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Ferroelectric Domains,Tensor Pairs and Magnetoelectric Polarisability Properties of Single Ferrotroiodic Crystal

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Abstract

In this paper the Tensor components of the ferroelectric and Magneto electric polarisability for the ferrotroidic crystal $Pb(Mg_{1/3}Nb_{1/3})O_3$-$xPbTiO_3$ are calculated theoretically using group theoretical methods at the transition temperature 5^ok, where magnetite undergoes a first order metal _insulator transition, which lowers the crystallographic symmetry from cubic (m3m/Oh) to Rhombohedra($3m/C_{3v}$), again this crystal changed its structure into orthorhombic($mm2/C_{2v}$) or tetragonal structure($4mm/C_{4v}$) at certain temps.

Introductions

It is a well known that the "Group Theory" can be effectively employed to a variety of problems in physics and chemistry. Group theory plays a major role in the solution of solid-state physics problems. The concept of symmetry plays an important role in our physical environment. The symmetry of a molecule can be used to determine the various physical property of a crystal using group theoretical methods. The concept of Ferro-Magnetism, Ferro-Electricity and Ferro-Elasticity species was introduced by Aizu (1970). D.B.Litvin, V.Janovec, T.R. Wike and E. Dvorakova (1989) calculated coset and double coset decomposition for the 32 crystallographic point groups. Aizu, (1970 & 1974); Janovec (1972) made an analysis of domains of Ferroic crystals by using coset decomposition of point groups and space groups.

Ferro electricity is a phenomenon which was discovered in 1921. Ferro electricity has been also called Seignette electricity. As Seignette or Rochelle Salt (RS) was the first material found to show ferroelectric properties such as a spontaneous polarization on cooling below the Curie point, Ferroelectric domains and a Ferroelectric hysteresis loop. A huge leap in the research on ferroelectric materials came in the 1950's, leading to the widespread use of Barium titanate ($BaTiO_3$) based ceramics in capacitor applications and piezoelectric transducer devices. Since then, many other ferroelectric ceramics including lead titanate ($PbTiO_3$), lead Zirconate titanate (PZT), lead lanthanum Zirconate titanate (PLZT), and relaxor ferroelectrics like lead magnesium niobate (PMN) have been developed and utilized for a variety of applications. With the development of ceramic processing and thin film technology, many new applications have emerged. The biggest use of ferroelectric ceramics have been in the areas such as dielectric ceramics for capacitor applications, ferroelectric thin films for non volatile memories.

The present paper is based on group theoretical analysis of crystal structures. These crystals Pb ($Mg_{1/3}$ $Nb_{2/3}$) O_3-$xPbTiO_3$ [PMN-xPT] have attracted a huge amount of attention over the last decade. The above crystal under different phase transitions exhibits "gaint piezo-electric coefficients" and high Electromechanical coupling factors. Around 5k temperature, the phase transitions occurred in the crystal (Pb ($Mg_{1/3}$ $Nb_{2/3}$) O_3 –$xPbTiO_3$). i.e cubic structure (m3m (Oh group) prototypic point group) is changed into Rhombohedra structure (3m (C_{3v} group) Ferroic point group). Again this crystal changes it's structure into Ortho rhombic (mm2 (C_{2v} group) Ferroic point group) or tetragonal structure (4mm (C_{4v} group) Ferroic point group) at different temperatures. In this way the crystal exhibits Ferro-electric, Ferro-elastic and magneto electric polarizability. Ferro-electric, Ferro-elastic and magneto-electric polarizability domain pairs and tensor pairs are calculated using coset decomposition and double coset decomposition respectively for the crystals Pb ($Mg_{1/3}$ $Nb_{2/3}$)O_3 –$xPbTiO_3$. While considering Ferro-electric & Ferro-elastic properties only ordinary 32 point group m3m is considered as prototypic point group, since they are non-magnetic properties. In case of magneto electric polarizability, grey group $m3m1^1$ is taken as prototypic point group.

