Phase Transitions
Publication details, including instructions for authors and subscription information:
http://www.tandfonline.com/loi/gpht20

Tensor component distinction of magnetic non-ferroelastic domain pairs

Daniel B. Litvin [a]

[a] Department of Physics, Eberly College of Science, The Pennsylvania State University, Penn State Berks, P.O. Box 7009, Reading, PA 19610, USA

Available online: 24 May 2011

To cite this article: Daniel B. Litvin (2011): Tensor component distinction of magnetic non-ferroelastic domain pairs, Phase Transitions, 84:9-10, 804-809

To link to this article: http://dx.doi.org/10.1080/01411594.2011.558290

Phase Transitions
Vol. 84, Nos. 9–10, September–October 2011, 804–809

Tensor component distinction of magnetic non-ferroelastic domain pairs

Daniel B. Litvin*

Department of Physics, Eberly College of Science, The Pennsylvania State University, Penn State Berks, P.O. Box 7009, Reading, PA 19610, USA

(*Received 18 September 2010; final version received 20 October 2010*)

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 ΔG in free energy of two domain states is the driving potential of domain switching. To second order in external fields, ΔG is given by

$$\begin{aligned}\Delta G = {} & \Delta P_{(s)i}E_i + \Delta M_{(s)i}H_i + \Delta\varepsilon_{(s)ij}\sigma_{ij} + \Delta T_{(s)i}S_i + 1/2\Delta\kappa_{ij}E_iE_j + 1/2\Delta\chi_{ij}H_iH_j \\ & + 1/2\Delta s_{ijkl}\sigma_{ij}\sigma_{kl} + 1/2\Delta\tau_{ij}S_iS_j + \Delta d_{ijk}E_i\sigma_{jk} + \Delta q_{ijk}H_i\sigma_{jk} + \Delta\alpha_{ij}H_iE_j \\ & + \Delta\gamma_{ijk}S_i\sigma_{jk} + \Delta\zeta_{ij}H_iS_j + \Delta\theta_{ij}E_iS_j + \text{higher order terms} \end{aligned} \tag{1}$$

$\Delta(\text{Physical Property})_{ij\ldots}$ 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, σ_{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].

*Email: u3c@psu.edu

ISSN 0141–1594 print/ISSN 1029–0338 online

DOI: 10.1080/01411594.2011.558290
http://www.informaworld.com

Table 1. Physical property nomenclature, ferroic type, and physical property tensor Jahn notation.

	Physical property	Ferroic type	Jahn notation
$P_{(s)i}$	Spontaneous polarization	Ferroelectric	V
$M_{(s)i}$	Spontaneous magnetization	Ferromagnetic	aeV
$\varepsilon_{(s)ij}$	Spontaneous strain	Ferroelastic	$[V^2]$
$T_{(s)i}$	Spontaneous toroidal moment	Ferrotoroidic	aV
κ_{ij}	Electric susceptibility	Ferrobielectric	$[V^2]$
χ_{ij}	Magnetic susceptibility	Ferrobimagnetic	$[V^2]$
s_{ijkl}	Elastic compliance	Ferrobielastic	$[[V^2]^2]$
τ_{ij}	Toroidic susceptibility	Ferrobitoroidic	$[V^2]$
d_{ijk}	Piezoelectric coefficient	Ferroelastoelectric	$V[V^2]$
q_{ijk}	Piezomagnetic coefficient	Ferroelastomagnetic	$aeV[V^2]$
γ_{ijk}	Piezotoroidic coefficient	Ferroelastotoroidic	$aV[V^2]$
α_{ij}	Magnetoelectric coefficient	Ferromagnetoelectric	aeV^2
ζ_{ij}	Magnetotoroidic coefficient	Ferromagnetotoroidic	eV^2
θ_{ij}	Electrotoroidic coefficient	Ferroelectrotoroidic	aV^2

