TENSOR PROPERTIES OF COHERENT DOMAIN CONFIGURATIONS IN POTASSIUM NIOBATE CRYSTALS

OUTLINE

1. INTRODUCTORY REMARKS

2. DOMAIN CONFIGURATIONS, AVERAGE TENSOR PROPERTIES AND EXTERNAL FIELDS

3. TENSOR PROPERTIES OF COHERENT CONFIGURATIONS

4. FERROELECTRIC COHERENT CONFIGURATIONS OF $Amm2$-PHASE OF POTASSIUM NIOBATE CRYSTALS

5. CONCLUSIONS

1. INTRODUCTORY REMARKS

Piezoelectric materials

$\hookrightarrow$ more than seven decades of commercial use

$\hookrightarrow$ a wide variety of applications ranging from crystal-controlled oscillators to small size active elements of modern electronic devices

Piezoelectric effect

material response to electric field $\boldsymbol{E} = (E_i)$, or stress field $\boldsymbol{T} = (T_{jk})$

piezoelectric tensor $\boldsymbol{d} = (d_{ijk}) \sim V[V^2]$: 18 components

direct effect: stress field (e.g. sound pressure) $\longrightarrow$ polarization, appearance of electric field

$$P_i = \sum_{j,k=1}^{3} d_{ijk} T_{jk} \qquad \ldots \text{transducers}$$

converse effect: electric field $\longrightarrow$ induced strain, change in shape

$$\sigma_{jk} = \sum_{i=1}^{3} d_{ijk} E_i \qquad \ldots \text{actuators}$$

piezolectric coefficient d_{333}:

(a) $P_3 = d_{333} T_{33}$ – induced polarization along [001] under stress applied in the 3-direction

(b) $\sigma_{33} = d_{333} E_3$ – induced strain in the 3-direction under $\boldsymbol{E} \parallel [001]$

Structural forms of piezoelectrics:

A single domain crystals

– SiO_2 (oscillators), $LiNbO_3$ (SAW devices), $\cdots$

B polycrystalline ceramics:

typical material: solid solution $Pb(Zr_{(1-x)}Ti_x)O_3$ (PZT)

compositional tuning of material parameters: doping

soft PZT (donors): sensors, ultrasonic imaging systems

hard PZT (acceptors): autofocusing in cameras, tuning of lasers

C single multidomain crystals:

1997 – ultrahigh piezoelectric coefficient d_{33} in rhombohedral single crystals of ferroelectric $Pb(Zn_{1/3}Nb_{2/3})O_3$-8%$PbTiO_3$ (PZN-PT) poled along the non-polar direction [001]

– new generation of high sensitive actuators and transducers

Table 1. Piezoelectric response of piezoelectric materials.

structural form	material	d_{33} $[pC/N]$
single domain crystals	SiO_2	$\sim$ 50
polycrystalline texture	'soft' PZT	$\sim$ 600
	'hard' PZT	$\sim$ 200
single crystals	PZN-PT	$>$ 2000

Engineered domain configurations

1999 – stable domain structure in the PZN-PT crystals after poling

suggestion: *equal distribution of four equivalent domain states* with polarizations along [111], [$\bar{1}\bar{1}$1], [$\bar{1}$11] and [1$\bar{1}$1] (S. Wada *et al.*)

QUERY: ¿ engineered domain configuration – is it a factor supporting enhanced piezoelectric response to appear ?

experiments with non-lead single crystals of $BaTiO_3$ and $KNbO_3$

$\longrightarrow$ similar enhancement of piezoelectric coefficient d_{33}

Table 2. Piezoelectric properties of $BaTiO_3$ and $KNbO_3$ single crystals.

poling direction	ferroic phase	compound (T $= 25\,°C$)	d_{33} [pC/N]	polarization vectors
[111]	$4mm$	$BaTiO_3$	203	[100], [010], [001]
	$3m$	[b]	145	[111][a]
[001]	$4mm$	$BaTiO_3$	125	[001][a]
	$3m$	[c]	350	[111], [$\bar{1}\bar{1}$1], [$\bar{1}$11], [1$\bar{1}$1]
[110]	$mm2_{xy}$	$KNbO_3$	18.4	[110][a]
[001]	$4mm$		51.7	[101], [$\bar{1}$01], [011], [0$\bar{1}$1]

[a] single domain state [b] $E > 40\,kV/cm$
[c] T $= -100\,°C$

PROBLEM:

DETERMINE ALL POSSIBLE ENGINEERED DOMAIN CONFIGURATIONS WHICH CAN BE PRODUCED BY EXTERNAL FIELDS

2. DOMAIN CONFIGURATIONS, AVERAGE TENSOR PROPERTIES AND EXTERNAL FIELDS

A simple model of a multidomain crystal

Basic characteristics:

- point groups of prototypic and ferroic phase, G and F, resp.
- $n = |\mathsf{G}|/|\mathsf{F}|$ possible single domain states $<1>, \ldots, <n>$

  $|\mathsf{G}|, |\mathsf{F}|$ - the number of operations in those point groups

  all states equivalent under G:

  $<j> = g_{i\to j}<i>$ for any $i \neq j$, $g_{i\to j} \notin \mathsf{F}_i = Stab_{\mathsf{G}}(<i>)$

  the stabilizer of the ith state

  numbering through left cosets of F_1 in G

  cosets $\mathsf{G} = \mathsf{F}_1 + g_2\mathsf{F}_1 + \cdots + g_n\mathsf{F}_1$

  states $<1>, <2> = g_2<1>, \ldots, <n> = g_n<1>$

- partial volumes v_i of the n states, $v_1 + \cdots + v_n = 1$

Domain configuration (DC)

$$C(v_i) = v_1{<1>} \sqcup v_2{<2>} \sqcup \ldots \sqcup v_n{<n>}$$

$\ldots \quad \sqcup \sim$ coexists with

Some concepts in use:

H-orbit of the state $<i>$, $\mathsf{H} \subset \mathsf{G}$: $\quad \mathsf{H} \star i = \{h<i>; h \in \mathsf{H}\}$

$\rightarrow$ H-decomposition: $\quad \{1, \ldots, n\} = \mathsf{H} \star i_1 \cup \cdots \cup \mathsf{H} \star i_p$

The closure H^c of the group H with respect to the group pair $\mathsf{G} \supset \mathsf{F}$:

$$\mathsf{H}^c = Stab_{\mathsf{G}}(\mathsf{H} \star i_1) \cap \cdots \cap Stab_{\mathsf{G}}(\mathsf{H} \star i_p) \supseteq \mathsf{H}$$

Characteristics of domain configurations

1. *Effective symmetry* K *of domain configuration* $C(v_i)$

$$\mathsf{K} = \{g \in \mathsf{G};\, gC(v_i) = v_1 g_{<1>} \sqcup \cdots \sqcup v_1 g_{<n>} = C(v_i)\}$$

... the stabilizer $\mathsf{K} = Stab_{\mathsf{G}}(C(v_i))$ of $C(v_i)$

stability condition of a DC $C(v_i)$ exposed to an external field $\boldsymbol{F}$:

$\mathsf{K} \subseteq \mathsf{J}^{\mathsf{c}}$, $\mathsf{J} = Stab_{\mathsf{O(3)}}(\boldsymbol{F}) \cap \mathsf{G}$

$Stab_{\mathsf{O(3)}}(\boldsymbol{F}) = \{g \in \mathsf{O(3)};\, g\boldsymbol{F} = \boldsymbol{F}\}$ ... orthogonal stabilizer of $\boldsymbol{F}$

Statement 1. A subgroup H of G is the stabilizer of some DC $C(v_i)$ if and only if it coincides with its closure, $\mathsf{H} = \mathsf{H}^{\mathsf{c}}$.

2. *Unique expression of any DC through coherent configurations*

Coherent DC $<j_1, \ldots, j_q>$ with the stabilizer K:

all states $<j_1>, \ldots, <j_q>$ form an orbit $\mathsf{K} \star j_1$

$$\Longrightarrow v_{j_1} = \cdots = v_{j_q} = \tfrac{1}{q} \quad \& \quad \mathsf{K} = Stab_{\mathsf{G}}(\mathsf{K} \star j_1)$$

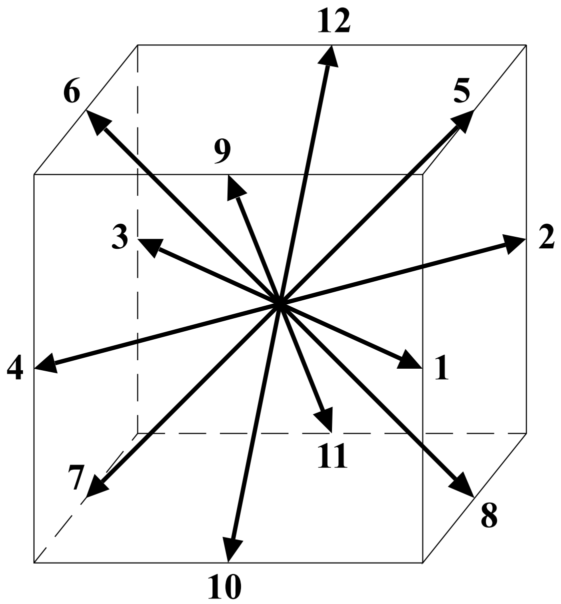
Statement 2. Any DC with stabilizer K is coherent or a unique combination of s coherent DC's $<i_{j,1}, \ldots, i_{j,r_j}>$, $s \leq n$:

$$C(u_j) = u_1 <i_{1,1}, \ldots, i_{1,r_1}> \sqcup \cdots \sqcup u_s <i_{s,1}, \ldots, i_{s,r_s}>$$

– $\mathsf{K} = Stab_{\mathsf{G}}(\mathsf{K} \star i_{1,1}) \cap \cdots \cap Stab_{\mathsf{G}}(\mathsf{K} \star i_{s,1})$