Many piezoelectric (including ferroelectric) ceramics such as Barium Titanate ($BaTiO_3$), Lead Titanate ($PbTiO_3$), Lead Zirconate Titanate (PZT), Lead Lanthanum Zirconate Titanate (PLZT), Lead Magnesium Niobate (PMN), Potassium Niobate ($KNbO_3$), Potassium Sodium Niobate ($K_xNa_{1-x}NbO_3$), and Potassium Tantalite Niobate (K (Ta_xNb_{1-x}) O_3) have a Perovskites type structure. Lead titanate is a ferroelectric material having a structure similar to $BaTiO_3$ with a high Curie point (490^0 C). On decreasing the temperature through the Curie point a phase transition from the par electric cubic phase to the ferroelectric tetragonal phase takes place. Relaxor ferroelectrics are a class of lead based Perovskite type compounds with the general formula $Pb(B_1,B_2)O_3$ where B_1 is a lower valency cation (like Mg^{2+}, Zn^{2+}, Ni^{2+}, Fe^{3+}) and B_2 is a higher valence cation (like Nb^{5+}, Ta^{5+}, W^{5+}). Pure lead magnesium niobate (PMN or Pb ($Mg_{1/3}Nb_{2/3}$) O_3) is a representative of this class of materials

with a Curie point at -10^0 C. Relaxor ferroelectrics like PMN can be distinguished from normal ferroelectrics such as $BaTiO_3$ and PZT, by the presence of a broad diffused and dispersive phase transition on cooling below the Curie point..

Ferro electrics are materials which posses a spontaneous electric polarization (Ps) and its direction can be reversed by applying a suitable electric field (E). In which the magnetization (I) may be reversed by a magnetic field (H). But in Ferro electric crystals no spontaneous magnetization or iron present. The significant characteristic of Ferro electrics is dielectric non-linearity.

Where the +ve and –ve signs are to be taken accordingly as the symmetry operation R is a pure rotation or a rotation reflection (Bhagavantham S. and Venkata Rayudu. T.V., 1962).

The phenomenon of magneto electric polarizability is the production of a magnetic field $\hat{H}$ (or $\bar{E}$) on the application of an electric field $\bar{E}$ (or $\hat{H}$) in a direction normal to it. Following a suggestion of Landau and Lifshitz (1960) had shown that this effect is likely to appear in crystals possessing magnetic structures. Its actual occurrence has been Verified in the trioxides of chromium (Astrov, 1960) and Titanium (AL'Shin and Astrov, 1963) in their anti-ferromagnetic state. $\bar{E}$ and $\hat{H}$ connected by the relation

$$\mathbf{H_i = \Sigma_j \chi_{ij} E_j \ (i, j = 1, 2, 3)}$$

Where χ_{ij} is represents a magneto electric polarizability tensor. Since $\bar{E}$ is polar vector and $\hat{H}$ is an axial vector, χ is a second rank tensor whose transformation law is the same as the product of the representations of $\bar{E}$ and $\hat{H}$. Thus, the character χ_ρ (R_φ); corresponding to a symmetry element R_φ in this representation, is

$$\mathbf{\chi_\rho\ (R_\varphi) = (1 \pm 2\cos\varphi)(\ 2\cos\varphi \pm 1)}$$

Where the +ve and –ve signs are to be taken accordingly as the symmetry operation R is a pure rotation or a rotation reflection.

Two domain states that have different spontaneous magnetization vector are denoted as a Ferro-Magnetic domain pairs. Consider a phase transition between phases of symmetry G and F. The crystal splits into $n = \left|\mathbf{G}\right| / \left|\mathbf{H}\right|$ single domain states denoted by $\mathbf{S_1, S_2 \ldots S_n}$. Let $\mathbf{S_i}$ and $\mathbf{S_j}$ be two arbitrary orientation states of Ferroic crystals. They are identical or an antimorphism in structure. For the given group G and subgroup F one writes the left coset decomposition of G with respect to F symbolically as

