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TENSORIAL COVARIANTS AND DOMAIN STATE TENSORS[1]

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The use of tensorial covariants, subduction, and domain structure tables are shown to facilitate the computation of physical property tensors, their matrix form, the relationships among these tensors in domain states which arise during a phase transition, and the relationship of these components to parameters that drive a phase transition. An example is given for phase transitions between a parent phase point group symmetry of $m\bar{3}m$ and the point group mmm.

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In describing the physical property of crystals by tensors, the components of the tensors are usually given in a cartesian coordinate system (Nye, 1957). However, in calculating these components, especially of higher rank tensors, relating components in different domain states that arise in phase transitions, and in relating these components to parameters that drive phase transitions, it is more

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appropriate and revealing , as we shall show below, to relate these cartesian components first to what are called *tensorial covariants*.

To show this we shall consider a specific equitranslational ferroic phase transition where the point group of the parent phase is $G = m\bar{3}m$ and the point group of the lower symmetry phase is $F = m_x m_y m_z$. This corresponds to phase transitions in lead zirconate (Landolt-Boernstein, 1982) and cesium lead chloride (Chabin & Gilletta ,1980). The physical property tensors which we shall consider, and their symbols are:

ϵ	enantiomorphism
P	polarization, pyroelectricity
u	deformation, permitivity, thermal expansion
g	gyrotropy, optical activity
d	piezoelectricity, electrooptics
A	electrogyration
s	elastic stiffness
Q	piezooptics, electrostriction

One can calculate (Kopsky, 1979) linear combinations of the cartesian components of tensors which transform as sets of basis functions of irreducible representations of the point group G of the parent phase. These are named *tensorial covariants*. These have been calculated (Kopsky 1970,2000) and in Table 1 we have listed these tensor covariants for the physical property tensors listed above and the group $G = m\bar{3}m$. Under each heading of symbols of basis functions of irreducible representations of $m\bar{3}m$ is a list of linear combinations of cartesian components, the tensorial covariants, which transform under G as those basis functions.

In Table 2 , information concerning the subduction of irreducible representations of the group $G = m\bar{3}m$ onto the subgroup $F = m_x m_y m_z$ is given (Kopsky 1982 and these proceedings). Each basis function of $m\bar{3}m$, when restricted to the subgroup $m_x m_y m_z$, transforms as a basis function of $m_x m_y m_z$ and is listed under that basis function of $m_x m_y m_z$.

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In this phase transition between G = $m\bar{3}m$ and F = $m_x m_y m_z$ there arises six domain states which we denote by S_i , i=1,2...,6 . In Table 3 we give the domain structure table (Kopsky 1982) with the information necessary to calculate the physical property tensors in these domain states. We note that only basis functions of the type x^+_1 , x^+_2 , and x^+_3, y^+_3 appear in Table 3. The consequences of this are:

1) Physical property tensors which have no tensor covariants which transform as these basis functions are identically zero in all six domains. That is, ϵ, P, g, and d are such tensors, which is anticipated by the fact that the point group F is centrosymmetric.

2) Tensor covariants of physical property tensors which do not transform as any of these basis functions are identically zero in all six domains. This immediately provides a list of cartesian components which are zero in all six domains. From Table 1, one sees, for example, that $A_{11} \equiv 0$, and from $s_{34} - s_{23} = 0$ and $s_{34} + s_{23} = 0$ that $s_{34} = s_{23} = 0$. For this particular transition we have in all six domain states that $u_4 = u_5 = u_6 = 0$; $A_{11} = A_{12} = A_{13} = A_{15} = A_{16} = A_{21} = A_{22} = A_{23} = A_{24} = A_{26} = A_{31} = A_{32} = A_{33} = A_{34} = A_{35} = 0$; $s_{14} = s_{15} = s_{16} = s_{24} = s_{25} = s_{26} = s_{34} = s_{35} = s_{36} = s_{45} = s_{46} = s_{56} = 0$; and $Q_{14} = Q_{15} = Q_{16} = Q_{24} = Q_{25} = Q_{26} = Q_{34} = Q_{35} = Q_{36} = Q_{41} = Q_{42} = Q_{43} = Q_{45} = Q_{46} = Q_{51} = Q_{52} = Q_{53} = Q_{54} = Q_{56} = Q_{61} = Q_{62} = Q_{63} = Q_{64} = Q_{65} = 0$.