– u_j is a partial volume of the jth coherent DC, $u_1 + \cdots + u_s = 1$

3. *Example of potassium niobate: ferroelectric Amm2-phase.*



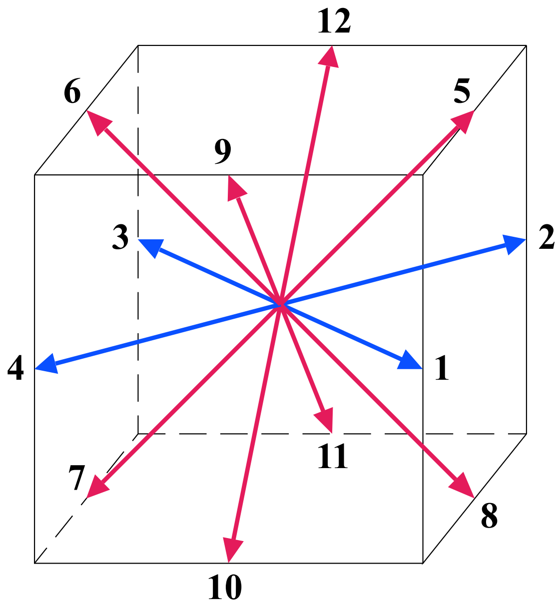
prototypic group $\mathsf{G} = \mathsf{m\bar{3}m}$
ferroic group $\mathsf{F} = \mathsf{2_{xy}m_{x\bar{y}}m_z}$

twelve ferroelectric states

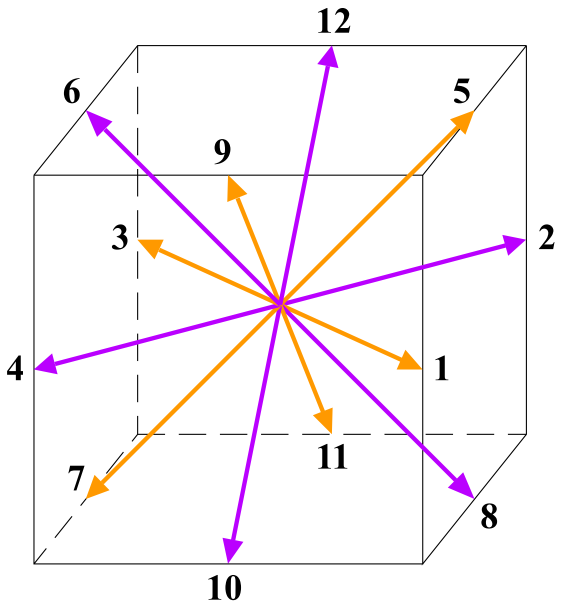
ith state – polarization $\boldsymbol{P}^{(i)}$
$\leftrightarrow$ oriented line with arrow

$\hookrightarrow$ initial non-ferroelectric coherent DC $<1, 2, \ldots, 12>$
Stabilizer $\mathsf{K} = \mathsf{m\bar{3}m}$

Non-ferroelectric coherent DC's produced by mechanical stress $\boldsymbol{T}$



Stress field $T_{11} = T_{22} \neq T_{33}$
$Stab_{\mathsf{O(3)}}(\boldsymbol{T}) = \mathsf{\infty_z/m_zmm}$
Configurations:
$<1, 2, 3, 4>$,
$<5, 6, 7, 8, 9, 10, 11, 12>$
Stabilizer $\mathsf{K} = \mathsf{4_z/m_zm_xm_{xy}}$



Stress field $T_{11} = T_{22} = T_{33}$,
$T_{23} = T_{31} = T_{12}$
$Stab_{\mathsf{O(3)}}(\boldsymbol{T}) = \infty_{\mathsf{xyz}}/\mathsf{m_{xyz}mm}$
Configurations:
$<1, 3, 5, 7, 9, 11>$,
$<2, 4, 6, 8, 10, 12>$
Stabilizer $\mathsf{K} = \bar{3}_{\mathsf{xyz}} 2_{\mathsf{x\bar{y}}}/\mathsf{m_{x\bar{y}}}$

4. *Average tensor properties of a DC* $C(v_i)$.

The average $\overline{\boldsymbol{T}}$ of a tensor property $\boldsymbol{T}$ (first approximation):

$$\sim \quad \overline{\boldsymbol{T}} = v_1 \boldsymbol{T}^{(1)} + \cdots + v_n \boldsymbol{T}^{(n)}$$

$\boldsymbol{T}^{(i)}$ – contribution from the ith state

Final expressions:

coherent DC $<j_1, \ldots, j_q>$ $\quad \sim \quad \overline{\boldsymbol{T}} = \frac{1}{q}(\boldsymbol{T}^{(j_1)} + \cdots + \boldsymbol{T}^{(j_q)})$

general DC $\quad C(u_j) = u_1 <i_{1,1}, \ldots, i_{1,r_1}> \sqcup \cdots \sqcup u_s <i_{s,1}, \ldots, i_{s,r_s}>$

$$\sim \quad \overline{\boldsymbol{T}} = u_1 \overline{\boldsymbol{T}}^{(1)} + \cdots + u_s \overline{\boldsymbol{T}}^{(s)}$$