$$\mathbf{G = F + g_1F + g_2F + \ldots + g_nF}$$

Where $\mathbf{g_iF,\ i = 1, 2, 3\ldots\ n}$ denotes the subset of elements of G, which is obtained by multiplying each element of the subgroup F from the left by the elements g_i of G. Each subset of elements of $\mathbf{g_iF,\ i = 1, 2\ldots n}$ of G are called left coset representatives of the left coset decomposition of G with respect to F (V. Janovec, 1989). Two domain states S_i and S_j form a domain pair (S_i,S_j) if $\mathbf{S_j = g_{ij}S_j}$ where $\mathbf{g_{ij}}$ is element of G. Here we calculated domain pairs of "Ferro electric, Ferro elastic and Magneto-electric polarizability for the Ferroic species" by using coset decomposition.

Let G be the prototypic point group, H is the Ferroic point group and T is the specific form of the physical property tensor T that keeps H invariant. The number N of crystallographically equivalent ordered distinct tensor pair classes is equal to the number of double cosets in the double coset decomposition of G with respect to $\mathbf{G_T}$.

$$\mathbf{G = G_T E G_T + G_T g_1 G_T + \ldots\ldots\ldots + G_T g_N G_T}$$

Where G_T is the stabilizer of T in G and g_k, k = 1, 2…N are the double coset representatives. Tables of the coset and double coset decomposition of the 32 crystallographic point groups with respect to one of each set of conjugate sub groups were given by Janovec and Dvorakova (1974).

Procedure:

FERRO-ELECTRIC DOMAIN PAIRS FOR Pb ($Mg_{1/3}$ $Nb_{2/3}$) O_3 – x$PbTiO_3$ IN THE STATE m3m F 3m:

Consider the ferroic specied m3m F 3m where m3m is a prototypic point group and 3m is a ferroic point group. The number of distinct domain pair classes is 4. The coset decompostion of m3m with respect to the group 3m is given by G = m3m = E (3m) + C_{2x} (3m) + C^+_{33}(3m) +σ_x (3m) + S^-_{61} (3m) + S^+_{64} (3m) + S^-_{4x} (3m) + C^+_{4x} (3m). The coset elements g_i's are E, C_{2x}, C^+_{33}, σ_x, S^-_{61}, S^+_{64}, S^-_{4x} and C^+_{4x}.

Now let $S_i = C^+_{33}(3m)$, $g_{ij} = S^-_{62}$ and $S_j = S^+_{64}$ (3m), then we have $S_i = g_{ij}Sj$ and

$Sj = g_{ij}S_j$ i.e., $C^+_{33}(3m) = S^-_{62}$ (S^-_{64} (3m)) and S^-_{64} (3m) = S^-_{62} ($C^+_{33}(3m)$) .

Hence, ($C^+_{33}(3m)$, $S^+_{64}(3m)$) forms a domain pair, instead of writing this we represent domain pair as (C^+_{33}, S^+_{64}). Similarly the remaining domain pair of

G = m3m are (E, C_{2x}), (S^-_{61}, σ_x), (C^+_{33}, S^+_{64}).and (C^+_{4X}, S^-_{4X})

Table: Ferroelectric Domain pairs for ferroic species m3m F 3m

Domain pair representatives	Domain Pairs
(E, C_{2x})	$((x+y+z)/3, (x-y-z)/3)$
(S^{-}_{61}, σ_x)	$((-z-x-y)/3, (-x+y+z)/3)$
(C^{+}_{33}, S^{+}_{64}).	$((-z-x+y)/3, (y+z-x)/3)$
(C^{+}_{4x}, S^{-}_{4x})	$((x-z+y)/3, (-x+z-y)/3)$

FERRO-ELASTIC TENSOR PAIRS FOR $Pb(Mg_{1/3} Nb_{2/3}) O_3 - xPbTiO_3$ IN THE STATE m3m F 3m:

Consider the ferroic species m3m F 3m, where m3m is a prototypic point group and 3m is a ferroic point group and the stabilizer G_T also 3m. The number of distinct tensor pair classes is 4. The double coset decomposition of m3m with respect to the stabilizer is also 3m is given by

$G = m3m = (3m) E (3m) + (3m) C_{2x} (3m) + (3m) S^{-}_{61} (3m) + (3m) C^{+}_{4x} (3m)$.

