SHORT COMMUNICATIONS

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Magnetic physical-property tensors.

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Abstract

A method is presented to determine the form of magnetic physical-property tensors from the form of non-magnetic physical-property tensors.

1. Introduction

The derivation and tabulation of physical-property tensors invariant under the non-magnetic crystallographic point groups have been considered by many authors (Jahn, 1949; Nye, 1957; Birss, 1964; Kopsky, 1979*a*; Sands, 1982; Brandmuller & Winter, 1985; and references contained in these sources). Tables of a wide variety of physical-property tensors invariant under non-magnetic point groups have been given by Sirotin & Shaskolskaya (1975) and Brandmuller, Bross, Bauer & Winter (1986) and will appear in the forthcoming Volume D of *International Tables for Crystallography* (1994).

The derivation and tabulation of physical-property tensors invariant under magnetic groups have been considered by Birss (1964) and Kopsky (1979*b*). An analysis of the relationships among the forms of tensors invariant under space inversion, time inversion, space–time inversion and all three inversions has been given by Grimmer (1991). What we present below is a two-step algorithm to read from tables of the form of physical-property tensors invariant under the non-magnetic point groups the form of tensors invariant under all magnetic point groups. This method has already been implemented by Litvin & Litvin (1991) in tabulating the form of rank 0, 1, 2 and 3 magnetic physical-property tensors and in work on non-ferroelastic magnetoelectric twin laws (Litvin, Janovec & Litvin, 1994).

2. Determining the form of magnetic physical-property tensors

Let V denote a polar vector tensor and $V^n = V \times V \times \ldots \times V$ the nth ranked product of V; e and a denote zero-rank tensors that change sign under spatial inversion $\bar{1}$ and time inversion $1'$, respectively. The form of magnetic physical-property tensors is determined by the invariance of the tensors under the elements of the magnetic point group. For example, the invariance of a tensor V^n and the transformation of its components under a pure rotation p gives

$$pV^n_{ij\ldots k} = V^n_{ij\ldots k} = D^{1-}(p)_{ii'}D^{1-}(p)_{jj'}\ldots D^{1-}(p)_{kk'}V^n_{i'j'\ldots k'},$$

where the first equality denotes the invariance and the second gives the corresponding constraints on the components of the tensor. For typographical simplicity, we write the above as $pV^n = V^n = D(p)V^n$. In Table 1, we give the invariance and corresponding constraints on the components of tensors V^n, eV^n, aV^n and aeV^n under elements p, $\bar{p}$, p' and $\bar{p}'$ of a magnetic point group. The two columns of Table 1 correspond to tensors of odd and even rank. These conditions are applicable not only to general tensors of rank n but also to tensors with additional intrinsic symmetry.

Table 1. *Invariance and constraints*

n odd	n even
$pV^n = V^n = D(p)V^n$	$pV^n = V^n = D(p)V^n$
$\bar{p}V^n = V^n = -D(p)V^n$	$\bar{p}V^n = V^n = D(p)V^n$
$p'V^n = V^n = D(p)V^n$	$p'V^n = V^n = D(p)V^n$
$\bar{p}'V^n = V^n = -D(p)V^n$	$\bar{p}'V^n = V^n = D(p)V^n$
$p(eV^n) = eV^n = D(p)(eV^n)$	$p(eV^n) = eV^n = D(p)(eV^n)$
$\bar{p}(eV^n) = eV^n = D(p)(eV^n)$	$\bar{p}(eV^n) = eV^n = -D(p)(eV^n)$
$p'(eV^n) = eV^n = D(p)(eV^n)$	$p'(eV^n) = eV^n = D(p)(eV^n)$
$\bar{p}'(eV^n) = eV^n = D(p)(eV^n)$	$\bar{p}'(eV^n) = eV^n = -D(p)(eV^n)$
$p(aV^n) = aV^n = D(p)(aV^n)$	$p(aV^n) = aV^n = D(p)(aV^n)$
$\bar{p}(aV^n) = aV^n = -D(p)(aV^n)$	$\bar{p}(aV^N) = aV^n = D(p)(aV^n)$
$p'(aV^n) = aV^n = -D(p)(aV^n)$	$p'(aV^n) = aV^n = -D(p)(aV^n)$
$\bar{p}'(aV^n) = aV^n = D(p)(aV^n)$	$\bar{p}'(aV^n) = aV^n = -D(p)(aV^n)$
$p(aeV^n) = aeV^n = D(p)(aeV^n)$	$p(aeV^n) = aeV^n = D(p)(aeV^n)$
$\bar{p}(aeV^n) = aeV^n = D(p)(aeV^n)$	$\bar{p}(aeV^n) = aeV^n = -D(p)(aeV^n)$
$p'(aeV^n) = aeV^n = -D(p)(aeV^n)$	$p'(aeV^n) = aeV^n = -D(p)(aeV^n)$
$\bar{p}'(aeV^n) = aeV^n = -D(p)(aeV^n)$	$\bar{p}'(aeV^n) = aeV^n = D(p)(aeV^n)$