Note in Table 3 under the first domain state that $*(x^+_3, y^+_3)$ appears with a "*" to the left. This indicates the physical property tensors and tensor components which can distinguish all domains. From this and Table 3 one can see immediately that tensors u, s, and Q can distinguish all six domains. In terms of an Aizu classification (Aizu 1970), these tensors are *fully ferroic*. In terms of parameters which drive this particular phase transitions, only tensor components, and cartesian components related to these tensor components, which transform as (x^+_3, y^+_3) can drive this transition, can uniquely characterize the six domains.

The consequences given above were easily determined due to the

Table 1. Tensorial covariants for the group $m\bar{3}m$.

X^+_1	X^+_2	(x^+_3, y^+_3)	(x^+_1, y^+_1, z^+_1)	(x^+_2, y^+_2, z^+_2)
$u_1+u_2+u_3$		$[u_3 - a(u_1+u_2), b(u_1 - u_2)]$		
	$A_{14}+A_{25}+A_{36}$	$[b(A_{14} - A_{25}), a(A_{14}+A_{25})-A_{36}]$	$(A_{13}+A_{12}, A_{21}+A_{23}, A_{32}+A_{31})$	$(A_{13} - A_{12}, A_{21} - A_{23}, A_{32} - A_{31})$
			$(A_{35}+A_{26}, A_{16}+A_{34}, A_{24}+A_{15})$	$(A_{35} - A_{26}, A_{16} - A_{34}, A_{24} - A_{15})$
			(A_{11}, A_{22}, A_{33})	
$s_{11}+s_{22}+s_{33}$		$[s_{33} - a(s_{11}+s_{22}), b(s_{11} - s_{22})]$	$(s_{34} - s_{24}, s_{15} - s_{35}, s_{26} - s_{16})$	$(s_{34}+s_{24}, s_{15}+s_{35}, s_{26}+s_{16})$
$s_{23}+s_{13}+s_{12}$		$[s_{12} - a(s_{23}+s_{13}), b(s_{23} - s_{13})]$		(s_{14}, s_{25}, s_{36})
$s_{44}+s_{55}+s_{66}$		$[s_{66} - a(s_{44}+s_{55}), b(s_{44} - s_{55})]$		(s_{56}, s_{46}, s_{45})
$Q_{11}+Q_{22}+Q_{33}$	$Q^a_{23}+Q^a_{31}+Q^a_{12}$	$[Q_{33} - a(Q_{11}+Q_{22}), b(Q_{11} - Q_{22})]$	$(Q_{34} - Q_{24}, Q_{15} - Q_{35}, Q_{26} - Q_{16})$	$(Q_{34}+Q_{24}, Q_{15}+Q_{35}, Q_{26}+Q_{16})$
$Q^s_{23}+Q^s_{13}+Q^s_{12}$		$[Q_{66} - a(Q_{44}+Q_{55}), b(Q_{44} - Q_{55})]$	$(Q_{43} - Q_{42}, Q_{51} - Q_{53}, Q_{62} - Q_{61})$	$(Q_{43}+Q_{42}, Q_{51}+Q_{53}, Q_{62}+Q_{61})$
$Q_{44}+Q_{55}+Q_{66}$		$[Q^s_{12} - a(Q^s_{23}+Q^s_{13}), b(Q^s_{23} - Q^s_{13})]$	$(Q_{56} - Q_{65}, Q_{64} - Q_{46}, Q_{45} - Q_{54})$	$(Q_{56}+Q_{65}, Q_{64}+Q_{46}, Q_{45}+Q_{54})$
		$[b(Q^a_{23} - Q^a_{13}), a(Q^a_{23}+Q^a_{13}) - Q^a_{12}]$		(Q_{14}, Q_{25}, Q_{36})
X^-_1	X^-_2	(x^-_3, y^-_3)	(x^-_1, y^-_1, z^-_1)	(x^-_2, y^-_2, z^-_2)
ϵ			(P_1, P_2, P_3)	
$g_1+g_2+g_3$		$[g_3 - a(g_1+g_2), b(g_1 - g_2)]$		
	$d_{14}+d_{25}+d_{36}$	$[b(d_{14} - d_{25}), d(d_{14}+d_{25})-d_{36}]$	$(d_{13}+d_{12}, d_{21}+d_{23}, d_{32}+d_{31})$	$(d_{13} - d_{12}, d_{21} - d_{23}, d_{32} - d_{31})$
			$(d_{35}+d_{26}, d_{16}+d_{34}, d_{24}+d_{15})$	$(d_{35} - d_{26}, d_{16} - d_{34}, d_{24} - d_{15})$
			(d_{11}, d_{22}, d_{33})	

