

Tenzorový popis fyzikálních vlastností

Typ veličin

- ◆ skalární - hmotnost, objem, energie, teplo, ...
- ◆ vektorové - intenzita elektrického a magnetického pole, gradient teploty a koncentrace, difúzní tok, ...
- ◆ tenzorové - mechanické a elektrické napětí, deformace, difúzní koeficient, ...

Tenzor vyjadřuje závislost fyzikální vlastnosti na krystalografickém směru.

Příklady

◆ Pyroelektrický jev

$$\Delta \vec{P} = \vec{p} \Delta T$$

max = 3 komponenty

◆ Elektrická vodivost $\vec{j} = \vec{\sigma} \vec{E}$

max = 9 komponent $\vec{j} = -\vec{D} \nabla c$

◆ Difúzní tok

$$\vec{\varepsilon} = \vec{S} \vec{\sigma}$$

max = 9 komponent

◆ Mechanická deformace

Nezávislé složky tenzorů vlastností

$$B_{ijk\dots} = T_{ijk\dots lmn\dots} A_{lmn\dots}$$

řád p

řád p + q

řád q

Skupina	Fyzikální veličiny		Nezávislé složky
1	skalár	skalár	1
2	skalár	vektor	3
3	skalár	symetrický tenzor	6
4	skalár vektor	nesymetrický tenzor vektor	9
5	vektor	symetrický tenzor	18
6	vektor	nesymetrický tenzor	27
7	symetrický tenzor	symetrický tenzor	36
8	symetrický tenzor	nesymetrický tenzor	54
9	nesymetrický tenzor	nesymetrický tenzor	81

Redukce nezávislých složek díky symetrii

Bodová grupa	1	2	3	4	5	6	7	8	9
2	1	1	4	5	8	13	20	28	41
<i>mm2</i>	1	1	3	3	5	7	12	15	21
<i>mmm</i>	1	0	3	3	0	0	12	15	21
4	1	1	2	3	4	7	10	14	21
<i>3m</i>	1	1	2	2	4	5	8	10	14
<i>6/m</i>	1	0	2	3	0	0	8	12	19
<i>6/mmm</i>	1	0	2	2	0	0	6	7	10
432	1	0	1	1	0	1	3	3	4
<i>m-3m</i>	1	0	1	1	0	0	3	3	4

Elektrická vodivost v kubických krystalech je skalár

Další redukce díky zákonu zachování energie ($a_{ik} = a_{ki}$)

Fyzikální vlastnost v určitém směru

Vlastnost T

$$p_i = \sum_k T_{ik} q_k$$

Hodnota vlastnosti T
ve směru \mathbf{q}

$$[T]_{\mathbf{q}} = \frac{p_{\parallel}}{q}$$

Směrové kosiny

$$c_k = \cos(\mathbf{q}, \mathbf{x}_k)$$

$$p_i = \sum_k T_{ik} q c_k = \sum_k q T_{ik} c_k$$

$$p_{\parallel} = \sum_i c_i p_i = \sum_i \sum_k c_i T_{ik} c_k$$

$$[T]_{\mathbf{q}} = \sum_i \sum_k c_i T_{ik} c_k$$

Pro symetrický tenzor

$$[T]_{\mathbf{q}} = T_{11}c_1^2 + T_{22}c_2^2 + T_{33}c_3^2 + 2T_{12}c_1c_2 + 2T_{23}c_2c_3 + 2T_{13}c_1c_3$$