Table 2. *Number of the column of Table* 3 *to be used in determining the non-magnetic point group is given at the intersection of the row denoting the magnetic physical-property tensor and the column denoting the parity of the rank of the tensor*

	n odd, V^n	n even, eV^n
V^n	2	1
eV^n	1	2
aV^n	4	3
aeV^n	3	4

From Table 1, we see that there are only two types of sets of constraints: (tensor) = $D(p)$(tensor) and (tensor) = $-D(p)$(tensor). Consequently, for odd- (even-) ranked tensors, the form of any magnetic physical-property tensor invariant under a magnetic group M is identical with the form of the physical-property tensor V^n (eV^n) invariant under a non-magnetic point group G. The non-magnetic point group G corresponding to the magnetic group M is determined by replacing those elements p, $\bar{p}$, p', $\bar{p}'$ that give rise to the constraint (tensor) = $D(p)$(tensor) with the element p and those elements that give rise to the constraint (tensor) = $-D(p)$(tensor) with the element $\bar{p}$. The resulting non-magnetic groups G are determined from Tables 2 and 3. In Table 2, at the intersection of the row

Table 3. *Magnetic-to-non-magnetic point-group conversion table*

		1	2	3	4
1	11'	1	1	$\bar{1}$	$\bar{1}$
2	$\bar{1}1'$	1	$\bar{1}$	$\bar{1}$	$\bar{1}$
3	$\bar{1}'$	1	$\bar{1}$	$\bar{1}$	1
4	21'	2	2	2/m	2/m
5	2'	2	2	m	m
6	m1'	2	m	2/m	2/m
7	m'	2	m	m	2
8	2/m1'	2	2/m	2/m	2/m
9	2'/m	2	2/m	2/m	m
10	2/m'	2	2/m	2/m	2
11	2'/m'	2	2/m	m	2/m
12	2221'	222	222	mmm	mmm
13	2'2'2	222	222	mm2	mm2
14	mm21'	222	mm2	mmm	mmm
15	m'm2'	222	mm2	m2m	2mm
16	m'm'2	222	mm2	mm2	222
17	mmm1'	222	mmm	mmm	mmm
18	m'mm	222	mmm	mmm	2mm
19	m'm'm	222	mmm	mm2	mmm
20	m'm'm'	222	mmm	mmm	222
21	41'	4	4	4/m	4/m
22	4'	4	4	$\bar{4}$	$\bar{4}$
23	$\bar{4}1'$	4	$\bar{4}$	4/m	4/m
24	$\bar{4}'$	4	$\bar{4}$	$\bar{4}$	4
25	4/m1'	4	4/m	4/m	4/m
26	4'/m	4	4/m	$\bar{4}$	4/m
27	4/m'	4	4/m	4/m	4
28	4'/m'	4	4/m	4/m	$\bar{4}$
29	4221'	422	422	4/mmm	4/mmm
30	4'22'	422	422	$\bar{4}2m$	$\bar{4}2m$
31	42'2'	422	422	4mm	4mm
32	4mm1'	422	4mm	4/mmm	4/mmm
33	4'm'm	422	4mm	$\bar{4}m2$	$\bar{4}2m$
34	4m'm'	422	4mm	4mm	422
35	$\bar{4}2m1'$	422	$\bar{4}2m$	4/mmm	4/mmm
36	$\bar{4}'2'm$	422	$\bar{4}2m$	$\bar{4}m2$	4mm
37	$\bar{4}'2m'$	422	$\bar{4}2m$	$\bar{4}2m$	422
38	$\bar{4}2'm'$	422	$\bar{4}2m$	4mm	$\bar{4}m2$
