International Journal of Theoretical & Applied Sciences, 10(1): 281-284(2018)

ISSN No. (Print): 0975-1718
ISSN No. (Online): 2249-3247

# Predictive Role of 0°, 90°, 180° and non-180° Aligned Domains in Backswitching and Switching Kinematics of Ferroelectrics

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*(Received 21 February, 2018, accepted 24 April, 2018)*
*(Published by Research Trend, Website: www.researchtrend.net)*

**ABSTRACT: The spontaneous polarization acquired during phase transition from paraelectric to ferroelectric is randomly distributed. The lattice conditions around 'the spontaneously ordered electric polarization vector prevailing in different regions' are different and they change with the change in the thermal state of the sample. These regions may consist of a single domain or a group of domains and as such may be classified into four broad categories of domain alignments. The domain alignment of a specific region can be represented by resultant polarization vector acquired spontaneously. These polarization vectors tend to rotate on the application of external field and acquire induced polarization. On the removal of external field, fraction of induced polarization gets permanently set-in while rest disappears. The disappeared part forms the backswitching. In this paper, an attempt is made to build theoretical concepts about backswitching and to predict the role of 0°, 90°, 180° and non-180° domain alignments in switching kinematics of ferroelectrics.**

**Keywords:** Backswitching, Domain Switching, Ferroelectricity, Free Energy, Polarization, 90° and 180°-aligned domain orientations.

## I. INTRODUCTION

In ferroelectric samples, the study of domain switching kinetics has become of much significance because the switching transients in thin ferroelectric films have shown their utility in a number of practical applications particularly in memory devices [1-4]. The reversal of polarization in these samples can be studied by measuring switching currents as a function of time [5]. A ferroelectric is characterized by two states of polarization and that for convenience can be labelled as up state (forward state of polarization) and down state (reverse state of polarization) [6-8]. The term switching actually refers to switching of domains whereby the ferroelectric material jumps from its one state of polarization to another or vice-a-versa under the influence of external electric field. Thus domain switching is a field dependent mechanism [9, 10]. It always remains on the priority of researchers to study switching kinetics of the domain structure amidst polarization reversal. So, it is important to conceptualize the idea of domain switching kinematics on the application of external alternating electric field to the ferroelectric specimen.

## II. CONCEPT OF BACK SWITCHING

To understand the concept of back switching, consider a ferroelectric sample that acquires a saturated polarization $P_s$ under an external electric field. When this field is totally withdrawn, the sample retains some remanant polarization $P_r$ owing to its intrinsic nature and thermodynamic conditions. The relative polarization retained by this sample is represented by the ratio $P_r/P_s$; and the polarization that could not be retained on withdrawal of the field is $(1 - P_r/P_s)$. It means that some of the domains choose to step out of the direction undertaken by resultant polarization vector acquired in saturated state of polarization once the polarizing field from the sample is withdrawn. This behaviour of the domains by which they become unable to remain in the mainstream of switched domains on withdrawal of applied field is known as back-switching.

$$\text{Back-switching (\%)} = [1 - P_r/P_s] \times 100$$

The back-switching represents the 'polarization retention-loss' of a ferroelectric capacitor. The retention-loss in ferroelectric capacitors is not counted as a good sign for memory operation [11, 12].

## III. CONCEPTUALIZING 0°, 90°, 180° AND NON-180° ALIGNED DOMAINS

The spontaneous polarization acquired during phase transition from paraelectric to ferroelectric is randomly distributed [13]. The lattice conditions around 'the spontaneously ordered electric polarization vector prevailing in different regions' are different and they change with the change in the thermal state of the sample. These regions may consist of a single domain or a group of domains. Previous to any kind of poling, all the pre-field (i.e. before the application of external electric field) domain orientations in any plane of the ferroelectric sample just at the start of first half cycle' of the applied field can broadly be divided into following four categories:

(a) **0$^o$-aligned domains**: Those which coincidently would find their spontaneous polarization along 'the direction of the first half cycle' of the applied field may be called as 0$^o$-aligned domains.

(b) **180$^o$-aligned domains**: Those domain orientations which would find their spontaneous polarization in a direction opposite to 'the direction of the first half cycle' of the applied field may be categorized as 180$^o$-aligned domains.

(c) **non-180°-aligned domains**: Those domains which would find their spontaneous polarization in an arbitrary direction other than the perpendicular direction to the applied field and also in directions other than the ones taken in the two former cases (a) and (b); such domains may be called as non-180°-aligned domains.

(d) **90°-aligned domains**: This category belongs to that group of domains which would be perpendicular to the direction of the applied field and may be called as 90°-aligned domains.

## IV. DISCUSSION

A plane containing aligned domains of the kind described in section III (a) to (d) is shown in the Fig. 1 (i) All the domains in the given ferroelectric sample can be spotted by turning an imaginary plane of this kind through 2π radians around the axis of applied field.