Kvadrík

$$\sum_i \sum_k x_i T_{ik} x_k = 1$$

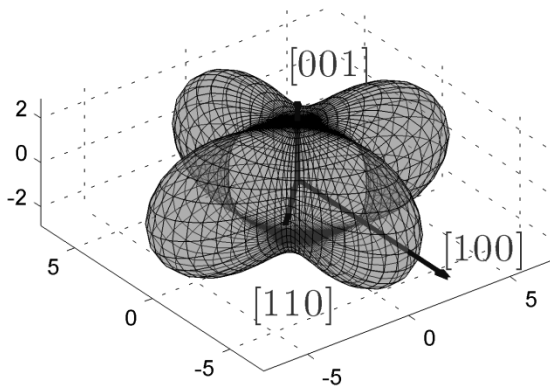
Plocha druhého stupně

pro kladné T_{ii} elipsoid

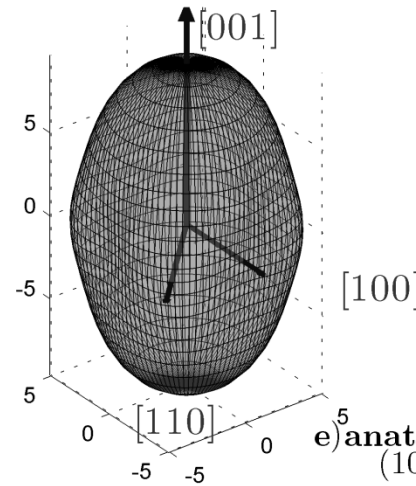
$$[T]_{c_1c_2c_3} = \frac{1}{r^2}$$

Young's modulus

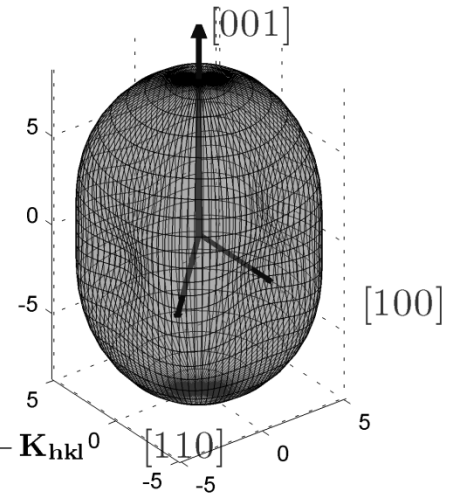
a) rutile - $1/E(\mathbf{q})$
(1/TPa)



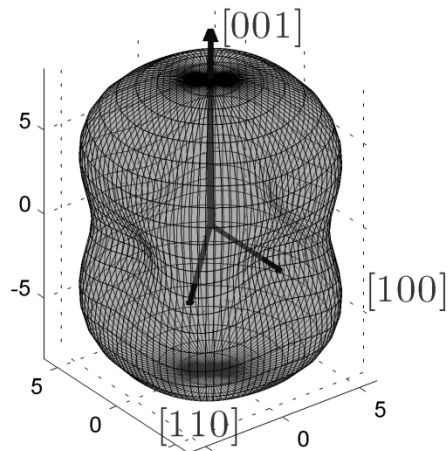
b) anatase - $1/E(\mathbf{q})$ [33]
(1/TPa)



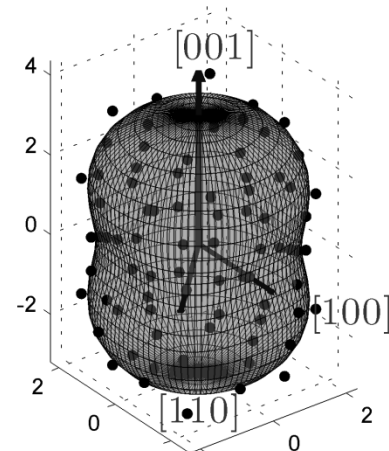
c) anatase - $1/E(\mathbf{q})$ [34]
(1/TPa)



d) anatase - $1/E(\mathbf{q})$ [35]
(1/TPa)



e) anatase - K_{hkl}^0
(10⁻³)



Neumannův princip

Symetrie fyzikální vlastnosti nemůže být nižší, než je symetrie daná bodovou grupou krystalu.

Grupa G_T operací symetrie fyzikální vlastnosti T krystalu musí obsahovat všechny operace symetrie bodové grupy K tohoto krystalu. Grupa K je tedy podgrupou grupy G_T , $K \subset G_T$.

Speciální aplikace: Index lomu kubických krystalů je popsán degenerovaným elipsoidem (koulí). Totéž platí pro (anizotropní) teplotní kmity atomů.

Naopak: Nejvyšší možnou symetrii krystalu lze určit ze symetrie jeho (fyzikálních) vlastností

Voigtův princip

Pro splnění Neumannova principu je postačující invariantnost složek tenzoru T (tenzoru fyzikálních vlastností) při operacích symetrie grupy K (krystalové symetrie).

Tenzor fyzikální vlastnosti se nesmí měnit při žádné operaci grupy symetrie K krystalu.

Aplikace: Vztahy mezi jednotlivými komponentami tenzoru T lze určit působením operací symetrie na T .