39	4/mmm1'	422	4/mmm	4/mmm	4/mmm
40	4/m'mm	422	4/mmm	4/mmm	4mm
41	4'/mm'm	422	4/mmm	$\bar{4}m2$	4/mmm
42	4'/m'm'm	422	4/mmm	4/mmm	$\bar{4}2m$
43	4/mm'm'	422	4/mmm	4mm	4/mmm
44	4/m'm'm'	422	4/mmm	4/mmm	422
45	31'	3	3	$\bar{3}$	$\bar{3}$
46	$\bar{3}1'$	3	$\bar{3}$	$\bar{3}$	$\bar{3}$
47	$\bar{3}'$	3	$\bar{3}$	$\bar{3}$	3
48	321'	32	32	$\bar{3}m$	$\bar{3}m$
49	32'	32	32	3m	3m
50	3m1'	32	3m	$\bar{3}m$	$\bar{3}m$
51	3m'	32	3m	3m	32
52	$\bar{3}m1'$	32	$\bar{3}m$	$\bar{3}m$	$\bar{3}m$
53	$\bar{3}'m$	32	$\bar{3}m$	$\bar{3}m$	3m
54	$\bar{3}m'$	32	$\bar{3}m$	3m	$\bar{3}m$
55	$\bar{3}'m'$	32	$\bar{3}m$	$\bar{3}m$	32
56	61'	6	6	6/m	6/m
57	6'	6	6	$\bar{6}$	$\bar{6}$
58	$\bar{6}1'$	6	$\bar{6}$	6/m	6/m
59	$\bar{6}'$	6	$\bar{6}$	$\bar{6}$	6
60	6/m1'	6	6/m	6/m	6/m
61	6'/m	6	6/m	6/m	$\bar{6}$
62	6/m'	6	6/m	6/m	6
63	6'/m'	6	6/m	$\bar{6}$	6/m
64	6221'	622	622	6/mmm	6/mmm
65	6'2'2	622	622	$\bar{6}m2$	$\bar{6}m2$
66	62'2'	622	622	6mm	6mm
67	6mm1'	622	6mm	6/mmm	6/mmm
68	6'm'm	622	6mm	$\bar{6}m2$	$\bar{6}2m$
69	6m'm'	622	6mm	6mm	622
70	$\bar{6}m21'$	622	$\bar{6}m2$	6/mmm	6/mmm
71	$\bar{6}'m'2$	622	$\bar{6}m2$	$\bar{6}m2$	622
72	$\bar{6}'m2'$	622	$\bar{6}m2$	$\bar{6}2m$	6mm
73	$\bar{6}m'2'$	622	$\bar{6}m2$	6mm	$\bar{6}2m$
74	6/mmm1'	622	6/mmm	6/mmm	6/mmm
75	6/m'mm	622	6/mmm	6/mmm	6mm
76	6'/mm'm	622	6/mmm	6/mmm	$\bar{6}2m$
77	6'/m'm'm	622	6/mm	$\bar{6}m2$	6/mmm
78	6/mm'm'	622	6/mmm	6mm	6/mmm
79	6/m'm'm'	622	6/mmm	6/mmm	622
80	231'	23	23	$m\bar{3}$	$m\bar{3}$
81	$m\bar{3}1'$	23	$m\bar{3}$	$m\bar{3}$	$m\bar{3}$
82	$m'\bar{3}'$	23	$m\bar{3}$	$m\bar{3}$	23
83	4321'	432	432	$m\bar{3}m$	$m\bar{3}m$
84	4'32'	432	432	$\bar{4}3m$	$\bar{4}3m$
85	$\bar{4}3m1'$	432	$\bar{4}3m$	$m\bar{3}m$	$m\bar{3}m$
86	$\bar{4}'3m'$	432	$\bar{4}3m$	$\bar{4}3m$	432
87	$m\bar{3}m1'$	432	$m\bar{3}m$	$m\bar{3}m$	$m\bar{3}m$
88	$m'\bar{3}'m$	432	$m\bar{3}m$	$m\bar{3}m$	$\bar{4}3m$
89	$m\bar{3}m'$	432	$m\bar{3}m$	$\bar{4}3m$	$m\bar{3}m$
90	$m'\bar{3}'m'$	432	$m\bar{3}m$	$m\bar{3}m$	432

corresponding to the type of magnetic physical-property tensor and the column corresponding to either the odd or even rank of the tensor, is a number denoting a column of Table 3. In Table 3, at the intersection of this column and the row corresponding to M, is the required non-magnetic group G.