$\overline{\boldsymbol{T}}^{(j)}$ – contribution from the jth coherent DC

3. TENSOR PROPERTIES OF COHERENT CONFIGURATIONS

Tensor representation S of rank m

Tensor space L : basis – $\{\boldsymbol{e}_{jk\ldots};\underbrace{j,k,\ldots}_{m-\text{indices}}=1,2,3\}$, $\dim L=3^m$

$S:\mathsf{O}(3)\ni g\rightarrow S(g)\in\mathsf{GL}(L)$,

$$S(g)\boldsymbol{e}_{jk\ldots}=\sum_{j'k'\ldots=1}^{3}\varepsilon(g)D_{j'j}(g)D_{k'k}(g)\cdots\boldsymbol{e}_{j'k'\ldots}\,,\quad j,k,\ldots=1,2,3$$

$$\varepsilon(g)=\left\{\begin{array}{ll}1 & -\text{ polar}\\ |D(g)| & -\text{ axial}\end{array}\right\}\ \text{tensors}\qquad m=1:S\sim\left\{\begin{array}{l}D_{1u}\\ D_{1g}\end{array}\right.$$

$m\geq 2$: a tensor property $\boldsymbol{T}=\sum_{jk\ldots=1}^{3}T_{jk\ldots}\boldsymbol{e}_{jk\ldots}$

permutational symmetry of m indices ... $Q_{\boldsymbol{T}}\subseteq\mathsf{S_m}$

$\pi\in Q_{\boldsymbol{T}}$: $S(\pi)\boldsymbol{e}_{j_1j_2\ldots}=\boldsymbol{e}_{j'_1j'_2\ldots},\ j'_k=j_{\pi^{-1}(k)}\,,\ k=1,2,\ldots$

projection operator $P_{Q_{\boldsymbol{T}}}=\frac{1}{|Q_{\boldsymbol{T}}|}\sum_{\pi\in Q_{\boldsymbol{T}}}S(\pi)$: $P_{Q_{\boldsymbol{T}}}L=L^{\boldsymbol{T}}$

... carrier space of tensor $\boldsymbol{T}$

polar tensor $\boldsymbol{T}$: $Q_{\boldsymbol{T}}=C_1\Longrightarrow L^{\boldsymbol{T}}=L,\ S\sim D_{1u}^m$

$Q_{\boldsymbol{T}}\neq C_1\Longrightarrow L^{\boldsymbol{T}}\subset L, S\sim[D_{1u}^m]^{Q_{\boldsymbol{T}}}$ ... *symmetrized power*

Neumann's principle: $Stab_{\mathsf{O(3)}}(\boldsymbol{T}^{(1)})\supseteq\mathsf{F}_1$

$\Longleftrightarrow$ $\mathsf{F}_1<1>=<1>\Rightarrow$ tensor property $\boldsymbol{T}^{(1)}\in L_{\mathsf{F}_1}\subseteq L^{\boldsymbol{T}}$

$L_{\mathsf{F}_1}=\{\boldsymbol{x}=\sum_{jk\ldots=1}^{3}x_{jk\ldots}\boldsymbol{e}_{jk\ldots}\in L^{\boldsymbol{T}};S(f)\boldsymbol{x}=\boldsymbol{x}\text{ for all }f\in\mathsf{F}_1\}$

... stability space of F_1

projection operator $P_{\mathsf{F}_1}=\frac{1}{|\mathsf{F}_1|}\sum_{f\in\mathsf{F}_1}S(f)$: $P_{\mathsf{F}_1}L^{\boldsymbol{T}}=L_{\mathsf{F}_1}$

a coherent DC $<j_1,\ldots,j_p>$, $Stab_{\mathsf{G}}(<j_1,\ldots,j_p>)=\mathsf{K}$:

$$\overline{\boldsymbol{T}}=\frac{1}{p}(\boldsymbol{T}^{(j_1)}+\cdots+\boldsymbol{T}^{(j_p)})=P_{\mathsf{K}}\boldsymbol{T}^{(j_1)}=\cdots=P_{\mathsf{K}}\boldsymbol{T}^{(j_p)}\in L_{\mathsf{K}}$$

Statement 3. The average property $\overline{\boldsymbol{T}}$ of a coherent configuration $<j_1, \ldots, j_p>$ will have the same form as the tensor $\boldsymbol{T}$ of a single domain crystal with equal macroscopic symmetry K if $P_{\mathsf{K}} L_{\mathsf{F}_{j_1}} = L_{\mathsf{K}}$.

Basic observations: $P_{\mathsf{K}} L_{\mathsf{F}_{j_1}} = 0 \Longleftrightarrow L_{\mathsf{K}} \perp L_{\mathsf{F}_{j_1}}$.