Př. – dvojčetná osa podél x_2 ,

$$c'_1 = -c_1, c'_2 = c_2, c'_3 = -c_3$$

$$T_{12} = T_{23} = 0$$

4 nezávislé složky

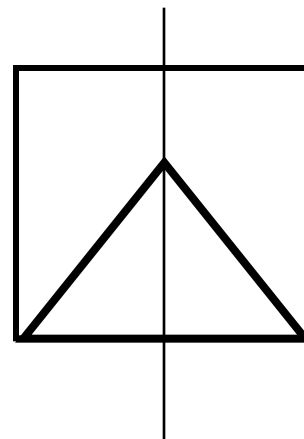
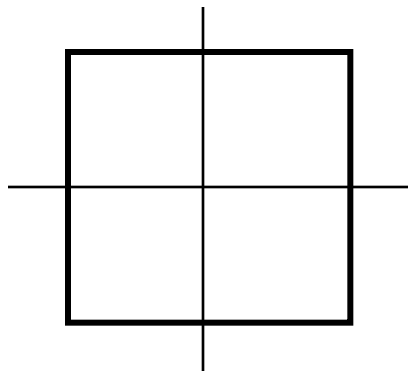
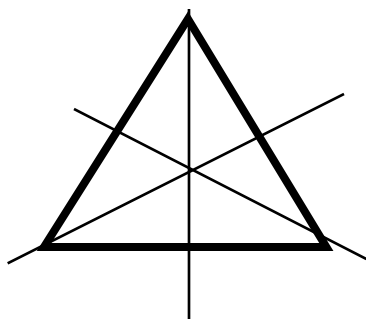
Curieův princip

Krystal změní svoji bodovou symetrii pod vlivem vnějšího působení tak, že zachová pouze ty prvky symetrie, které jsou společné s prvky symetrie tohoto působení.

$$\tilde{K} = K \cap G$$

K ... bodová grupa symetrie krystalu

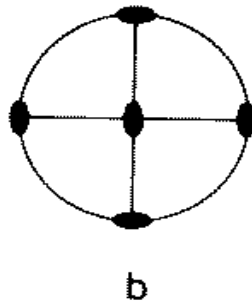
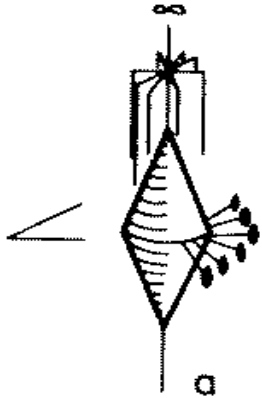
G ... grupa prvků symetrie vnějšího působení



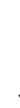
Při skalárním působení nemůže dojít ke změně symetrie (např. teplotní roztažnost).

Kubický krystal $m-3$

Homogenní jednoosé mechanické napětí ve směru $[001]$

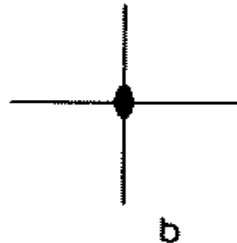


$\infty/m (2/m, 2/m, 2/m \dots)$



Ortorombická mmm

Elektrické pole ve směru $[001]$

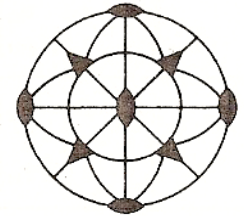


$\infty mmm \dots$



Ortorombická $mm2$

Ztráta středu symetrie



Strukturní fázové přechody

BaTiO₃ nad 405 K kubický, $m-3m$, paraelektrický

278 K < T < 405 K

Polarizace $\parallel \langle 001 \rangle$

Grupa $4mm$, tetragonální ferroelektrická fáze

183 K < T < 278 K

Polarizace $\parallel \langle 110 \rangle$

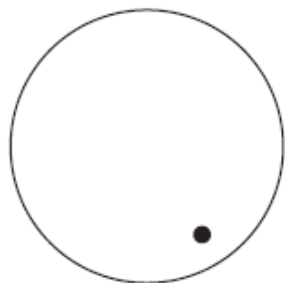
Grupa $mm2$, ortorombická ferroelektrická fáze

T < 183 K

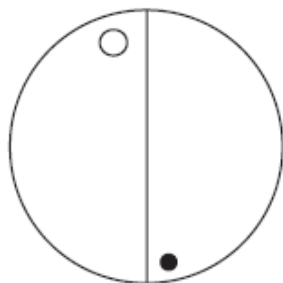
Polarizace $\parallel \langle 111 \rangle$