Table: Ferro-electric Tensor pairs for ferroic species m3m F 3m

Double coset Representations	Tensor Pairs	
(a)	*(b)*	*(c)*
E	$(x+y+z)/3$	$(x+y+z)/3$
C_{2x}	$(x+y+z)/3$	$(x-y-z)/3$
S^{-}_{61}	$(x+y+z)/3$	$(-z-x-y)/3$
C^{+}_{4x}	$(x+y+z)/3$	$(x-z+y)/3$

THE MEP DOMAIN PAIRS FOR $Pb (Mg_{1/3} Nb_{2/3}) O_3 - xPbTiO_3$ IN THE STATE $m3m1^{'}$ Fmm2:

Consider the Ferroic $m3m1^{'}$ F mm2 where $m3m1^{'}$ is a prototypic point group and mm2 is a ferroic point group. The number of distinct domain pair classes is 12. The coset decomposition of $m3m1^{'}$ with respect to the group mm2 is given by

$G = m3m1^{I} = E (mm2) + R_2 (mm2) + C_{2x} (mm2) + R_2C_{2x} (mm2) + C^{+}_{31} (mm2) + R_2C^{+}_{31} (mm2) + S^{-}_{61} (mm2) + R_2S^{-}_{61} (mm2) + C^{-}_{31} (mm2) + R_2C^{-}_{31} (mm2) + S^{+}_{61} (mm2) + R_2S^{+}_{61} (mm2) + C^{+}_{4x} (mm2) + R_2C^{+}_{4x} (mm2) + C^{-}_{4x} (mm2) + R_2C^{-}_{4x} (mm2) + C_{2a} (mm2) + R_2C_{2a} (mm2) + \sigma_{da} (mm2) + R_2\sigma_{da} (mm2) + S^{-}_{4y} (mm2) + R_2S^{-}_{4y} (mm2) + S^{+}_{4y} (mm2) + R_2S^{+}_{4y} (mm2)$.

The coset elements g_i's are $E, R_2, C_{2x}, R_2C_{2x}, C^{+}_{31}, R_2C^{+}_{31}, S^{-}_{61}, R_2S^{-}_{61}, C^{-}_{31}, R_2C^{-}_{31}, S^{+}_{61}, R_2S^{+}_{61}, C^{+}_{4x}, R_2C^{+}_{4x}, C^{-}_{4x}, R_2C^{-}_{4x}, C_{2a}, R_2C_{2a}, \sigma_{da}, R_2\sigma_{da}, S^{-}_{4y}, R_2S^{-}_{4y}, S^{+}_{4y}, R_2S^{-}_{4y}$.

The domain pair classes are (E, R_2), $(C2x, R_2C_{2x})$, $(C^{+}_{31}, R_2C^{+}_{31})$, $(C^{-}_{31}, R_2C^{-}_{31})$, $(S^{-}_{61}, R_2S^{-}_{61})$, $(S^{+}_{61}, R_2S^{+}_{61})$, $(C^{+}_{4x}, R_2C^{+}_{4x})$, $(C^{-}_{4x}, R_2C^{-}_{4x})$, (C_{2a}, R_2C_{2a}), $(\sigma_{da}, R_2\sigma_{da})$, $(S^{-}_{4y}, R_2S^{-}_{4y})$, $(S^{+}_{4y}, R_2S^{-}_{4y})$.

