Ferro electric, ferro elastic & magneto electric polarizability
domain and tensor pairs of magnetite (Fe$_3$O$_4$)

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Abstract: The present work is based on group theoretic analysis of crystal structures. Group theory can be employed to a variety of problems in physics and chemistry. It 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 various physical properties of a crystal using group theoretical methods. The applications of magneto-electric devices lie in the regions of millimeter and sub-millimeter wavelengths and in the areas of reducing electrical conductivity, improving dielectric magnetic or magneto-electric properties by solid solutions improving optical quality and obtaining larger crystals. Ferro-electric, Ferro-elastic and magneto-electric polarized domain pairs and tensor pairs are calculated using coset decomposition and double coset decomposition respectively for the crystal magnetite (Fe$_3$O$_4$). While considering Ferro-electric and Ferro-elastic properties only ordinary point group m$_3$m is considered as prototypic point group since they are non-magnetic properties. In case of magneto-electric polarizability grey group m$_3$m$_1$ is taken as prototypic point group.

Keywords: Coset, Double coset, Domain pairs, Tensor pairs, Magnetite.

1. Introduction

Magnetite was the first magnetic material to be discovered and utilized. It still has wide spread usage in modern society as it is a rather strong permanent ferrimagnet (T$_c$ =858 K) [19]. It exhibits a metal-non metal transition at a ~120°C. Above this temperature it has the cubic inverse spinel structure. At 120°C a phase transition to a slight orthorhombic distortion occurs. Verwey’s transition temperature T$_v$ [16] magnetic adopts a cubic inverse spinel structure with fd$_3$m space group. They are two different iron symmetry sites labeled A and B. The two A sites reside in the tetrahedral coordinated oxygen intensities. The four B sites have octahedral coordination. The magnetic structure is a collinear ferri-magnet with A and B moments aligned anti parallel. From Figure 1, it is noticed that at 123°C magnetite undergoes a first order metal insulator transition, the transition which lowers the crystallographic symmetry from cubic to monoclinic. Ignoring the small monoclinic distortion, the low temperature structure can also be described in a slight less orthorhombic structure in the pmca space group. Here the phase transitions for the inverse spinel Fe$_3$O$_4$ from the high order cubic symmetry to the lower orthorhombic symmetry below 123°C and the domain orientations are calculated theoretically using the group theory.
Ferro electrics are materials which possess a spontaneous electric polarization \( P_s \) and its direction can be reversed by applying a suitable electric field \( E \). In many ways these materials are electrical analogues of ferromagnetics, in which the magnetization \( I \) may be reversed by a magnetic field \( H \). But in ferro electric crystals no spontaneous magnetization or iron present. Examples for ferro electric crystals are Barium titanate (BaTiO₃), Barium strontium titanate (BST) & Lead zirconate titanate (PZT). The materials exhibit interesting electrical properties, the binding forces in many solid materials are largely electric and ferro electrics may show up these forces in exaggerated fashion. Most ferro electrics cease to be ferro electric above a temperature known as the transition temperature. The significant characteristic of ferro electrics is dielectric non-linearity. It is represented by the polar vector with the character 

\[
\chi(\varphi) = 2 \cos \varphi \pm 1
\]

the +ve and -ve signs are taken according to the symmetry operation \( R \), which is a pure rotation reflection [5]. The ferro-elastic behavior can be understood in a simple way by going back to the case of spontaneous distortion of a square to a rectangle. The rectangle has spontaneous strain (that is strain occurring without the application of any mechanical stress) with respect to the square. Ferro elastic property is represented by symmetrical stress tensor with the character 

\[
\chi(\varphi) = 4 \cos^2 \varphi \pm 2 \cos \varphi
\]

where the +ve and -ve signs are to be taken accordingly as the symmetry operation \( R \) is a pure rotation or a rotation reflection [5]. In the present work, we discussed the properties ferro-electric, ferro-elastic and magneto electric polarizability of Magnetite (Fe₃O₄).

