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Tensor component distinction of magnetic non-ferroelastic domain pairs

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Global tensor distinction considers whether or not a physical property tensor can distinguish among all domains that arise in a phase transition. Domain pair tensor distinction considers whether or not a property tensor can distinguish between a pair of domains. To determine how switching of a pair of domains may be accomplished requires in addition tensor component distinction, i.e. the determination of which components of a property tensor distinguish the two domains. These tensor component distinctions are necessary but not sufficient conditions for switching. Here, we consider all magnetic non-ferroelastic domain pairs and determine the tensor component distinction for each for a wide variety of physical property tensors.

Keywords: tensor distinction; tensor components; domains; switching

1. Introduction

Switching between domains is determined by the differences in the components of physical property tensors in the domains [1,2]. The difference $\Delta G$ in free energy of two domain states is the driving potential of domain switching. To second order in external fields, $\Delta G$ is given by

$$
\Delta G = \Delta P_{(s)i}E_i + \Delta M_{(s)i}H_i + \Delta \varepsilon_{(s)ij}\sigma_{ij} + \Delta T_{(s)i}S_i + \frac{1}{2}\Delta \kappa_{ij}E_iE_j + \frac{1}{2}\Delta \chi_{ij}H_iH_j + \frac{1}{2}\Delta \sigma_{ijk}\sigma_{ijkl} + \frac{1}{2}\Delta \tau_{ij}S_iS_j + \Delta \sigma_{ij}H_i\sigma_{jk} + \Delta \sigma_{ij}H_i\sigma_{jk} + \Delta \alpha_{ij}H_iE_j + \Delta \eta_{ij}S_i\sigma_{jk} + \Delta \xi_{ij}H_iS_j + \Delta \theta_{ij}E_iS_j + \text{higher order terms}
$$

(1)

$\Delta (\text{Physical Property})_{ij}$ represents the differences in the components of a physical property tensor in a pair of domains, e.g. $\Delta P_{(s)i}$, $\Delta M_{(s)i}$, $\Delta \varepsilon_{(s)ij}$ and $\Delta T_{(s)i}$ represent, respectively, the differences in the components of the spontaneous polarization, magnetization, strain and toroidal moment. In Table 1, we list the nomenclature of the physical property tensors associated with the free-energy terms given above along with the nomenclature of the type of ferroic domains which are distinguished by that physical property. The Jahn [3] notation of the physical property tensors is also given. $E_i$, $H_i$, $\sigma_{ij}$ and $S_i$ are, respectively, the components of the external electric field, magnetic field, stress, and $S_i \sim (E \times H)_i$ [4].

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As an example of switching [5,6], consider the form of the electric susceptibility tensor of a domain invariant under the point group \(2\) and in a second domain related to the first by the mirror plane \(m_x\), these two tensors are
\[
\begin{pmatrix}
\kappa_{xx} & \kappa_{xy} & 0 \\
\kappa_{xy} & \kappa_{yy} & 0 \\
0 & 0 & \kappa_{zz}
\end{pmatrix}
\quad \text{and} \quad
\begin{pmatrix}
\kappa_{xx} & -\kappa_{xy} & 0 \\
-\kappa_{xy} & \kappa_{yy} & 0 \\
0 & 0 & \kappa_{zz}
\end{pmatrix}.
\]
Consequently,
\[
\Delta \kappa_{ij} = \begin{pmatrix}
0 & 2\kappa_{xy} & 0 \\
2\kappa_{xy} & 0 & 0 \\
0 & 0 & 0
\end{pmatrix}
\]
and \(\Delta G = \cdots + 2\kappa_{xy}E_xE_y \cdots\), the domains are ferrobielectric and can be switched with crossed electric fields.

2. Non-ferroelastic twin laws
Consider a phase transition between phases of point group symmetry \(G\) and \(F\). The crystal splits into \(n = |G|/|F|\) single domain states denoted by \(S_1, S_2, \ldots, S_n\). Writing the coset decomposition of \(G\) with respect to \(F\) as \(G = F + g_2F + \cdots + g_nF\), we have \(S_i = g_iS_1\), \(i = 1, 2, \ldots, n\), i.e. the orientation of the \(i\)-th domain \(S_i\) is related to the orientation of domain \(S_1\) by the element \(g_i\) of the coset decomposition, and \(F_i = g_iF_1g_i^{-1}\) is the symmetry group of the \(i\)-th domain.