For example, consider the magnetoelectric effect tensor, which is of the type aeV^2, invariant under the magnetic group $M = \bar{4}'2'm$. From Table 2, we have that the form of this tensor is the same as the form of the tensor eV^2 invariant under the non-magnetic group G in the fourth column of Table 3 on the row corresponding to the magnetic group $M = \bar{4}'2'm$. From Table 3, we have $G = 4mm$. The form of the physical-property tensor aeV^2 invariant under $M = \bar{4}'2'm$ is then the same as the form of the tensor eV^2 invariant under $G = 4mm$. The latter is given by Sirotin & Shaskolskaya (1975) as

$$\begin{bmatrix} 0 & A & 0 \\ -A & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix},$$

which agrees with the form of the magnetoelectric physical-property tensor invariant under $\bar{4}'2'm$ given by Birss (1964).

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References

BIRSS, R. R. (1964). *Symmetry and Magnetism*. Amsterdam: North-Holland.

BRANDMULLER, J., BROSS, H., BAUER, W. G. & WINTER, F. X. (1986). Tables to accompany Brandmuller & Winter (1985), 2nd ed.

BRANDMULLER, J. & WINTER, F. X. (1985). *Z. Kristallogr.* **172**, 191–231.

GRIMMER, H. (1991). *Acta Cryst.* **A47**, 226–232.

International Tables for Crystallography (1994). Vol. D: *Physical Properties of Crystals*, edited by A. AUTHIER. In preparation.

JAHN, H. A. (1949). *Acta Cryst.* **2**, 30–33.

KOPSKY, V. (1979*a*). *Acta Cryst.* A**35**, 83–95.
KOPSKY, V. (1979*b*). *Acta Cryst.* A**35**, 95–101.
LITVIN, D. B., JANOVEC, V. & LITVIN, S. Y. (1994). *Ferroelectrics.* In the press.
LITVIN, S. Y. & LITVIN, D. B. (1991). *Acta Cryst.* A**47**, 290–292
NYE, J. F. (1957). *Physical Properties of Crystals.* Oxford: Clarendon Press.
SANDS, D. E. (1982). *Vectors and Tensors in Crystallography.* Reading, MA: Addison-Wesley.
SIROTIN, YU. & SHASKOLSKAYA, M. P. (1975). *Osnovi Kristallogfiziki.* Moscow: Nauka.

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Normalization factors for Kubic harmonic density functions.

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Abstract

Normalization factors N_{lj} for the Kubic harmonics K_{lj} defined by

$$\int_{\theta=0}^{\pi}\int_{\varphi=0}^{2\pi} N_{lj}|K_{lj}|\sin\theta\,d\theta\,d\varphi = 2-\delta_{l0}$$

have been evaluated numerically for $l\leq 10$.

Introduction

For cubic site symmetries, the symmetry-adapted functions for describing the angular dependence of the atomic charge density are the Kubic harmonics K_{lj} (Kurki-Suonio, 1977; Dawson, 1967). However, the normalization factors available in the literature, defined by

$$(1/M_{lj}^2)\int_{\theta=0}^{\pi}\int_{\varphi=0}^{2\pi} K_{lj}^2\sin\theta\,d\theta\,d\varphi = 1 \quad (1)$$

(Von der Lage & Bethe, 1947; Kurki-Suonio, 1977), apply to the normalization of wave functions. For density functions, the normalization

$$N_{lj}\int_{\theta=0}^{\pi}\int_{\varphi=0}^{2\pi} |K_{lj}|\sin\theta\,d\theta\,d\varphi = 2-\delta_{l0} \quad (2)$$

is appropriate. With this normalization, a population coefficient $P_{lj}=1$ implies, for $l=0$, a population of one electron and, for $l>0$, that one electron has been transferred from the negative to the positive lobes of the function $R_l(r)N_{lj}K_{lj}$, where $R_l(r)$ is a normalized radial function.