$Q^s_{ij} = Q_{ij} + Q_{ji}$ $\quad$ $Q^a_{ij} = Q_{ij} - Q_{ji}$

consideration not of the cartesian components, but of the tensor covariants of physical property tensors. The cartesian components can be calculated from these tensor covariants: From Table 1, one has a list of tensor covariants in terms of linear combinations of cartesian components, e.g. $u^+_1 = u_1+u_2+u_3$; $u^+_{3x} = u_3 + (u_1+u_2)/2$; and $u^+_{3y} = \sqrt{3}(u_1-u_2)/2$, where the superscript and subindices on the left-hand-side of each equation denote the transformation properties of the specific tensor covariants. These equations can be inverted to obtain *conversion equations*, i.e. the cartesian components in terms of the tensor covariants. For this phase transition, this has been done and is given in Table 4 for u_1 , u_2 , u_3 , and all non-identically zero cartesian components. These are also the non-zero components of the tensors u, A, s, and Q in the first of the six domain states.

The cartesian components of the tensors in the remaining domains are derived from the dependence of the cartesian components on the tensor covariants given in the first domain state.
How the tensor covariants change from one domain state to another is given explicitly in Table 3. For example, each tensor covariant which transforms as x^+_3 changes from the first to the second domain state from x^+_3 to $-x^+_3/2 + \sqrt{3}y^+_3/2$, as y^+_3 from y^+_3 to $\sqrt{3}x^+_3/2 + y^+_3/2$, and as x^+_1 and x^+_2 remain the same. Consequently, $u_1(S_1) = u^+_1/3 - u^+_{3x}/3 + u^+_{3y}/\sqrt{3}$ in the first domain state becomes in the second domain state $u_1(S_2) = u^+_1/3 + 2u^+_{3x}/3$. The cartesian components of the non-identically zero cartesian components of the tensors u and A are given in Table 5. From these tables one can also find relationships among the cartesian components of the domains. For example, for the A tensor one has: $A_{14}(S_2) = -A_{14}(S_5) = A_{36}(S_1) = -A_{36}(S_4)$ and $A_{25}(S_3) = -A_{25}(S_6)$.

References:

Aizu, K. (1970) Phys. Rev. B2, 754-772.
Chabin, M. & Gilletta, F., (1980) J. Appl. Cryst. 533-538.
Landolt-Boernstein, III/16b *Ferroelectrics and Related Substances* (1982).
Kopsky, V. (1982) *Group Lattices Subduction of Basis and Fine*

Domain Structures for Magnetic Crystal Point Groups, (Academia, Praha).
Kopsky, V. (1979) Acta Cryst. A35, 83-95 .
Kopsky, V. (2000 in *International Tables for Crystallography*, *Volume D: Physical Properties of Crystals* (edited by Authier), in preparation.
Kopsky, V. these proceedings.
Nye, J.F. (1957) *Physical Properties of Crystals*, (Clarendon Press, Oxford).

Table 2. $m\bar{3}m$ to $m_xm_ym_z$ subduction

$m_xm_ym_z$	x^+_1	x^+_2	x^+_3	x^+_4
$m\bar{3}m$	x^+_1, x^+_2, x^+_3, y^+_3	z^+_1, z^+_2	x^+_1, x^+_2	y^+_1, y^+_2

$m_xm_ym_z$	x^-_1	x^-_2	x^-_3	x^-_4
$m\bar{3}m$	x^-_1, x^-_2, x^-_3, y^-_3	z^-_1, z^-_2	x^-_1, x^-_2	y^-_1, y^-_2

Table 3.