The phenomenon of magneto electric polarizability is the production of magnetic field \( \vec{H} \) (or \( \vec{E} \)) on the application of an electric field \( \vec{E} \) (or \( \vec{H} \)) in directions normal to it. Following a suggestion of Landau and Lifshitz [8] had shown that this effect is likely to appear in crystals processing magnetic structures. Its actual occurrence has been verified in the trioxides of Chromium [3] and Titanium [3] in their anti-ferromagnetic state. \( \vec{E} \) and \( \vec{H} \) are connected by the relation

\[
\sum_{ij} x_{ij} E_i = H_j
\]

where \( x_{ij} \) is a magneto electric polarizability tensor. Since \( \vec{E} \) is a polar vector and \( \vec{H} \) in an axial vector, \( \chi \) is a second rank tensor whose transformation law is the same as the product of the representations of \( \vec{E} \) and \( \vec{H} \). Thus, the character \( \chi(R_\theta) \); corresponding to a symmetry elementary \( R_\theta \) in the representation is \( \chi(R_\theta) = (1 \pm 2 \cos \phi)(2 \cos \phi \pm 1) \) where +v end –ve signs are to be taken accordingly as he symmetry operation \( R \) is a pure rotation or rotation reflection.

A ferroic crystal contains two or more equally stable domains of the same structure but different spatial orientation. These domains can coexist in a crystal and may be distinguished by the values of components of certain macroscopic tensorial physical properties of the domain [1,14&17]. Aizu [1] has given tensorial classification of ferroic crystals based on a rank one physical property tensors ability to distinguish some or all the domains. This method was extended by Litvin [9] to an arbitrary physical property tensor and used to determine the tensorial classification of non-magnetic crystals for all physical property tensors of rank less than or equal to four [10]. A vast amount of literature exists on the derivation of physical property tensor invariant under the crystallographic point groups [15, 6 & 18]. Litvin and Litvin [12] has tabulated the representative tensor pairs for all 32 point groups \( G \), subgroups \( H \) and all physical property tensors \( T \) of rank 0,1 and 2. This constitutes the basics for the tensorial classification of domain pairs in ferroic crystals using group theoretical classification of the corresponding physical property of tensor property of tensor pairs. Here the magneto electric polarizability tensor pairs are calculated using double coset decomposition for the crystal Fe₃O₄ taking grey group m3m1 as prototypic point group. Using Aizu [1] we have calculated domain pairs and tensor pairs for the three properties ferro-electric, ferro-elastic & magneto electric polarizability of the material Magnetite (Fe₃O₄).
2. Mathematical formulation

2.1. Ferro-Electric Domain Pairs for Fe₃O₄ ferroic species m₃m F mm2
Consider the ferroic species m₃m F mm2 where m₃m is a prototypic point group and mm2 is a ferroic point group. The number of distinct domain pair classes is 6. The coset decomposition of m₃m with respect to the group mm2 is given by G=m₃m=E(mm2) +C₂ₓ (mm2) +C⁺₃₁ (mm2) +C⁻₃₁ (mm2) +C₂₄ (mm2) +C⁺₄₄ (mm2) +C⁻₄₄ (mm2) +S⁺₆₁ (mm2) +S⁻₆₁ (mm2) +σ₆₆ (mm2) +C₂₅ (mm2) +C₂₆ (mm2). The coset elements gᵢ’s are E, C₂ₓ, C⁺₃₁, C⁻₃₁, C₂₄, C⁺₄₄, C⁻₄₄, S⁺₆₁, S⁻₆₁, σ₆₆, C₂₅ & C₂₆.