As an example of switching [5,6], consider the form of the electric susceptibility tensor of a domain invariant under the point group $\mathbf{2}_z$ 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 $\Delta G = \cdots + 2\kappa_{xy}E_xE_y \ldots$, 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 $\boldsymbol{G}$ and $\boldsymbol{F}$. The crystal splits into $n = |\boldsymbol{G}|/|\boldsymbol{F}|$ single domain states denoted by $S_1, S_2, \ldots, S_n$. Writing the coset decomposition of $\boldsymbol{G}$ with respect to $\boldsymbol{F}$ as $\boldsymbol{G} = \boldsymbol{F} + g_2\boldsymbol{F} + \cdots + g_n\boldsymbol{F}$, 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 $\boldsymbol{F}_i = g_i\boldsymbol{F}_1g_i^{-1}$ is the symmetry group of the i-th domain.

A domain pair is denoted by (S_i, S_k) with $S_k = g_{ik}S_i$ 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 $\boldsymbol{J}_{ik}$ of a domain pair (S_i, S_k) is defined [7] as

$$\boldsymbol{J}_{ik} = (\boldsymbol{F}_i \cap \boldsymbol{F}_k) + g_{ik}^*(\boldsymbol{F}_i \cap \boldsymbol{F}_k)$$

where g^*_{ik} is an element that interexchanges 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: $\boldsymbol{F}_i \cap \boldsymbol{F}_k$ is the group that simultaneously leaves each domain invariant and $g^*_{ik}(\boldsymbol{F}_i \cap \boldsymbol{F}_k)$ 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

$$\boldsymbol{J}_{ik} = \boldsymbol{F} + g_{ik}\boldsymbol{F}$$

where $\boldsymbol{F}$ is the symmetry group of S_i and g_{ik} can be chosen such that $g^2_{ik} = 1$, the identity element of $\boldsymbol{F}$. 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 $\boldsymbol{J}_{ik}$ and $\boldsymbol{F}$ 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 $\boldsymbol{T}$ in the domains S_i and S_k of a non-ferroelastic domain pair (S_i, S_k) whose twin law is $\boldsymbol{J}_{ik} = \boldsymbol{F} + g_{ik}\boldsymbol{F}$. As $\boldsymbol{F}$ is the symmetry group of domain S_i, the matrix form of $T(i)$ is invariant under $\boldsymbol{F}$. For non-magnetic groups $\boldsymbol{F}$, $T(i)$ can be found in printed [11,12] or computerized [13,14] tabulations of physical property tensors. For magnetic groups $\boldsymbol{F}$, $T(i)$ 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 $\boldsymbol{T}$ 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.

Table 2. Example of supplementary material table.

	$\boldsymbol{F}$	g_{ik}	$\boldsymbol{J}_{ik}$	aV^2
050.	$\mathbf{4}_z$	$2'_x 2'_y 2'_{xy} 2'_{\bar{x}y}$	$\mathbf{4}_z\mathbf{2}'_x\mathbf{2}'_{xy}$	2/1
	$T(i)=\begin{pmatrix} T_{xx} & T_{xy} & 0 \\ -T_{xy} & T_{xx} & 0 \\ 0 & 0 & T_{zz} \end{pmatrix}$		$g_{ik}T(i)=\begin{pmatrix} -T_{xx} & T_{xy} & 0 \\ -T_{xy} & -T_{xx} & 0 \\ 0 & 0 & -T_{zz} \end{pmatrix}$	

Notes: In the heading, $\boldsymbol{F}$ denotes the point group symmetry of the first domain S_i, of a domain pair (S_i, S_k). g_{ik} denotes an element of the twin law such that $g_{ik}^2=1$ and transforms the first domain state into the second domain state, $g_{ik}S_i=S_k$, all such elements are listed. $\boldsymbol{J}_{ik}=\boldsymbol{F}+g_{ij}\boldsymbol{F}$ is the twin law of the domain pair followed by the type of physical property tensor in Jahn notation. The following line gives the serial number of this class of magnetic non-ferroelastic twin laws, and its $\boldsymbol{F}$, g_{ij}, and $\boldsymbol{J}_{ik}$. The numbers N/M give the number N of non-zero distinct components which change sign in the two domains, and the number M which stay the same. $T(i)$ is the form of the physical property tensor in the first domain and $g_{ik}T(i)=T(k)$ its form in the second domain.