Four cases: ○ $P_{\mathsf{K}} L_{\mathsf{F}_{j_1}} = 0 \Longrightarrow \overline{\boldsymbol{T}} = 0$

● $P_{\mathsf{K}} L_{\mathsf{F}_{j_1}} = L_{\mathsf{K}} \Longrightarrow Stab_{\mathsf{O}(3)}(\overline{\boldsymbol{T}}) = Stab_{\mathsf{O}(3)}(\boldsymbol{T})$

□ $0 \subset P_{\mathsf{K}} L_{\mathsf{F}_{j_1}} \subset L_{\mathsf{K}}$ & $Stab_{\mathsf{O}(3)}(\overline{\boldsymbol{T}}) = Stab_{\mathsf{O}(3)}(\boldsymbol{T})$

△ $0 \subset P_{\mathsf{K}} L_{\mathsf{F}_{j_1}} \subset L_{\mathsf{K}} \Longleftarrow Stab_{\mathsf{O}(3)}(\overline{\boldsymbol{T}}) \supset Stab_{\mathsf{O}(3)}(\boldsymbol{T})$

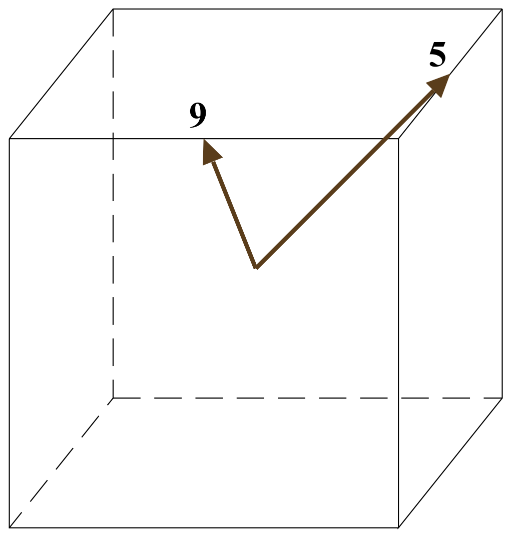
Similar four cases after projection $P^{R_{q_i}}: L^{\boldsymbol{T}} \rightarrow L^{\boldsymbol{T}, R_{q_i}}, \boldsymbol{T} \rightarrow \boldsymbol{T}^{R_{q_i}}$

R_{q_i} - *an irreducible representation (irep)* of G

$L^{\boldsymbol{T}, R_{q_i}}$ - maximal G-invariant subspace of $L^{\boldsymbol{T}}$ whose G-irreducible subspaces afford just the irep R_{q_i}

$L_{\mathsf{F}_{j_1}} \rightarrow L_{\mathsf{F}_{j_1}}^{R_{q_i}} = L_{\mathsf{F}_{j_1}} \cap L^{\boldsymbol{T}, R_{q_i}}$, $L_{\mathsf{K}} \rightarrow L_{\mathsf{K}}^{R_{q_i}} = L_{\mathsf{K}} \cap L^{\boldsymbol{T}, R_{q_i}}$

Ferroelectric monoclinic coherent DC produced by electric field



Electric field (E_1, E_1, E_3), $|E_1| < |E_3|$

$Stab_{\mathsf{O}(3)}(\boldsymbol{E}) = \infty_{[11\kappa]} \mathsf{m}_{\mathsf{x}\bar{\mathsf{y}}} \mathsf{m}$.

Configuration $<5, 9>$

Stabilizer $\mathsf{K} = \mathsf{m}_{\mathsf{x}\bar{\mathsf{y}}}$

TENSOR PROPERTIES OF A COHERENT DOMAIN CONFIGURATION

with average symmetry K= mx-y in $KNbO_3$

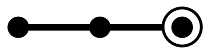
L= $Stab_{O(3)}(\boldsymbol{T})$ - orthogonal stabilizer of a tensor $\boldsymbol{T}$

coherent DC <5,9>

single domain state

stabilizer K= mx-y

tensor components

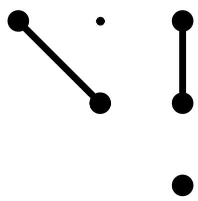


Polarization

P_1 P_2 P_3

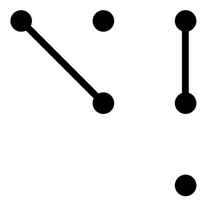
L= $\infty_{\parallel \boldsymbol{P}}$mm

$\boldsymbol{P} \sim \boldsymbol{V}$



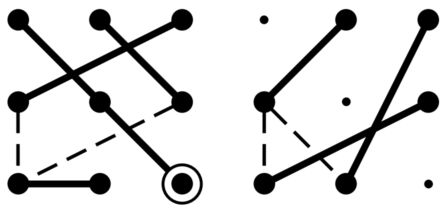
Strain tensor

$\boldsymbol{e} \sim [\boldsymbol{V}^2]$



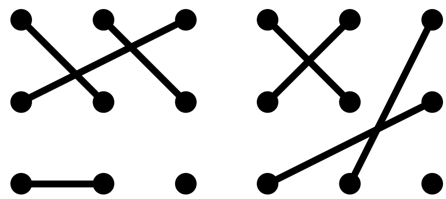
e_{11} e_{12} e_{13}
e_{22} e_{23}
e_{33}