Now let Sᵢ=C⁻₃₁ (mm2), gᵢ=C₂ₓ and Sᵢ=S⁺₆₁ (mm2), then we have Sᵢ=gᵢSᵢ & Sᵢ=gᵢSᵢ i.e. C⁻₃₁ (mm2) =C₂ₓ (S⁺₆₁ (mm2)). Hence (C⁻₃₁ (mm2), S⁺₆₁ (mm2)) forms a domain pair, instead of writing this we represent domain pair as (C⁻₃₁ , S⁺₆₁), similarly the remaining domain pairs of G = m₃m are given in the table 1.

| Domain Pairs | Domain Pairs |
|--------------|--------------|
| (E, C₂ₓ)     | (0, 0, z), (0, 0, -z) |
| (C⁺₃₁ , S⁻₆₁) | (z, 0, 0), (-z, 0, 0) |
| (C⁺₄₄ , C⁻₄₄) | (0, -z, 0), (0, z, 0) |
| (C⁻₃₁ , S⁺₆₁) | (0, z, 0), (0, -z, 0) |
| (C₂₅ , σ₆₆) | (z, 0, 0), (-z, 0, 0) |
| (C₂₆) | (0, 0, -z), (0, 0, z) |

2.2. Ferro-Electric Tensor Pairs for Fe₃O₄ ferroic species m₃m F mm2
Consider the ferroic species m₃m F mm2 where m₃m is a prototypic point group and mm2 is a ferroic point group and the stabilizer Gₗ is 4mm. The numbers of distinct tensor pair classes are 3. The double coset decomposition of m₃m with respect to the stabilizer 4mm is given by G=m₃m= (4mm)E(4mm) + (4mm)C₂ₓ(4mm) + (4mm) C⁺₃₁ (4mm).
Table 2: Tensor pairs for ferroic species m3m Fmm2

| Double coset representatives | Tensor pairs |
|-----------------------------|-------------|
| (a)                         | (b)         |
| E                           | (0, 0, z)   |
| C2x                         | (0, 0, z)   |
| C+31                        | (0, 0, z)   |

2.3. Ferro-Elastic Domain Pairs for Fe3O4 ferroic species m3m Fmm2

Consider the ferroic species m3m F mm2 where m3m is a prototypic point group and mm2 is a ferroic point group. The number of distinct domain pair classes is 6. The coset decomposition of m3m with respect to the group mm2 is given by G=m3m= E(mm2) +C2x (mm2) +C+31 (mm2) +C−31 (mm2) +C2a (mm2) +C4x (mm2) C−4x (mm2) +S−61 (mm2) +S+61 (mm2) +σda (mm2) +C2c (mm2) +C2e (mm2). The coset elements g,i’s are E, C2x, C+31, C−31, C2a, C+4x, C−4x, S−61, S+61, σda, C2c & C2e.

Now let S1=C2a(mm2), g1=I and S2=σda(mm2), then we have S1=g1S1 and S2=σda i.e. C2a(mm2)=I (σda(mm2)). Hence (C2a(mm2),σda(mm2)) forms a domain pair, instead of writing this we represent domain pair as (C2a,σda), similarly the remaining domain pairs of G = m3m are mentioned in the table 3.

Table 3: Domain pairs for ferroic species m3m F mm2

| Domain Pairs |
|--------------|
| (E, C2a)     |
| (C+31, S−61) |
| (C+31, S+61) |
| (C2a, σda)   |
| (C4x, C−4x)  |
| (C2c, C2e)   |

2.4. Ferro-Elastic Tensor Pairs for Fe3O4 ferroic species m3m F mm2

Consider the ferroic species m3m F mm2 where m3m is a prototypic point group and mm2 is a ferroic point group and the stabilizer G_T is mmm. The numbers of distinct tensor pair classes are 6. The double coset decomposition of m3m with respect to the stabilizer mmm is given by G=m3m=(mmm)E (mmm)+(mmm)C+31 (mmm)+(mmm)C−31 (mmm)+(mmm)C4x (mmm)+(mmm)C−4x (mmm)+(mmm)C2a(mmm)+(mmm)σda(mmm).

Table 4: Tensor pairs for ferroic species m3m F mm2

| Double coset representatives | Tensor pairs |
|-----------------------------|-------------|
| (a)                         | (b)         |
| E                           | (xx, yy, zz)|
| C+31                        | (xx, yy, zz)|

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double coset decomposition of $m_3m_1$ with respect to the stabilizer $4/m\bar{1}m\bar{1}m\bar{1}$ is given by $G = m_3m = \sigma_{31}(mm2)+R_2C_{2c}(mm2)+C_{2a}(mm2)+R_2C_{2d}(mm2)+\sigma_{dc}(mm2)+R_2C_{2e}(mm2)$.