4. Switching example

We consider a domain pair pair (S_i, S_k) whose non-ferroelastic twin law $\mathbf{6}_z\mathbf{2}_x\mathbf{2}_1=\mathbf{3}_z\mathbf{2}_x+2_z\mathbf{3}_z\mathbf{2}_x$, i.e. the symmetry group of domain S_i is $\boldsymbol{F}=\mathbf{3}_z\mathbf{2}_x$ and domain S_k is obtained from the domain S_i with the rotation 2_z, i.e. $S_k=2_zS_i$. 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 $V[V^2]$, $aV[V^2]$, $aeV[V^2]$, and $[[V^2]^2]$ can possibly distinguish the domains and consequently possibly lead to switching of the domains. For this non-ferroelastic twin law and tensor type $V[V^2]$, we have [16]

$$T(i)_{m\mu}=\begin{pmatrix} T_{xxx} & -T_{xxx} & 0 & T_{xyz} & 0 & 0 \\ 0 & 0 & 0 & 0 & -T_{xyz} & -T_{xxx} \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

$$T(k)_{m\mu}=\begin{pmatrix} -T_{xxx} & T_{xxx} & 0 & T_{xyz} & 0 & 0 \\ 0 & 0 & 0 & 0 & -T_{xyz} & T_{xxx} \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix},$$

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

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

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

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

The twin law $\mathbf{6}_z\mathbf{2}_x\mathbf{2}_1=\mathbf{3}_z\mathbf{2}_x+2_z\mathbf{3}_z\mathbf{2}_x$ does not contain spatial or time inversion, independently or coupled with other elements. The form of tensors of the type $aV[V^2]$ and

$aeV[V^2]$, for this twin law, are then identical with the form of tensor $V[V^2]$. Therefore Equation (1) has two additional sets of terms, those associated with the piezomagnetic coefficient 'q' and the piezotoroidic coefficient 'γ':

$$\Delta G = \cdots - q_{xxx}(H_x\sigma_{xx} - H_x\sigma_{yy} - 2H_y\sigma_{xy}) - \gamma_{xxx}(S_x\sigma_{xx} - S_x\sigma_{yy} - 2S_y\sigma_{xy})\ldots$$

For the fourth tensor type $[[V^2]^2]$, we have

$$T(i)_{\mu\nu} = \begin{pmatrix} T_{xxxx} & T_{xxyy} & T_{xxzz} & T_{xxyz} & 0 & 0 \\ & T_{xxxx} & T_{xxzz} & -T_{xxyz} & 0 & 0 \\ & & T_{zzzz} & 0 & 0 & 0 \\ & & & T_{yzyz} & 0 & 0 \\ & & & & T_{xzxz} & T_{xxyz} \\ & & & & & \dfrac{T_{xxxx} - T_{yyyy}}{2} \end{pmatrix},$$

$$T(k)_{\mu\nu} = \begin{pmatrix} T_{xxxx} & T_{xxyy} & T_{xxzz} & -T_{xxyz} & 0 & 0 \\ & T_{xxxx} & T_{xxzz} & T_{xxyz} & 0 & 0 \\ & & T_{zzzz} & 0 & 0 & 0 \\ & & & T_{yzyz} & 0 & 0 \\ & & & & T_{xzxz} & -T_{xxyz} \\ & & & & & \dfrac{T_{xxxx} - T_{yyyy}}{2} \end{pmatrix},$$

where $T_{mnpq} = T_{nmpq} = T_{mnqp} = T_{pqmn}$, and in the contracted notation $T_{\mu\upsilon}$, the values $\mu,\upsilon = xx$, yy, zz, yz, xz, xy. Therefore

$$\Delta T_{\mu\nu} = 2\begin{pmatrix} 0 & 0 & 0 & T_{xxyz} & 0 & 0 \\ & 0 & 0 & -T_{xxyz} & 0 & 0 \\ & & 0 & 0 & 0 & 0 \\ & & & 0 & 0 & 0 \\ & & & & 0 & T_{xxyz} \\ & & & & & 0 \end{pmatrix}$$

