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Numerical Study of The Spontaneous Polarization near The Ferroelectric Surface

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Abstract

The ferroelectric materials signified by the existence of electric potential that can be reversed using an external electric field. Hence, the polarization was an important parameter. It was well known that the polarization in a bulk ferroelectric was homogenous. However, when it was noticed, the electric polarization at the region near the surface was in-homogeneous. This inhomogeneous polarization was important since it affected the physical behaviour of ferroelectric. In this paper, we studied the inhomogeneity in the surface of ferroelectrics by using lattice model. In this model, we included the interaction between lattices. We obtained that in-homogeneous ferroelectric appeared near surface. We predicted that this happened since above the lattice at the surface, there was no other existed lattice. The difference of interaction constant lattice at the surface and the other interaction constant of the lattice inside material also contributed to the inhomogeneity.

Keyword: lattice model, inhomogeneous, ferroelectrics

Introduction

The ferroelectrics ws a type of material which retained spontaneous electric polarization. This electric polarization can be reversed by applying an external electric field [1]. Spontaneous polarization occurred when temperature was lower than Curie temperature T_C. The electric polarization was an important parameter in ferroelectric since it affected the resonance frequency of the permittivity [2]. In the bulk geometry, the polarization was homogeneous. However, if we noticed the polarization near surface, we found that the electric polarization was inhomogeneous. This inhomogeneous property was also found in the film geometry [3]. This behavior appeared from the size effect where the value of polarization near surface was different from the value inside material [4].

The inhomogeneous polarization can be studied by assuming that the bulk geometry comprised of the lattices. In this model, we focused on the lattices near surface of the ferroelectrics. There were interactions of the polarization at a lattice and the polarization at the nearest neighbor lattices [5]. The equation of density energy was derived for each lattice. The solutions of the minimization of the energy in each lattice illustrated the inhomogeneity of the electric polarization near surface.

The method and formulation

The geometry of this study was given in Figure 1. A ferroelectric material was placed with the surface set at *x*-*y* plane. Here, we considered the model of ten lattices, with the first lattice was at surface. The density energy of this lattice model can be written as[5]

$$F = \sum_{i=1}^{n} \left[\frac{a_0 T_c}{2}\left(\frac{T}{T_C} - 1\right)\right] P_i^2 + \frac{\beta}{4} P_i^4 + \frac{K}{2}(P_i - P_{i-1})^2 - E P_i. \quad (1)$$

Here, a_0 and β represented the ferroelectric stiffness constant, T_c was Curie temperature, E symbolized external electric field. Parameter P_i signified the electric polarization in i^{th} lattice.

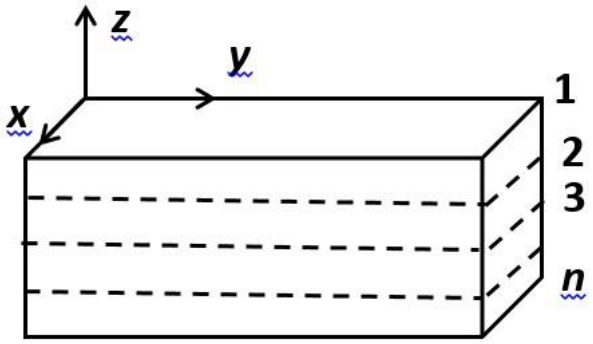

Figure 1. Geometry of the study. The lattice model with lattice 1 at the surface. Here, the surface of ferroelectric was arranged at *x*-*y* plane.

Then, using substitution $P_i = p_0 \wp_i$ with $p_0 = (a_0 T_C/\beta)^{1/2}$ and performed rescaling process, we obtained the unit-less form. The minimization of energy density toward the polarization $\left(\frac{\partial F}{\partial P} = 0\right)$, resulted the equation in each lattice as

$$\mathbb{C}_i \wp_i + \wp_i^3 - \kappa_i \wp_{i-1} = 0 \quad (2)$$

where $\mathbb{C}_i = \left[\left(\frac{T}{T_C} - 1\right) + \left(\frac{K_i}{a_0 T_C}\right)\right]$, $\kappa_i = \frac{K_i}{a_0 T_C}$. Here, the electric field was excluded. The solution can be obtained by solving simultaneously Eq. (2) for involved lattices. In the numerical calculation, we set the value of interaction constant between lattice 2 and lattice different from the value of the rest lattices.