The unnormalized Kubic harmonics K_{lj} have been expressed in different forms (Kurki-Suonio, 1977; Dawson, 1967; Von der Lage & Bethe, 1947). We adopt the expressions given by Kurki-Suonio (1977).

The calculation

Table 1 lists the definitions of K_{lj} up to $l=10$, together with the N_{lj} values. Except for K_0 ($N_0=1/4\pi$) and K_3 ($N_3=1/15$), the values have been calculated by numerical integration using the Gaussian quadrature (Press, Flannery, Teukolsky & Vetterling, 1986). Satisfactory results have been obtained by dividing the intervals of integration for θ and φ into about 200 parts, evaluating the integral in each small solid angle by the 10-point Gaussian formula and subsequently summing the integrals. Finer divisions did not change the values to seven significant figures. For example, the numerical result for N_3 is 0.9999999997/15 for both a 200-by-200 and a 300-by-300 division of $\theta\varphi$ space.

Table 1. *Normalization factors for Kubic harmonics*

$u_{lm\pm}$ is given here as $P_l^m(\cos\theta)\,{}^{\cos(m\varphi)}_{\sin(m\varphi)}$.

Unnormalized $K_{lj}(0, 0)$	Normalization factor N_{lj}
$K_0=u_{00+}=1$	$1/4\pi=0.07957747$
$K_3=u_{32-}$	$2/30=1/15=0.06666667$
$K_4=u_{40+}+(1/168)u_{44+}$	$2/4.602568=0.4345400$
$K_{6,1}=u_{60+}-(1/360)u_{64+}$	$2/7.930299=0.2521973$
$K_{6,2}=u_{62+}-(1/792)u_{66+}$	$2/96.00000=0.02083333$
$K_7=u_{72-}+(1/1560)u_{76-}$	$2/136.8711=0.01461229$
$K_8=u_{80+}+(1/5940)[u_{84+}+(1/672)u_{88+}]$	$2/3.552877=0.5629241$
$K_{9,1}=u_{92-}-(1/2520)u_{96-}$	$2/335.7424=0.005956948$
$K_{9,2}=u_{94-}-(1/4080)u_{98-}$	$2/13513.50=0.0001480001$
$K_{10,1}=u_{10,0+}-(1/5460)[u_{10,4+}+(1/4320)u_{10,8+}]$	$2/5.480931=0.3649015$
$K_{10,2}=u_{10,2+}+(1/43680)[u_{10,6+}-(1/456)u_{10,10+}]$	$2/210.1611=0.009516509$

Table 2. *Some high-order* $y_{lm\pm}$ $[z=\cos(\theta)]$

u_{80+}	$(1/128)(6435z^8-12012z^6+6930z^4-1260z^2+35)$
u_{84+}	$(1/8)(10395)(z^2-1)^2(65z^4-26z^2+1)\cos(4\varphi)$
u_{88+}	$2027025(z^2-1)^4\cos(8\varphi)$
u_{92-}	$(495/16)z(1-z^2)(221z^6-273z^4+91z^2-7)\sin(2\varphi)$
u_{94-}	$(135135/8)z(z^2-1)^2(17z^4-10z^2+1)\sin(4\varphi)$
u_{96-}	$(675675/2)z(1-z^2)^3(17z^2-3)\sin(6\varphi)$
u_{98-}	$34459425z(z^2-1)^4\sin(8\varphi)$
$u_{10,0+}$	$(1/256)(46189z^{10}-109395z^8+90090z^6-30030z^4+3465z^2-63)$
$u_{10,2+}$	$(495/128)(1-z^2)(4199z^8-6188z^6+2730z^4-364z^2+7)$
$u_{10,4+}$	$(45045/16)(z^2-1)^2(323z^6-255z^4+45z^2-1)\cos(4\varphi)$
$u_{10,6+}$	$(675675/8)(1-z^2)^3(323z^4-102z^2+3)\cos(6\varphi)$
$u_{10,8+}$	$(34459425/2)(z^2-1)^4(19z^2-1)\cos(8\varphi)$
$u_{10,10+}$	$654729075(1-z^2)^5\cos(10\varphi)$

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