A domain pair is denoted by \((S_i, S_k)\) with \(S_k = g_kS_i\) where \(g_{ik} = g_kg_i^{-1}\), the operation \(g_{ik}\) transforms the domain state \(S_i\) into the domain state \(S_k\). The twin law \(J_{ik}\) of a domain pair \((S_i, S_k)\) is defined [7] as
\[
J_{ik} = (F_i \cap F_k) + g_{ik}^* (F_i \cap F_k)
\]
where $g^*_{ik}$ is an element that interchanges the two domains, i.e., $g^*_{ik}S_i = S_k$ and $g^*_{ik}S_k = S_i$, the operation $g^*_{ik}$ simultaneously transforms the domain state $S_i$ into domain state $S_k$ and the domain state $S_k$ into the domain state $S_i$. A twin law describes the symmetry of a domain pair: $F_i \cap F_k$ is the group that simultaneously leaves each domain invariant and $g^*_{ik}(F_i \cap F_k)$ a set of elements that interexchanges the two domains.

The two domains in a non-ferroelastic domain pair $(S_i, S_k)$ possess the same spontaneous strain. Consequently [8,9], the twin law of a non-ferroelastic domain pair is of the form

$$J_{ik} = F + g_{ik}F$$

where $F$ is the symmetry group of $S_i$ and $g_{ik}$ can be chosen such that $g^2_{ik} = 1$, the identity element of $F$. All twin laws can be classified into equivalence classes of twin laws [7]. There are 43 classes of non-magnetic twin laws of non-ferroelastic domain pairs [8] and 309 classes of magnetic twin laws of non-ferroelastic domain pairs [9]. The latter are a subset, the subset where both $J_{ik}$ and $F$ belong to the same crystal family, of the 380 classes of magnetic completely transposable twin laws [10].

3. Tensor component distinction

To determine the tensor component distinction of a pair of domains requires the form of the physical property tensors in each of the domains. Let $T(i)$ and $T(k)$ denote, respectively, the matrix forms of a physical property tensor of type $T$ in the domains $S_i$ and $S_k$ of a non-ferroelastic domain pair $(S_i, S_k)$ whose twin law is $J_{ik} = F + g_{ik}F$. As $F$ is the symmetry group of domain $S_i$, the matrix form of $T(i)$ is invariant under $F$. For non-magnetic groups $F$, $T(i)$ can be found in printed [11,12] or computerized [13,14] tabulations of physical property tensors. For magnetic groups $F$, $T(i)$ can be found from the form of the physical property tensor invariant under a related non-magnetic group [15]. The form of the physical property tensor $T(k)$ is related to $T(i)$ by the element $g_{ik}$

$$T(k)_p = \sum_{q=1}^{m} D(g_{ik})_{pq} T(i)_q,$$

where $T(i)_q$, $q = 1, 2, \ldots, m$, are the components of the form of the tensor of type $T$ in domain $S_i$ and $T(k)_p$, $p = 1, 2, \ldots, m$, are the components in domain $S_k$. It has been shown [9] that for every magnetic non-ferroelastic twin law, there exists a coordinate system where $D(g_{ik})_{pq}$ is diagonal. Consequently, there exists a coordinate system for every magnetic non-ferroelastic domain pair in which physical property tensors distinguish between the two domains in a simple manner: corresponding tensor components are either the same or differ only in sign.

For each of the 309 classes of magnetic non-ferroelastic twin laws of domain pairs $(S_i, S_k)$ and the each of the physical property tensors in Table 1, we have tabulated (The tables of the Component distinction of magnetic non-ferroelastic domain pairs can be found in the supplementary material in the online edition of this journal and at the author’s website: http://www.bk.psu.edu/faculty/litvin/) the explicit form of the physical property tensors $T(i)$ and $T(k)$ in the two domains. An example of these tables is given in Table 2.
4. Switching example

We consider a domain pair pair $(S_i, S_k)$ whose non-ferroelastic twin law $6_z^2 x^2 y^2 x^2 y^2 = 3 z^2 x^2 + 2 z^2 y^2 z^2 x^2 y^2$, i.e. the symmetry group of domain $S_i$ is $F = 3 z^2 x^2$ and domain $S_k$ is obtained from the domain $S_i$ with the rotation $2_z$, i.e. $S_k = 2_z S_i$. For the types of physical property tensors listed in Table 1, from the table [16] listing the component distinction of the non-ferroelastic twin laws, only physical properties of the Jahn type $V[2^2], aV[2^2], a_e V[2^2]$, and $[[2^2]^2]$ can possibly distinguish the domains and consequently possibly lead to switching of the domains. For this non-ferroelastic twin law and tensor type $V[2^2]$, we have [16]