Grupa $-3m$, trigonální ferroelektrická fáze

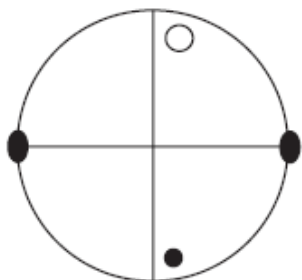
Symetrie 32 bodových grup



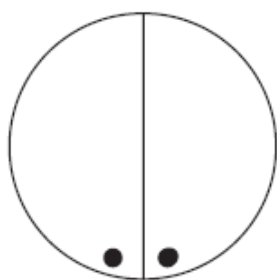
1



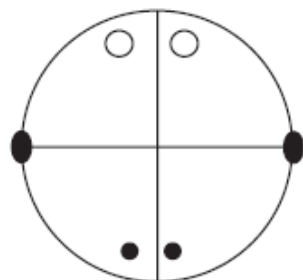
$\bar{1}$



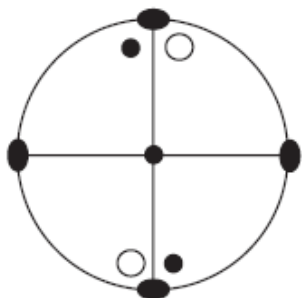
2



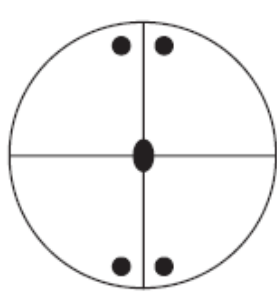
m



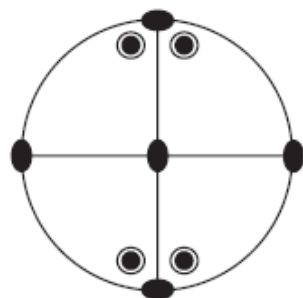
$2/m$



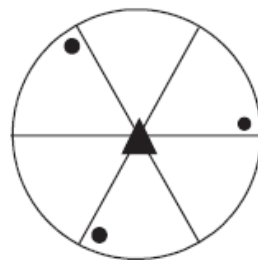
222



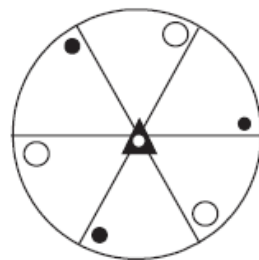
$mm2$



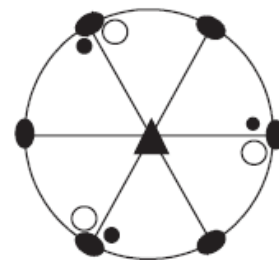
mmm



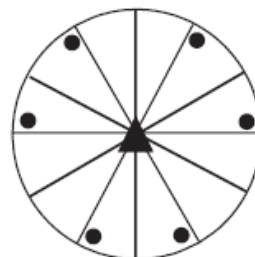
3



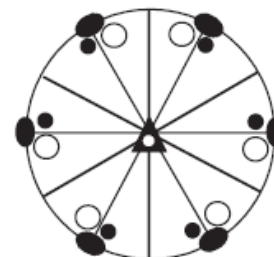
$\bar{3}$



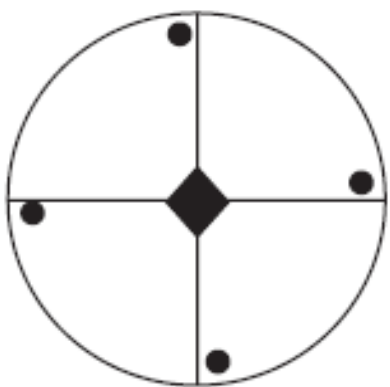
32



