FERROELECTRICS in press

DOMAIN AVERAGE ENGINEERING IN FERROICS

B. SHAPARENKO, J. SCHLESSMAN & D.B. LITVIN

Department of Physics, The Pennsylvania State University, Penn State Berks Campus, P.O. Box 7009, Reading PA 19610-6009, U.S.A.
E-mail: u3c@psu.edu

In a domain average engineered sample of a multidomain ferroic, the sample is divided into a very large number of domains, representing m domain states where m is less than the theoretically allowed maximum number n of domain states. The response to external fields is described by tensorial properties averaged over all the involved domain states. We have developed a program to classify subsets of m < n domain states which can arise in a ferroic phase transition. We calculate properties of these subsets of domain states, including the symmetry of the subset, the subset domain polarizations and magnetizations, and, if they exist, the poling directions which gives rise to the subsets of domain states.

Keywords: domain states, domain engineering, polarization, magnetization

INTRODUCTION

Practical applications of multidomain ferroics can be classified into those which depend on dynamical domain processes and those which depend on a static distribution of domains. The latter can be subdivided into three cases [1] : *domain geometry engineered* samples, where the spatial distribution of domains is tuned to correspond to the k-vectors of fields propagating through the material, *domain average engineered* samples, where the sample is divided into a very large number of domains, representing m domain states where m is less than the theoretically allowed maximum number n of domain states, and *domain wall engineered* samples where the static walls play an essential role. Here we shall consider only the second case, that of domain average engineering.

The response of a domain average engineered sample to external fields is roughly described by tensorial properties averaged over all of the domain states involved. In a recent paper, Fousek & Litvin [2] have introduced a classification of subsets of the domain states which arise in a ferroic phase transition from a parent phase of point group **G** to a ferroic phase of symmetry **F** $\subset$ **G**, and have shown how to calculate the effective symmetry of domain average engineered samples. The phase transition from $\mathbf{m\bar{3}m}$ to **3m** was considered there because of the piezoelectric properties of PZN-PT single crystals poled along one of the {001} directions [3-6].

In this paper we present the contents of a program[7] which calculates the classification of subsets of m < n domain states which arise in a ferroic phase transition and determine properties of the subsets including, their symmetry, and , if they exist, the poling directions to obtain the subsets of domain states.

THE PROGRAM

[1] Selection of point groups:

For a phase transition from a point group **G** to a point group **F**, one can select for **G** the magnetic point group $\mathbf{m\bar{3}m1'}$, one of its 420 subgroups, **6/mmm1'** , or one of its 236 subgroups. The group **F** is chosen from among the subgroups of **G**. Three notations can be used, International primed, International G[H], and Schoenflies notations.

[2] Coset and Double Coset Decomposition of G with respect to F:

This group theoretical decomposition of G with respect to F provides information for calculating the classification and properties of the subsets of domain states [8].

[3] Index, Point Group, Polarization and Magnetization of the Domain States:

"i" is the index of the domain state S_i , g_i an element of **G** which relates S_i to S_1 , i.e. $S_i = g_i S_1$, , F_i the symmetry group, and P_i and M_i are, respectively, the polarization and magnetization of the ith domain state. As an example here and also below, we consider the phase transition from $\mathbf{G} = \mathbf{m\bar{3}m}$ to $\mathbf{F} = \mathbf{m_{\bar{x}y} m_z 2_{xy}}$. The index, point group, and polarization of the domain states (the magnetization is identically zero) are:

i	g_i	F_i	P_i	i	g_i	F_i	P_i
1	1	$\mathbf{m_{\bar{x}y} m_z 2_{xy}}$	(A,A,0)	7	m_{yz}	$\mathbf{m_y m_{xz} 2_{\bar{x}z}}$	(A,0,-A)
2	2_x	$\mathbf{m_{xy} m_z 2_{\bar{x}y}}$	(A,-A,0)	8	$m_{\bar{x}z}$	$\mathbf{m_x m_{\bar{y}z} 2_{yz}}$	(0,A,A)
3	2_y	$\mathbf{m_{xy} m_z 2_{\bar{x}y}}$	(-A,A,0)	9	$2_{\bar{y}z}$	$\mathbf{m_y m_{\bar{x}y} 2_{xz}}$	(-A,0,-A)
4	$\bar{1}$	$\mathbf{m_{\bar{x}y} m_z 2_{xy}}$	(-A,-A,0)	10	2_{xy}	$\mathbf{m_x m_{yz} 2_{\bar{y}z}}$	(0,-A,A)
5	$m_{\bar{y}z}$	$\mathbf{m_y m_{\bar{x}z} 2_{xz}}$	(A,0,A)	11	2_{yz}	$\mathbf{m_y m_{xz} 2_{\bar{x}z}}$	(-A,0,A)
6	m_{xy}	$\mathbf{m_x m_{yz} 2_{\bar{y}z}}$	(0,A,-A)	12	$2_{\bar{x}z}$	$\mathbf{m_x m_{\bar{y}z} 2_{yz}}$	(0,-A,-A)

In Figure 1 we show diagrammatically these polarizations as vectors within a cube.