$$
T(i) = \begin{pmatrix}
T_{xx} & T_{xy} & 0 \\
-T_{xy} & T_{xx} & 0 \\
0 & 0 & T_{zz}
\end{pmatrix}
$$

and

$$
g_{ik} T(i) = \begin{pmatrix}
-T_{xx} & T_{xy} & 0 \\
-T_{xy} & -T_{xx} & 0 \\
0 & 0 & -T_{zz}
\end{pmatrix}
$$

where $T_{mnp} = T_{mpn}$, and in the contracted notation $T_{m\mu}$, the values $\mu = xx, yy, zz, yz, xz, xy$. Therefore

$$
\Delta T_{m\mu} = 2 \begin{pmatrix}
-T_{xx} & 0 & 0 & 0 & 0 \\
0 & T_{xx} & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & T_{xx}
\end{pmatrix}
$$

and as the piezoelectric coefficient ‘$d$’ is a physical property tensor of the type $V[2^2]$, this leads to the following terms in Equation (1):

$$
\Delta G = \cdots -d_{xxx}(E_x \sigma_{xx} - E_x \sigma_{yy} - 2E_y \sigma_{xy}) \cdots
$$

The twin law $6_z^2 x^2 y^2 = 3_z^2 x^2 + 2_z^2 y^2 x^2 y^2$ does not contain spatial or time inversion, independently or coupled with other elements. The form of tensors of the type $aV[2^2]$ and
\[ \Delta G = \cdots -q_{xxx} (H_x \sigma_{xx} - H_y \sigma_{yy} - 2H_y \sigma_{xy}) - \gamma_{xxx} (S_x \sigma_{xx} - S_x \sigma_{yy} - 2S_y \sigma_{xy}) \cdots \]

For the fourth tensor type \([V^2]^2\), we have

\[
T(i)_{\mu\nu} = \begin{pmatrix}
T_{xxx} & T_{xyy} & T_{xxz} & T_{xyz} & 0 & 0 \\
T_{xxx} & T_{xyy} & -T_{xyz} & 0 & 0 \\
T_{xxx} & T_{xyy} & T_{xyz} & 0 & 0 \\
T_{xxx} & T_{xyy} & 0 & 0 & 0 \\
T_{xxx} & T_{xyy} & 0 & 0 & 0 \\
T_{xxx} & T_{xyy} & 0 & 0 & 0 \\
T_{xxx} & T_{xyy} & 0 & 0 & 0 \\
\end{pmatrix},
\]

\[
T(k)_{\mu\nu} = \begin{pmatrix}
T_{xxx} & T_{xyy} & T_{xxz} & -T_{xyz} & 0 & 0 \\
T_{xxx} & T_{xyy} & T_{xyz} & 0 & 0 \\
T_{xxx} & T_{xyy} & 0 & 0 & 0 \\
T_{xxx} & T_{xyy} & 0 & 0 & 0 \\
T_{xxx} & T_{xyy} & 0 & 0 & 0 \\
T_{xxx} & T_{xyy} & 0 & 0 & 0 \\
\end{pmatrix},
\]

where \(T_{mnpq} = T_{nmqp} = T_{mpqn} = T_{pgmn}\), and in the contracted notation \(T_{\mu\nu}\), the values \(\mu, \nu = xx, yy, zz, yz, xz, xy\). Therefore

\[
\Delta T_{\mu\nu} = 2
\begin{pmatrix}
0 & 0 & 0 & T_{xyz} & 0 & 0 \\
0 & 0 & -T_{xyz} & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & T_{xyz} & 0 & 0 & 0 & 0 \\
\end{pmatrix}
\]

and as the elastic compliance ‘s’ is a physical property tensor of the type \(V[V^2]\), this leads to the following terms in Equation (1):

\[ \Delta G = \cdots + 4s_{xxx} \sigma_{xx} \sigma_{yy} - 4s_{xyy} \sigma_{yy} \sigma_{yy} + 8s_{xyy} \sigma_{xy} \sigma_{xy} \cdots \]

The term \(d_{xxx} E_x \sigma_{xx}\) in Equation (2) implies the possibility of ferroelastoelectric switching in \(\alpha\)-quartz by the simultaneous application of \(\sigma_{xx}\) and \(E_x\) and such switching has been found [16].

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