L= 2x-y / mx-y



Piezoelectric tensor

$\boldsymbol{d} \sim \boldsymbol{V}[\boldsymbol{V}^2]$



L= mx-y

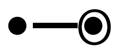
· = Ø

• ≠ Ø

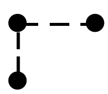
$d_{i\lambda}$: $i = 1,2,3$
$\lambda = 1,...,6$

 *equal components*

$d_{i\lambda} = d_{ijj}$, $\lambda = j$

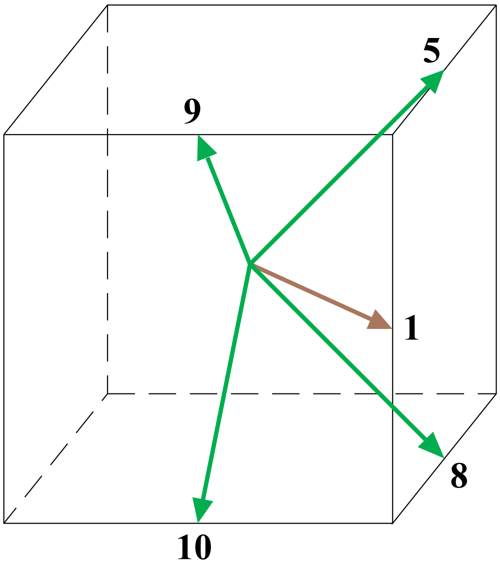
 2 x *former comp.*

$d_{i\lambda} = 2d_{ijk}$, $j \neq k$,
$\lambda = 9 - j - k$

 *2 dashed lines intersect in the sum of connected comps.*

4. FERROELECTRIC COHERENT CONFIGURATIONS OF $\boldsymbol{Amm2}$-PHASE OF POTASSIUM NIOBATE CRYSTALS

Coherent configurations



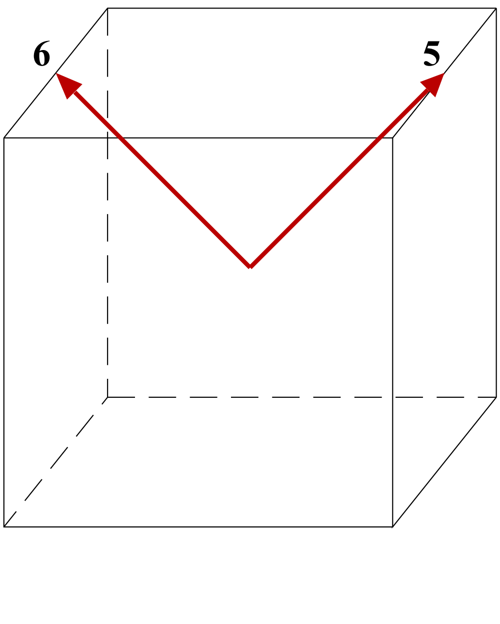
Electric field $(E_1, E_1, 0)$

$Stab_{\mathsf{O(3)}}(\boldsymbol{E}) = \infty_{\mathsf{xy}}\mathsf{m}_{\mathsf{x\bar{y}}}\mathsf{m}_{\mathsf{z}}$

Configurations

$<1>$ and $<5, 8, 9, 10>$

Stabilizer $\mathsf{K} = 2_{\mathsf{xy}}\mathsf{m}_{\mathsf{x\bar{y}}}\mathsf{m}_{\mathsf{z}}$



Electric field $(0, 0, E_3)$

mech. stress T_{11}, T_{22}, T_{33}

$Stab_{\mathsf{O(3)}}(\boldsymbol{E}) = \infty_{\mathsf{z}}\mathsf{m}_{\mathsf{x}}\mathsf{m}_{\mathsf{y}}$

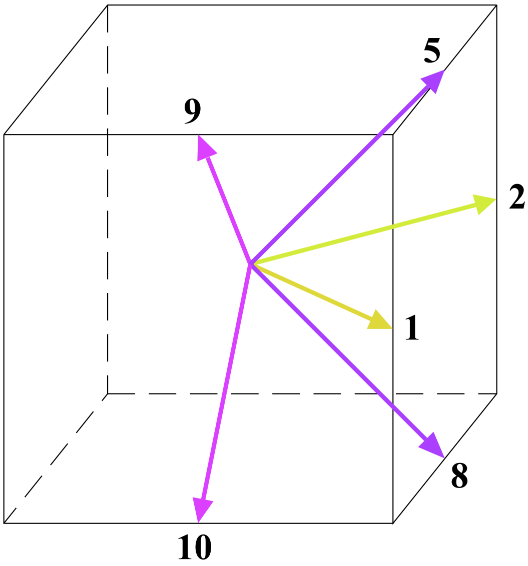
$Stab_{\mathsf{O(3)}}(\boldsymbol{T}) = \mathsf{m}_{\mathsf{z}}\mathsf{m}_{\mathsf{x}}\mathsf{m}_{\mathsf{y}}$

Configuration

$<5, 6>$

Stabilizer $\mathsf{K} = \mathsf{m}_{\mathsf{x}}\mathsf{m}_{\mathsf{y}}2_{\mathsf{z}}$