S_1	$S_2 = 3_{xyz}S_1$	$S_3 = 3^2_{xyz}\, S_1$
x^+_1	x^+_1	x^+_1
x^+_2	x^+_2	x^+_2
*(x^+_3, y^+_3)	$(-ax^+_3 - by^+_{3,}\, bx^+_3 - ay^+_3)$	$(-ax^+_3+by^+_{3,}\, -bx^+_3 - ay^+_3)$

$S_4 = 2_{\bar{x}y}\, S_1$	$S_5 = 2_{\bar{y}z}\, S_1$	$S_6 = 2_{\bar{x}z}\, S_1$
x^+_1	x^+_1	x^+_1

$S_4 = 2_{\bar{x}y}\, S_1$	$S_5 = 2_{\bar{y}z}\, S_1$	$S_6 = 2_{\bar{x}z}\, S_1$
$- x^+_2$	$- x^+_2$	$- x^+_2$
$(x^+_3, -y^+_3)$	$(-ax^+_3 + by^+_3, bx^+_3 + ay^+_3)$	$(-ax^+_3 - by^+_3, -bx^+_3 + ay^+_3)$

Table 4. Conversion Equations

$u_1 = u^+_1/3 - u^+_{3x}/3 + u^+_{3y}/\sqrt{3}$
$u_2 = u^+_1/3 - u^+_{3x}/3 - u^+_{3y}/\sqrt{3}$
$u_3 = u^+_1/3 + 2u^+_{3x}/3$

$A_{14} = A^+_2/3 + A^+_{3x}/\sqrt{3} + A^+_{3y}/3$

$A_{25} = A^+_2/3 - A^+_{3x}/\sqrt{3} + A^+_{3y}/3$

$A_{36} = A^+_2/3 - 2A^+_{3y}/3$

$s_{11} = s^+_{1,1}/3 - s^+_{3x,1}/3 + s^+_{3y,1}/\sqrt{3}$

$s_{22} = s^+_{1,1}/3 - s^+_{3x,1}/3 - s^+_{3y,1}/\sqrt{3}$

$s_{33} = s^+_{1,1}/3 + 2s^+_{3x,1}/3$

$s_{44} = s^+_{1,3}/3 - s^+_{3x,3}/3 + s^+_{3y,3}/\sqrt{3}$

$s_{55} = s^+_{1,3}/3 - s^+_{3x,3}/3 - s^+_{3y,3}/\sqrt{3}$

$s_{55} = s^+_{1,3}/3 - s^+_{3x,3}/3 - s^+_{3y,3}/\sqrt{3}$
$s_{66} = s^+_{1,3}/3 + 2s^+_{3x,3}/3$

$Q_{11} = Q^+_{1,1}/3 - Q^+_{3x,1}/3 + Q^+_{3y,1}/\sqrt{3}$

$Q_{22} = Q^+_{1,1}/3 - Q^+_{3x,1}/3 - Q^+_{3y,1}/\sqrt{3}$

$Q_{33} = Q^+_{1,1}/3 + 2\, Q^+_{3x,1}/3$

$Q_{44} = Q^+_{1,2}/3 - Q^+_{3x,2}/3 + Q^+_{3y,2}/\sqrt{3}$

$Q_{55} = Q^+_{1,2}/3 - Q^+_{3x,2}/3 - Q^+_{3y,2}/\sqrt{3}$

$Q_{66} = Q^+_{1,2}/3 + 2\, Q^+_{3x,2}/3$

$Q^s_{23} = Q^+_{1,3}/3 - Q^+_{3x,3}/3 + Q^+_{3y,3}/\sqrt{3}$

$Q^s_{13} = Q^+_{1,3}/3 - Q^+_{3x,3}/3 - Q^+_{3y,3}/\sqrt{3}$

$Q^s_{12} = Q^+_{1,3}/3 + 2\, Q^+_{3x,3}/3$

$Q^a_{23} = Q^+_2/3 + Q^+_{3x,4}/\sqrt{3} + Q^+_{3y,4}/3$

$s_{66} = s^{+}_{1,3}/3 + 2s^{+}_{3x,3}/3$ $Q^{a}_{31} = Q^{+}_{2}/3 - Q^{+}_{3x,4}/\sqrt{3} + Q^{+}_{3y,4}/3$