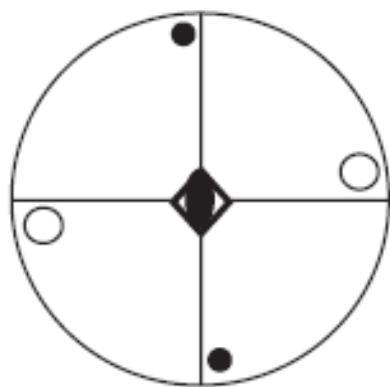
$3m$



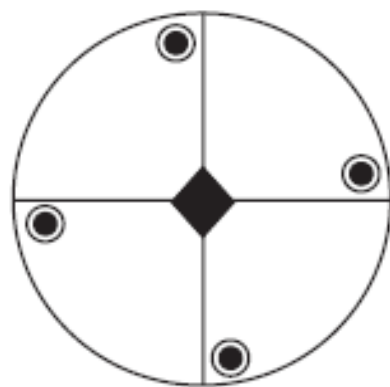
$\bar{3}m$



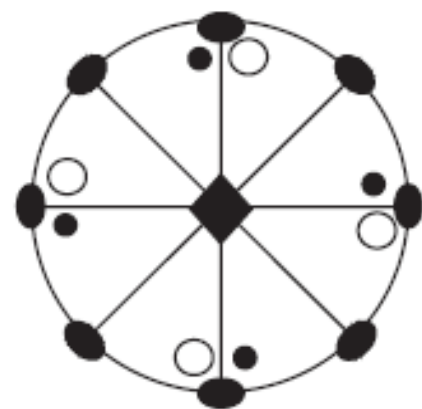
4



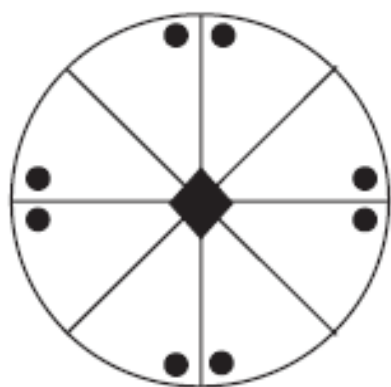
$\bar{4}$



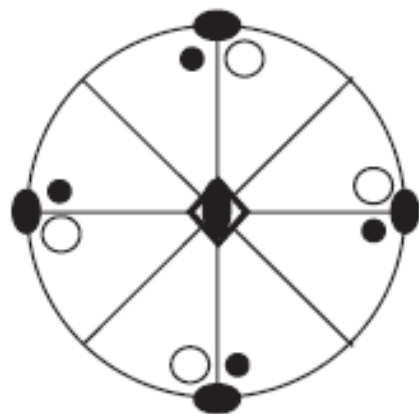
$4/m$



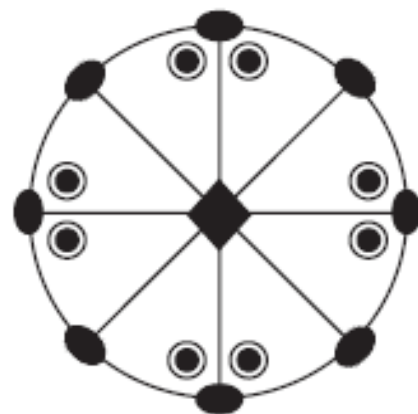
422



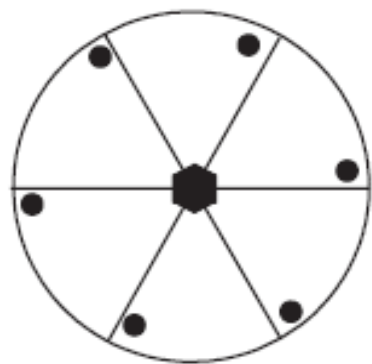
$4mm$



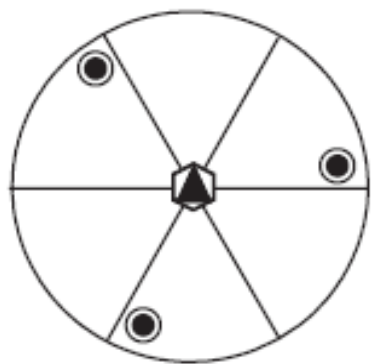
$\bar{4}2m$



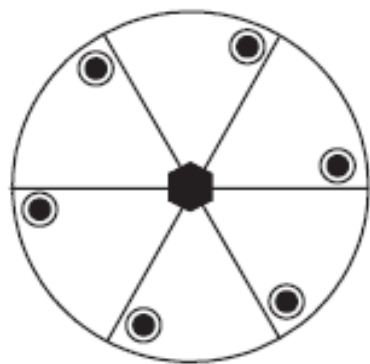
$4/mmm$



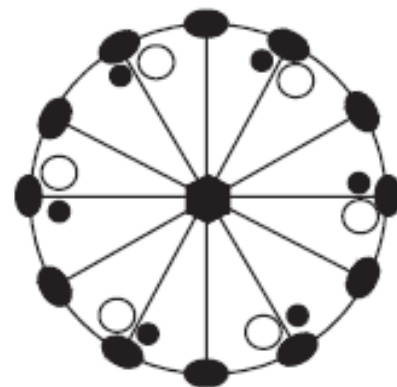
6



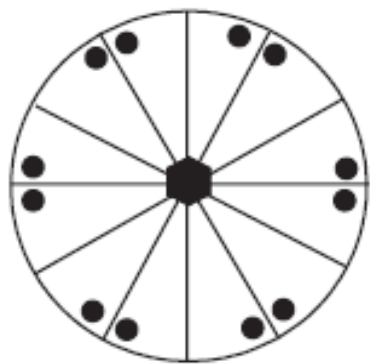
$\bar{6}$



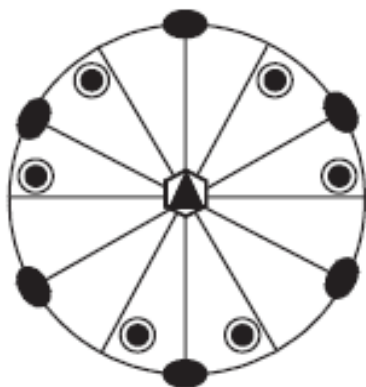
$6/m$



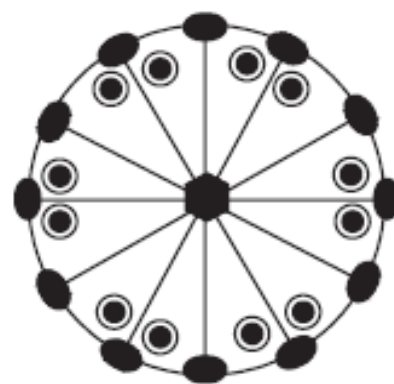