Minimal incoherent configurations



Electric field $(E_1, E_2, 0)$

$Stab_{\mathsf{O(3)}}(\boldsymbol{E}) = \infty_{[1\kappa 0]}\mathsf{m_z m}.$

Configurations

$u_1{<}1{>} \sqcup u_2{<}2{>}$,

$u_1{<}5, 8{>} \sqcup u_2{<}9, 10{>}$,

$u_1{<}1{>} \sqcup u_2{<}5, 8{>}$,

$u_1{<}2{>} \sqcup u_2{<}9, 10{>}$

Stabilizer $\mathsf{K} = \mathsf{m_z}$

Non-coherent DC $C(u_j)$:

$$C(u_j) = u_1{<}i_{1,1}, \ldots, i_{1,r_1}{>} \sqcup \cdots \sqcup u_s{<}i_{s,1}, \ldots, i_{s,r_s}{>}$$

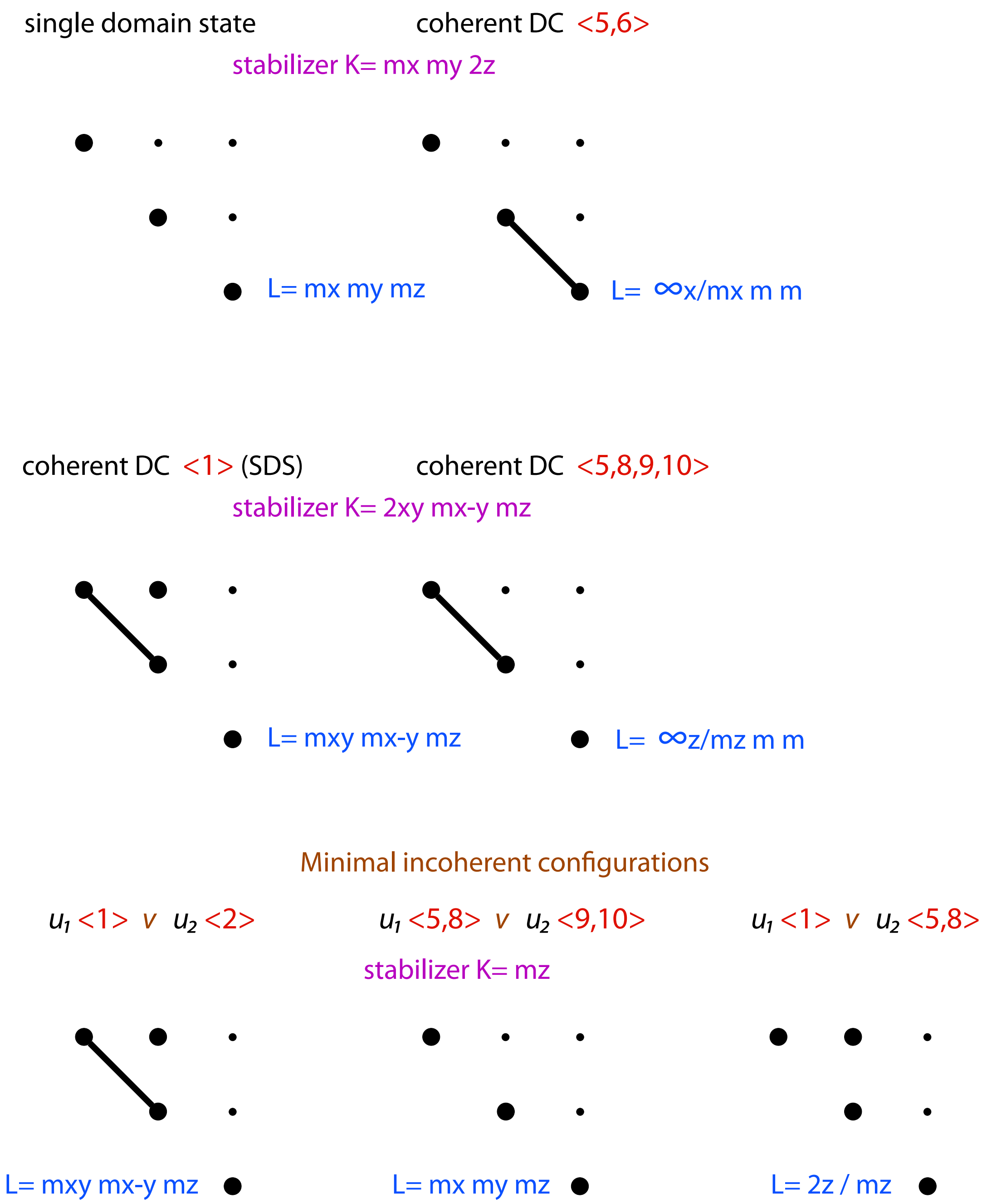
$Stab_{\mathsf{G}}({<}i_{j,1}, \ldots, i_{j,r_j}{>}) = \mathsf{K}_j,\ j = 1, \ldots, s$

$Stab_{\mathsf{G}}(C(u_j)) = \mathsf{K} = \mathsf{K}_1 \cap \cdots \cap \mathsf{K}_s = \bigcap_{j=1}^{s} \mathsf{K}_j$

$\mathsf{K} \neq \bigcap_{j\neq k} \mathsf{K}_j,\ k = 1, \ldots, s \quad \Longrightarrow$ minimal incoherent DC

DOMAIN CONFIGURATIONS IN POTASSIUM NIOBATE:

FORM OF STRAIN TENSOR ***e*** and its orthogonal stabilizer $L = Stab_{O(3)}(\boldsymbol{e})$



5. CONCLUSIONS

Tensor properties (summary): Coherent DC's vs. single domain states

Table 3. Non-equivalent coherent DC's produced by electric field. Comparison with hypothetic single domain states of same symmetry.