The switching behaviour of different category of domains defined in the previous section may be understood as follow:

(i) In the beginning, growth of first half cycle of the external field helps in the growth of sample polarization through: (i) the growth of only the arm length of 0°-aligned dipoles; (ii) rotation of 180°, non-180° and 90°-aligned dipoles respectively of 'domain categories (b), (c) and (d) as described in section III. With the subsequent growth of field overall polarization of the sample increases with subsequent growth of arm lengths of all the dipoles till

(1) The applied field attains its peak value or

(2) The 'arms of the dipoles' aligned 'along the field' attains their optimum length.

The resultant induced polarization in case of domains of category (a) and (b) is acquired by only 'one dimensional movement' of the 'constituent dipole moment vectors' of the unit cells along 'the direction of applied field' and the associated dipole moment vectors do not sweep across the lattice; whereas in case of category (c) and (d) the polarization is acquired by two dimensional motion of the said vectors around the field axis which sweep across the lattice making their switching mechanism comparatively difficult.

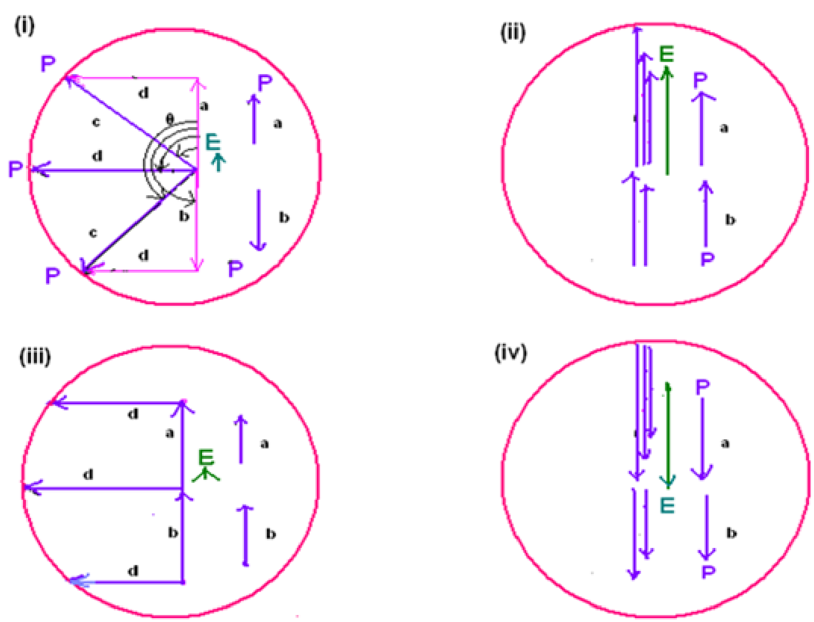


**Fig. 1.** In part (i) of this Figure, the meaning of respective symbols θ, a, b, c, and d is: symbol θ is the angle between any domain alignment and electric field E; symbol a represents 0$^o$-aligned domain/domain component(s); symbol b represents 180$^o$-aligned domain/domain component(s); symbol c represents non-180$^o$-aligned domains and symbol d represents 90$^o$-aligned domain/domain component(s). In Figure (ii) it is shown that with increase in electric field, the domain alignments start turning and align along applied field. Some domains/domain components switch through 180$^o$ while others switch through 90$^o$. Former attain more stability while later become lesser stable. Part (iii) of this Figure shows that the domains/domain components switched through 180$^o$ prefer to stay in their new state unlike 90$^o$ switched domain/domain component(s) when applied field decays to zero from its maximum value during first half cycle. Figure (iv) shows switched 'domain states' with respect to the states shown in Figure (ii); domains switch between states shown in Figure (ii) and Figure (iv) on attainment of peak field value every half cycle passing every time through state (iii).

Just at the beginning of applied field (say positive half cycle) 0°, 90°, 180°, non-180°-aligned domains with respect to applied field are shown in Fig. 1 (i); blue vectors are shown to represent domain orientations where the pink vectors are shown to represent their (domains') components resolved along, opposite and perpendicular to the applied field. Vector E in green is shown to represent applied field. Some pre-field domain orientations are arbitrarily taken. Any non-180° domain can be regarded as equivalent to its two rectangular orientation component: one perpendicular to the field axis and other along/opposite to the axis of the field; former may be called as '90°-aligned dipole component' while later may be any of the two kinds of components: component along the field direction i.e. 0°-aligned component or that aligned opposite to field direction i.e.180°-aligned dipole component. In a given region, none of the 'non-180° domains' has its '90°-aligned dipole component' more than that of the 90°-aligned domain. More an area the polarization vector of a domain has to sweep through the lattice more difficult is for it to switch its state. So, 90°-aligned domains are most difficult to switch. It also distinguishes switching behaviour of 90°-aligned domains or 90°-aligned domain components from 180°-aligned domains and 180°-aligned domain components; it makes easy to understand that it is difficult for the former to switch their polarization states in comparison to the later. This behaviour decides stability of switched state. The 90° domain switching places it into lesser stable state while 180° domain switching takes it into a more stable state. Thus, out of (c) and (d) domain/domain component categories, domains of latter category (90°-aligned domain/domain component(s)) are most difficult to switch as is clear from its comparison that may be made with switching of domains of category d (non-180°-aligned domains).