Consider the ferroic species $m_3m_1F$ mm2 where $m_3m_1$ is a prototypic point group and mm2 is a ferroic point group. The number of distinct tensor pair classes is 6. The coset decomposition of $m_3m_1$ with respect to the group mm2 is given by $G=m_3m_1¹=E(mm2)+R_2C_{2e}(mm2)+R_2C_{2c}(mm2)+C_{2a}(mm2)+R_2C_{2d}(mm2)+\sigma_{dc}(mm2)+R_2C_{2e}(mm2)$.

The coset elements $g_i's$ are $E, R_2, C_{2a}, C_{31}, R_2C_{31}', C_{31}, R_2C_{31}', C_{31}, R_2C_{31}'$, $C_{31}, R_2C_{31}'$ respectively.

Table 5: Domain pairs for ferroic species $m_3m_1 F$ mm2

| Domain Pairs | Tensor Pairs |
|--------------|-------------|
| $(E, R_2)$   | $(xy^', yx^')$, $(-xy^', -yx^')$ |
| $(C_{2a}, R_2C_{2a})$ | $(-xy^', -yx^')$, $(xy^', yx^')$ |
| $(C_{31}, R_2C_{31}')$ | $(zx^', xz^')$, $(-zx^', -xz^')$ |
| $(C_{4a}, R_2C_{4a})$ | $(-yz^', -zy^')$, $(yz^', zy^')$ |
| $(C_{4a}, R_2C_{4a})$ | $(-yz^', -zy^')$, $(yz^', zy^')$ |
| $(S_{61}, R_2S_{61})$ | $(-zx^', -xz^')$, $(zx^', xz^')$ |
| $(S_{61}', R_2S_{61}')$ | $(-yz^', -zy^')$, $(yz^', zy^')$ |
| $(\sigma_{dc}, R_2\sigma_{dc})$ | $(-yx^', -xy^')$, $(yx^', xy^')$ |
| $(C_{2a}, R_2C_{2a})$ | $(-zy^', -yz^')$, $(zy^', yz^')$ |
| $(C_{2a}, R_2C_{2a})$ | $(-zy^', -yz^')$, $(zy^', yz^')$ |

2.5. Magneto-Electric Polarizability Domain Pair for Fe$_3$O$_4$ ferroic species $m_3m_1F$ mm2

2.6. Magneto-Electric Polarizability Tensor Pairs for Fe$_3$O$_4$ ferroic species $m_3m_1F$ mm2
\[ m¹ \] + (4/m¹m¹m¹)R₂C₂c(4/m¹m¹m¹) + (4/m¹m¹m¹)R₂C₂d (4/m¹m¹m¹).

### Table 6: Tensor pairs for ferroic species m3m1 F mm2

| Double coset representatives | Tensor Pairs |
|------------------------------|--------------|
| (a)                          | (b)          | (c)          |
| E                            | (xy¹, xy¹)   | (xy¹, xy¹)   |
| R₂                           | (xy¹, xy¹)   | (-xy¹, -yx¹) |
| C₂c                          | (xy¹, xy¹)   | (-zy¹, -yz¹) |
| C₂d                          | (xy¹, xy¹)   | (-xz¹, -zx¹) |
| R₂C₂c                        | (xy¹, xy¹)   | (zy¹, yz¹)   |
| R₂C₂d                        | (xy¹, xy¹)   | (xz¹, zx¹)   |

### 3. Conclusions

In this paper, ferro electric, ferro elastic and magneto-electric polarizability of the Magnetite (Fe₃O₄) material are discussed. From these properties domain pairs and tensor pairs are calculated for Magnetite using group theoretical techniques. While considering ferro electric & ferro elastic properties only ordinary point group m3m is considered as prototypic point group because of non-magnetic properties. In case of magneto-electric polarizability grey group m3m1¹ is taken as prototypic point group. From these results we conclude that these studies will be applicable to ferro electric thin films in computer for making DRAM (Dynamic random access memory).

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