profile of magnetization and polarization in the discussed system with the external fields are set to zero. The condition without magnetoelectric coupling is illustrated with the solid line. The dashed line represents the material with ME coupling \( \alpha_1 \). The profile at the condition with the bigger ME coupling \( \alpha_2 \) is drawn by the dotted line.

Figure 2 above is illustrating three condition. The solid line represents the condition without magnetoelectric (ME) coupling. The profile of the condition with ME coupling \( \alpha_1 \) is represented by the dashed line. The condition with the bigger ME coupling \( \alpha_2 \) yield the profile which is represented by the dotted line. The magnetic profile of the sub-lattices is started at the saturation magnetization \( M_s(0) \) and decrease as the temperature increase. The shape of the magnetization in Fig.(2) is similar to that which is discussed in Ref.[10]. The sub-lattice magnetization become zero when temperature reach Neel temperature \( T_N \) since above that temperature the phase become paramagnet. It can also be seen from the Fig.(2) above that the magnetoelectric coupling gives contribution to the value of Neel temperature. It tends to increase the Neel temperature compare to that in the condition without coupling. This happen since the electric polarization tend to increase the sub-lattice magnetization through the magnetoelectric coupling.
Figure 3. The profile with the inclusion of external field. (a). The profile when the external electric field is applied to the magnetoelectric multiferroics. (b). The profiles when the external magnetic field is applied.

The polarization profile, as it is illustrated in Fig.(2), starts from $P(0)$ at zero temperature and decrease to zero at Curie temperature. Compare to the Ref.[11], The shape of the polarisation is similar. Figure 2 above also shows that magnetoelectric coupling give rise a ‘bump’ in the polarization profile. The ‘bump’ exist between zero temperature and Neel temperature. It is resulted from magnetization which increase the electric polarization through the magnetoelectric coupling.

Next, we present the result when the external field is applied into the system as it is illustrated in Fig.(3). In the
Fig. (3a), the profiles are resulted from the condition where the electric field is applied while the magnetic field is zero. The condition when the magnetic field is applied while the electric field is zero yield the profile which is drawn in Fig (3b).

It is clear from Fig. (3a) that the applied electric field are not only influence the electric polarization, but also increase slightly the magnetization. It is also shown in Fig. (3b) that the application of the external magnetic field increase slightly the electric polarization. The described phenomena above is resulted from the existence of magnetoelectric coupling.

Conclusion

We present the numerical calculation to study magnetoelectric phenomena. It is shown that the existence of magnetoelectricity can be represented by ‘bump’ in the electric polarization profile.

Bibliography