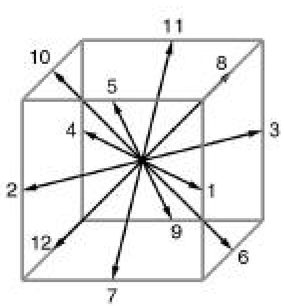


Figure 1: Polarization Indices

[4] Permutation of Domain States:

An element g of G permutes the domain states S_i , i = 1, 2, … , n. This is given in the notation:

$$\begin{pmatrix} S_1 & S_2 & . & . & S_i & . & . & S_n \\ gS_1 & gS_2 & . & . & gS_i & . & . & gS_n \end{pmatrix}$$

For $g = 3_{xyz}$ we have, listing only the indices of the domain states:

$$\begin{pmatrix} 01 & 02 & 03 & 04 & 05 & 06 & 07 & 08 & 09 & 10 & 11 & 12 \\ 08 & 06 & 10 & 12 & 01 & 11 & 03 & 05 & 04 & 07 & 02 & 09 \end{pmatrix}$$

[5] Subsets of Domain States:

Two (unordered) subsets of (distinct) domain states $\{S_1, S_2, \dots, S_m\}$ and $\{S'_1, S'_2, \dots, S'_{m'}\}$ are defined to be in the same class if $m = m'$ and there exists an element g of G such that:

$$g\{S_1, S_2, \dots, S_m\} \equiv \{gS_1, gS_2, \dots, gS_m\} = \{S'_1, S'_2, \dots, S'_m\}$$

For m = 2, there are four classes. Listing one representative subset from each class along with its symmetry group we have:

Subset	Symmetry	Subset	Symmetry
$\{S_1, S_2\}$	$\mathbf{m_y m_z 2_x}$	$\{S_1, S_5\}$	$\mathbf{m_{\bar{y}z}}$
$\{S_1, S_4\}$	$\mathbf{m_z m_{xy} m_{\bar{x}y}}$	$\{S_1, S_5\}$	$\mathbf{2_{\bar{y}z}}$

All subsets of a class can also be listed, for example, all subsets of the class with representative subset $\{S_1, S_4\}$ are:

Subset	Symmetry	Subset	Symmetry
$\{S_1, S_4\}$	$\mathbf{m_z m_{xy} m_{\bar{x}y}}$	$\{S_6, S_{10}\}$	$\mathbf{m_x m_{yz} m_{\bar{y}z}}$
$\{S_2, S_3\}$	$\mathbf{m_z m_{xy} m_{\bar{x}y}}$	$\{S_7, S_{11}\}$	$\mathbf{m_y m_{xz} m_{\bar{x}z}}$
$\{S_5, S_9\}$	$\mathbf{m_y m_{xz} m_{\bar{x}z}}$	$\{S_8, S_{12}\}$	$\mathbf{m_x m_{yz} m_{\bar{y}z}}$

One can also calculate the symmetry group of individual subsets of domain states.

[6] Polarizations:

One can list the polarizations of domain states in representative and arbitrary subsets of domain states and the average polarizations of subsets.

[7] Poling with an Electric Field:

Only some of the subsets of domain states can be obtained by poling with an electric field. This program calculates which of the subsets of domain states can be obtained by poling, and what is the poling direction. For m = 3 there is only a single representative subset which can be obtained by poling with an electric field, this is the representative subset $\{S_1, S_5, S_8\}$ and the poling direction is [1,1,1]. If there is no possible poling direction for a class representative subset, there is no possible poling direction for any subset of that class.

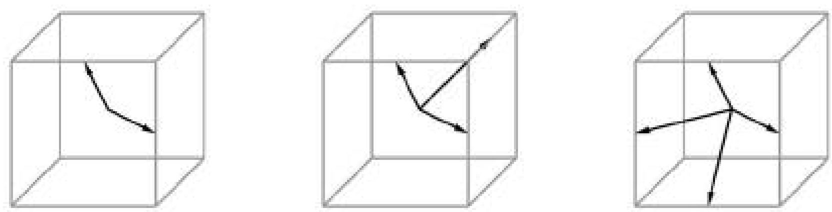
One can also calculate the poling direction for arbitrary subsets, e.g. the poling directions for all subsets of domain states in the class with representative subset $\{S_1, S_5, S_8\}$ are:

Subset	Poling Direction	Subset	Poling Direction
$\{S_1, S_5, S_8\}$	[1, 1, 1]	$\{S_1, S_6, S_7\}$	[1, 1,-1]
$\{S_2, S_5, S_{10}\}$	[1,-1, 1]	$\{S_2, S_7, S_{12}\}$	[1,-1,-1]
$\{S_3, S_6, S_9\}$	[-1, 1,-1]	$\{S_3, S_8, S_{11}\}$	[-1, 1, 1]
$\{S_4, S_9, S_{12}\}$	[-1,-1,-1]	$\{S_4, S_{10}, S_{11}\}$	[-1,-1, 1]

In this example of a phase transition from **G** = $\mathbf{m\bar{3}m}$ to **F** = $\mathbf{m_{\bar{x}y} m_z 2_{xy}}$ there are only three classes of subsets which can be obtained by poling with an electric field. The representative subsets of these classes and the poling directions are:

Representative subset	Poling Direction
{S_1, S_5}	[2,1,1]
{ S_1, S_5, S_8}	[1,1,1]
{ S_1, S_2, S_5, S_7}	[1,0,0]

and shown diagrammatically as:



For cases where the magnetization is not identically zero, one can also calculate magnetizations and poling with a magnetic field.

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