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):

$$\Delta G = \cdots + 4s_{xxyz}\sigma_{xx}\sigma_{yz} - 4s_{xxyz}\sigma_{yy}\sigma_{yz} + 8s_{xxyz}\sigma_{xy}\sigma_{xz}\ldots$$

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

Acknowledgements

The author would like to thank the Penn State Berks Science Division for its travel support.

References

[1] H. Schmid, *Magnetoelectric effects in insulating magnetic materials*, in *Introduction to complex mediums for optics and electromagnetics*, W.S. Weiglhofer and A. Lahhtakia, eds., SPIE Press, Bellingham, WA, 2003, pp. 167–195.
[2] R.E. Newnham, *Properties of Materials: Anisotropy, Symmetry, Structure*, Oxford University Press, Oxford, 2004.
[3] H.A. Jahn, *Note on the Bhagavantam-Suryanarayana method of enumerating the physical constants of crystals*, Acta Cryst. 2 (1949), pp. 30–33.
[4] H. Schmid, *On ferrotoroidics and electrotoroidic, magnetotoroidic and piezotoroidic effects*, Ferroelectrics 252 (2001), pp. 41–50.
[5] V.K. Wadhawan, *Ferroelasticity and related properties of crystals*, Phase Transitions 3 (1982), pp. 3–103.
[6] V.K. Wadhawan, *Introduction to Ferroic Materials*, Gordon and Breach, New York, 2000.
[7] V. Janovec, *Symmetry and structure of domain walls*, Ferroelectric 35 (1981), pp. 105–110.
[8] D.B. Litvin and V. Janovec, *On tensor distinction of Non-ferroelastic domains*, Ferroelectrics 303 (2004), pp. 43–46.
[9] D.B. Litvin and V. Janovec, *Distinction of magnetic non-ferroelastic domains*, Acta Cryst. A62 (2006), pp. 98–102.
[10] D.B. Litvin, S.Y. Litvin, and V. Janovec, *Magnetic completely transposable twin laws and tensor distinction*, Acta Cryst. A51 (1995), pp. 524–529.
[11] Yu. Sirotin and M.P. Shaskolskaya, *Fundamentals of Crystal Physics*, Mir, Moscow, 1982.
[12] J. Brandmuller, H. Bross, W.G. Bauer, and F.X. Winter, *Tables to accompany J. Brandmuller and F.X. Winter: Influence of symmetry on the static and dynamic properties of crystals*, Z Kristallogr. 172 (1985), pp. 191–231 (second corrected edition with extension to non-crystallographic point groups (1986)).
[13] M. Ephraim, T. Jannsen, A. Janner, and A. Thiers, *Introduction to the accompanying software Tenχar*, in *International Tables for Crystallography*, A. Authier, ed., Volume D: Physical Properties of Crystals, Kluwer Academic, Dordrecht, 2003, pp. 62–70.
[14] S.V. Popov, Yu.P. Svirko, and N.I. Zheludev, *Encyclopedia of Material Tensors on CD*, John Wiley, Chichester, 1999.
[15] D.B. Litvin, *Magnetic physical property tensors*, Acta Cryst. A50 (1994), pp. 406–408.
[16] J.W. Laughner, R.E. Newnham, and L.E. Cross, *Ferroelastoelectricity in quartz*, Phys. Stat. Sol. a56 (1979), pp. K83–K86.