Table: The MEP Domain pairs for ferroic species m3m F mm2

Domain pair representatives	Domain pairs	
(E, R_2)	$(xy^{'},yx^{'})$	$(-xy^{'},-yx^{'})$
(C_{2x}, R_2C_{2x})	$(-xy^{'},-yx^{'})$	$(xy^{'},yx^{'})$
$(C^{+}_{31}, R_2C^{+}_{31})$	$(zx^{'}, xz^{'})$	$(-zx^{'}, -xz^{'})$
$(C^{-}_{31}, R_2C^{-}_{31})$	$(yz^{'},zy^{'})$	$(-yz^{'},-zy^{'})$
$(S^{-}_{61}, R_2S^{-}_{61})$	$(-zx^{'},-xz^{'})$	$(zx^{'},xz^{'})$
$(S^{+}_{61}, R_2S^{+}_{61})$	$(-yz^{'},-zy^{'})$	$(yz^{'},zy^{'})$
$(C^{+}_{4x}, R_2C^{+}_{4x})$	$(-xz^{'},-zx^{'})$	$(xz^{'},zx^{'})$
$(C^{-}_{4x}, R_2C^{-}_{4x})$	$(xz^{'},zx^{'})$	$(-xz^{'},-zx^{'})$
(C_{2a}, R_2C_{2a})	$(yx^{'},xy^{'})$	$(-yx^{'},-xy^{'})$
$(\sigma_{da}, R_2\sigma_{da})$	$(-yx^{'},-xy^{'})$	$(yx^{'},xy^{'})$
$(S^{-}_{4y}, R_2S^{-}_{4y})$	$(-zy^{'},-yz^{'})$	$(zy^{'},yz^{'})$
$(S^{+}_{4y}, R_2S^{-}_{4y})$	$(zy^{'},yz^{'})$	$(-zy^{'},-yz^{'})$

THE MEP TENSOR PAIRS FOR Pb ($Mg_{1/3}$ $Nb_{2/3}$) O_3 –x$PbTiO_3$ IN THE STATE OF m3m1^1 F mm2:

Consider the ferroic species m3m1^1 F mm2, where m3m is a prototypic point group and mm2 is a ferroic point group and the stabilizer G_T is $4/m^1m^1m^1$. The number of distinct tensor pair classes is 6. The double coset decomposition of m3m with respect to the stabilizer $4/m^1m^1m^1$ is given by

$G = m3m = (4/m^1m^1m^1)\ E\ (4/m^1m^1m^1) + (4/m^1m^1m^1)\ R_2\ (4/m^1m^1m^1) + (4/m^1m^1m^1)\ S^-_{4y}\ (4/m^1m^1m^1) + (4/m^1m^1m^1)\ R_2S^-_{4y}\ (4/m^1m^1m^1) + (4/m^1m^1m^1)\ S^+_{4y}\ (4/m^1m^1m^1) + (4/m^1m^1m^1)\ R_2S^+_{4y}\ (4/m^1m^1m^1)$.

Table: **The MEP Tensor pairs for Ferroic species m3m1^1 F mm2**

Double coset representatives	**Tensor pairs**	
(a)	*(b)*	*(c)*
E	(xy^1,yx^1)	(xy^1,yx^1)
R_2	(xy^1,yx^1)	$(-xy^1,-yx^1)$
S^-_{4y}	(xy^1,yx^1)	$(-zy^1,-yz^1)$
$R_2S^-_{4y}$	(xy^1,yx^1)	(zy^1,yz^1)
S^+_{4y}	(xy^1,yx^1)	(zy^1,yz^1)
$R_2S^+_{4y}$	(xy^1,yx^1)	$(-zy^1,-yz^1)$

Conclusion

Ferro electric and Magneto Electric polarizability properties of Lead Magnesium (Pb ($Mg_{1/3}$ $Nb_{2/3}$) O_3, PMN) Lead Titanate ($PbTiO_3$, PT) were discussed in various structural transitions. By using Group theoretical techniques both Domain pairs and Tensor pairs calculated for these Ferroic & Magnetic properties in crystal. Actually these materials exhibits a gaint electromechanical response, that is used in ultrasonic (Uchino, K. Piezoelectric Actuators and Ultrasonic Motors (Kluwer Academic,Boston, 1996). and medical applications, as well as in telecommunications. These Properties make them very attractive for next generation Sensors and Actuators.

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