Results and Discussion

In this paper, we used the lattice model with the number of lattices was 10. The solution of Eq. (2) was presented in Figure 2 below.

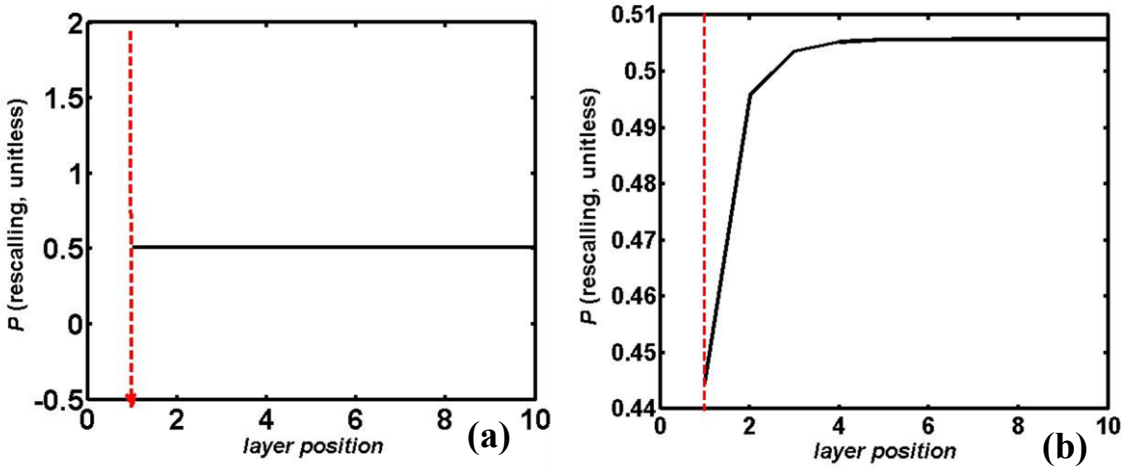

Figure 2. The electric polarization. (a) The homogeneous polarization in bulk ferroelectric. (b) Inhomogeneous polarization around the surface of ferroelectrics. The shaded red lines illustrated surface of ferroelectric.

In the numerical calculation, we set the number of lattices was ten. We considered that that number can illustrate the condition near surface and also bulk. Here, we used parameters as: $T_C = 391$, $a_0 = 6.65 \times 10^5$ K^{-1}, $\beta = 3.56 \times 10^9$ cm^3/erg, which is appropriate for ferroelectric $BaTiO_3$. Since we did not have any information about the value of inter-lattice constant, we set $K = 1.5 \times 10^6$ for the interaction between lattice one and two, and $K = 3.5 \times 10^7$ for the rest of lattice interactions. For the case of homogeneous polarization in Figure 2a, we use the same interaction constant for all lattices, which was $K = 3.5 \times 10^7$. Since the parameters in homogeneous case (bulk) were similar for all lattices, Then the polarization in each lattice showed the same value as illustrated in figure 2a. In bulk, the effect of inhomogeneity at the surface covered by homogeneous polarization in the ferroelectric. Hence, the non-homogeneous polarization near surface was not significant and it was difficult to observe.

The result for non-homogeneous case presented in figure 2b. At the picture, the red line represented the surface. Here, the lattice at the surface did not have neighbor lattice above it since the lattices was limited at the surface. The interaction between surface's lattice and a lattice below it had different value with the other value of inter-lattice interaction. These conditions generated the in-homogeneity of the electric polarizations near the surface. The effect can be observed if we only involved a few lattices in the model. Here the in-homogeneity is only about 10% from the electric polarization of the bulk.

Conclusion

The inhomogeneity of the electric polarization near the surface was contributed by two factors. One, the condition that the lattice at the surface only have one neighbour. Two, the value of constant inter-lattice between lattice at the surface and its neighbour was different from the value of other constant inter-lattice at the body of the ferroelectrics.

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