$s_{44} = s^{+}_{1,3}/3 - s^{+}_{3x,3}/3 + s^{+}_{3y,3}/\sqrt{3}$ $Q^{a}_{12} = Q^{+}_{2}/3 - 2Q^{+}_{3y,4}/3$

Table 5.

	u_1	u_2
S_1	$u^{+}_{1}/3 - u^{+}_{3x}/3 + u^{+}_{3y}/\sqrt{3}$	$u^{+}_{1}/3 - u^{+}_{3x}/3 - u^{+}_{3y}/\sqrt{3}$
S_2	$u^{+}_{1}/3 + 2u^{+}_{3x}/3$	$u^{+}_{1}/3 - u^{+}_{3x}/3 + u^{+}_{3y}/\sqrt{3}$
S_3	$u^{+}_{1}/3 - u^{+}_{3x}/3 - u^{+}_{3y}/\sqrt{3}$	$u^{+}_{1}/3 + 2u^{+}_{3x}/3$
S_4	$u^{+}_{1}/3 - u^{+}_{3x}/3 - u^{+}_{3y}/\sqrt{3}$	$u^{+}_{1}/3 - u^{+}_{3x}/3 + u^{+}_{3y}/\sqrt{3}$
S_5	$u^{+}_{1}/3 + 2u^{+}_{3x}/3$	$u^{+}_{1}/3 - u^{+}_{3x}/3 - u^{+}_{3y}/\sqrt{3}$
S_6	$u^{+}_{1}/3 - u^{+}_{3x}/3 + u^{+}_{3y}/\sqrt{3}$	$u^{+}_{1}/3 + 2u^{+}_{3x}/3$
	u_3	A_{14}
S_1	$u^{+}_{1}/3 + 2u^{+}_{3x}/3$	$A^{+}_{2}/3 + A^{+}_{3x}/\sqrt{3} + A^{+}_{3y}/3$
S_2	$u^{+}_{1}/3 - u^{+}_{3x}/3 - u^{+}_{3y}/\sqrt{3}$	$A^{+}_{2}/3 - 2A^{+}_{3y}/3$
S_3	$u^{+}_{1}/3 - u^{+}_{3x}/3 - u^{+}_{3y}/\sqrt{3}$	$A^{+}_{2}/3 - A^{+}_{3x}/\sqrt{3} + A^{+}_{3y}/3$
S_4	$u^{+}_{1}/3 + 2u^{+}_{3x}/3$	$-A^{+}_{2}/3 + A^{+}_{3x}/\sqrt{3} - A^{+}_{3y}/3$
S_5	$u^{+}_{1}/3 - u^{+}_{3x}/3 + u^{+}_{3y}/\sqrt{3}$	$-A^{+}_{2}/3 + 2A^{+}_{3y}/3$
S_6	$u^{+}_{1}/3 - u^{+}_{3x}/3 + u^{+}_{3y}/\sqrt{3}$	$-A^{+}_{2}/3 - A^{+}_{3x}/\sqrt{3} - A^{+}_{3y}/3$
	A_{25}	A_{36}
S_1	$A^{+}_{2}/3 - A^{+}_{3x}/\sqrt{3} + A^{+}_{3y}/3$	$A^{+}_{2}/3 - 2A^{+}_{3y}/3$
S_2	$A^{+}_{2}/3 + A^{+}_{3x}/\sqrt{3} + A^{+}_{3y}/3$	$A^{+}_{2}/3 - A^{+}_{3x}/\sqrt{3} + A^{+}_{3y}/3$
S_3	$A^{+}_{2}/3 + 2A^{+}_{3y}/3$	$A^{+}_{2}/3 + A^{+}_{3x}/\sqrt{3} + A^{+}_{3y}/3$

	A_{25}	A_{36}
S_4	$-A^+_2/3 - A^+_{3x}/\sqrt{3} - A^+_{3y}/3$	$-A^+_2/3 + 2A^+_{3y}/3$
S_5	$-A^+_2/3 + A^+_{3x}/\sqrt{3} - A^+_{3y}/3$	$-A^+_2/3 + A^+_{3x}/\sqrt{3} - A^+_{3y}/3$
S_6	$-A^+_2/3 - 2A^+_{3y}/3$	$-A^+_2/3 - A^+_{3x}/\sqrt{3} - A^+_{3y}/3$