Electric field $\boldsymbol{E}$	Coherent DC's	Stabilizer K of DC	Stabilizers: $\overline{\boldsymbol{T}}$ vs. $\boldsymbol{T}$	Tensor form
$(0, 0, E_3)$	$<5, 6, 9, 12>$	$4_z m_x m_{x\bar{y}}$	$=$	$=$
(E_1, E_1, E_1)	$<1, 5, 9>$	$3_{xyz} m_{x\bar{y}}$	$=$	$\neq$
$(E_1, E_1, 0)$	$<1>$; $<5, 8, 9, 10>$	$2_{xy} m_{x\bar{y}} m_z$	$=$; $\neq$	$=$; $\neq$
(E_1, E_1, E_3) $\lvert E_1\rvert < \lvert E_3\rvert$	$<5, 9>$	$m_{x\bar{y}}$	$=$	$\neq$
	Minimal incoherent DC's			
$(E_1, E_2, 0)$	$u_1<1> \sqcup u_2<2>$;	m_z	$\neq$	$\neq$
	$u_1<5, 8> \sqcup u_2<9, 10>$;		$\neq$	$\neq$
	$u_1<1> \sqcup u_2<5, 8>$;		$=$	$\neq$
	$u_1<1> \sqcup u_2<6, 7>$		$=$	$\neq$

DC's will not have minimal free energy in electric field alone

Table 4. Non-equivalent coherent DC's produced by electric field and mechanical stress.

El. field $\boldsymbol{E}$	Stress $\boldsymbol{T}$	Coherent DC's	Stabilizer K of DC	Stabilizers: $\overline{\boldsymbol{T}}$ vs. $\boldsymbol{T}$	Tensor form
$(0, 0, E_3)$	T_{11}, T_{22}, T_{33}	$<5, 6>$	$m_x m_y 2_z$	$\neq$	$\neq$
$(E_1, -E_1, 0)$	$T_{11} = T_{22}, T_{33}$, $T_{23} = T_{31}$	$<5, 11>$	$2_{x\bar{y}}$	$=$	$\neq$

Main results

- *6* non-equivalent *coherent DC's can be*, theoretically, *produced by electric field*, possibly in combination with additional stress

- *In 5 coherent DC's form of* odd rank and/or even rank *tensors differs from* tensor form in a *single domain crystal with same symmetry*:

  – for 2 orthorhombic coherent DC's the stabilizers of even rank tensors are different than for respective single domain states

  – in 4 cases, $\mathsf{3_{xyz}m_{x\bar{y}}}$, $\mathsf{m_x m_y 2_z}$, $\mathsf{2_{x\bar{y}}}$ and $\mathsf{m_{x\bar{y}}}$, pseudo-spontaneous tensor components are forbidden in the ferroelectric $Amm2$-phase

  – for coherent DC's whose stabilizer is one of ferroic groups, certain spontaneous tensor component(s) will be zero due to the orthogonality of relevant stability spaces, e.g.

  $$<5, 8, 9, 10> : \; L^{T_{2g}}_{\mathsf{K=2_{xy}m_{x\bar{y}}m_z}} \perp L^{T_{2g}}_{\mathsf{F_5=m_x 2_{yz} m_{y\bar{z}}}} \Rightarrow \bar{e}_{12} = 0$$

- *Quite similar features were established for* 4 *incoherent DC's* with the monoclinic stabilizer $\mathsf{m_z}$.

Concluding remarks

non-equivalent coherent configurations $\longrightarrow$ new materials

- stabilizer K of a coherent DC stands as 'fake' ferroic symmetry
- average properties are given by single domain parameters

Five basic cases:

Comparison of average tensor form with single domain form for odd- and even-parity tensors.

case		tensor parity odd	even	stabilizer K of coherent DC $[\boldsymbol{T}]$
A		same	same	4mm
B		different	different	$m_{x\bar{y}}$
C		same	different	$m_x m_y 2_z, 2_{xy} m_{x\bar{y}} m_z$
D		different	same	-
E	a_1	same	mixed case	-
	a_2	mixed case	same	$3m\ [\boldsymbol{P}] \quad \approx D$
	b_1	different	mixed case	-
	b_2	mixed case	different	$2_{x\bar{y}}\ [\boldsymbol{P}] \quad \approx B$
	c	mixed case	mixed case	-

mixed case - not for all tensors with same parity both forms coincide

$[\boldsymbol{T}]$ - both forms coincide/differ for tensor $\boldsymbol{T}$