(ii) When a ferroelectric sample is subjected to some external electric field, the lattice conditions around some regions are such that they allow them (regions) to accept energy from the applied field, to surmount the energy barrier that forbids the 'spontaneously oriented polarization vector' to attain a 'maximum stable state' marked with 'lowest free energy'. Thus lattice conditions around some regions facilitate the rotation of their spontaneously oriented polarization vector to attain 'a stimulated state of polarization' along the direction of applied field. Here, the lattice conditions and the direction of applied field act on that region in unison ending up with lowering of its (region's) free energy. The final 'stimulated state of polarization' of such domain or group of domains is maximum stable and once that state is attained then respective region would not leave that state even on the removal of the applied field. Such regions may be identified to have suffered 180° domain switching under applied field [14, 15]. It may be seen that 90°-aligned domains switch through 90°; 180°-aligned domains switch through 180° while the others i.e. non-180°-aligned domains switch through an angle lying above 90° and below 180°.

(iii) However, the 'lattice conditions' around some regions are not constructively placed to accept naturally, the energy from the applied field to surmount the energy barrier that forbids their 'spontaneously oriented polarization vector' to attain a 'maximum stable state' marked with 'lowest free energy'. Actually, the direction of applied field with respect to the direction of spontaneous polarization in such regions is not suitable to let their 'spontaneously oriented polarized vector' to 'a new orientation state of polarization' which may be expected to be energetically more viable to enhance more stability accompanied with further lowering of free energy. It can be said that such regions are forced to align along the direction of applied field in a new state of polarization that is not their natural state of polarization. The new state so attained in the presence of external field may be called as a 'forced state of polarization'. The free energy of such regions in the so called 'forced state of polarization' is increased making their final state energetically less stable. The forced state of polarization' of such regions may be retained only in the presence of applied field and once the polarizing field is withdrawn, polarization vector of such regions return to their natural orientation previously held just before the application of polarizing field. As we know on the basis of laws of statistics that there is no 'a priori probability' for any such region to align its spontaneously held polarization vector along any preferred direction, so these regions are found to revert back to their natural states with their polarization vectors randomly distributed all over the sample. In this situation, there could be no resultant polarization from such regions and eventually they cannot contribute anything to the retained polarization of the ferroelectric sample after withdrawal of polarizing field. Such regions may be identified to have suffered 90° domain switching under applied field [14, 15].

(iv) At the end of every half cycle i.e. at the time of withdrawal of applied field, previously held 90°-aligned domains and 90°-aligned components of 'non-180° domain orientations' revert back to their initial state but the previously held 180°-aligned domains or components of non-180°-aligned domains along the field remain in their new states providing the sample a remnant polarization; At the beginning of next half cycle of the applied field, the sample is mostly associated with only 90° and 180°-aligned domains and the hysteresis behaviour is the result of 'repeatable switching' of these states with respect to the applied alternating field.

## V. SUMMARY

When a ferroelectric sample is subjected to a polarizing field and in the active process of attaining more and more degree of electric polarization it may not be the case that every domain, on aligning along the direction of applied field, ends up with lowering of its fee energy. Some regions, which are forced to attain a state of polarization, end up with increase of free energy in the said exercise and hence cannot contribute to the retained or remanant polarization of the sample.

During withdrawal time of the applied field, the domains in these regions prefer to revert back to their pre-field states of polarization from their switched state of polarization.

The tendency of a domain to desist from accompanying the switched state of saturation polarization attained under some external field may be proportional to its degree of opposition to leave the pre-field polarization state. The switched orientations from some of the pre-field domain orientations may not be their natural orientations thereby making difficult to attain as well as difficult to retain the forced state of polarization. It can be said that the energy barrier to switch the state may depends upon the degree of orientation any domain shall have with respect to the applied field. Furthermore, the '90° and 180° domain switching' proceeds through different mechanisms of domain wall movement [16-18]. They are associated with different 'switching dissipation' energy, so they are affronted by different energy barriers before switching.

The contribution to the dynamic polarization in the hysteresis loop comes from both 90° as well as 180° domain switching. The back-switching is proportional to the 90° domain-switching only as 90° domain switching is difficult than 180° domain switching. Since the degree of viability of a ferroelectric sample to act as a 'potential source of memory storage' in electronic devices depends upon the degree of polarization it retains on the withdrawal of 'the polarizing field, so the calculation of 'backswitching percentage of the saturation polarization' is very significant to know 'domain-wise' composition of the ferroelectric sample.

## ACKNOWLEDGMENTS

All the authors acknowledge IKG Punjab Technical University Kapurthala, Punjab (India) and MRS Punjab Technical University Bathinda, Punjab (India) for facilitating present research work. The first three authors also acknowledge their parent organization Punjabi University Patiala (Punjab) India for having been allowed to pursue their respective research work.

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