622



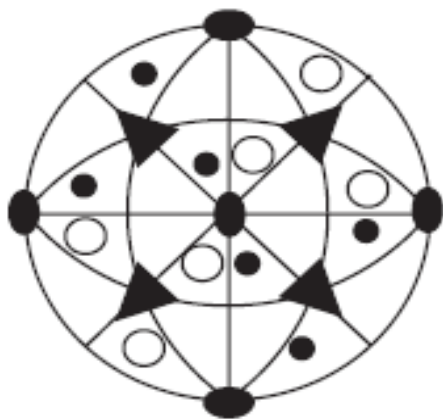
$6mm$



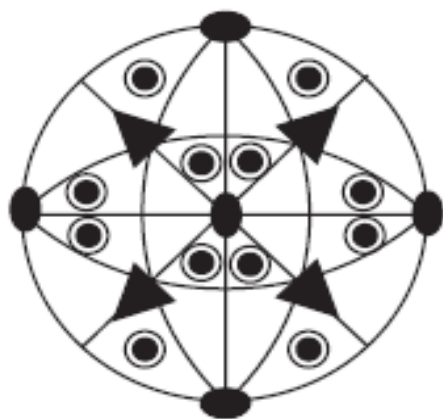
$\bar{6}m2$



$6/mmm$



23



$m\bar{3}$



432



$\bar{4}3m$



$m\bar{3}m$

$1 = C_1$	Kaolinite	$\text{Al}_2\text{Si}_2\text{O}_5(\text{OH})_4$
$\bar{1} = C_i$	Copper sulfate	$\text{CuSO}_4 \cdot 5\text{H}_2\text{O}$
$2 = C_2$	Sucrose	$\text{C}_{12}\text{H}_{22}\text{O}_{11}$
$m = C_s$	Potassium nitrite	KNO_2
$2/m = C_{2h}$	Orthoclase	KAlSi_3O_8
$222 = D_2$	Iodic acid	HIO_3
$mm2 = C_{2v}$	Sodium nitrite	NaNO_2
$mmm = D_{2h}$	Forsterite	Mg_2SiO_4
$3 = C_3$	Nickel tellurate	Ni_3TeO_6
$\bar{3} = C_{3i}$	Ilmenite	FeTiO_3
$32 = D_3$	Low-quartz	SiO_2
$3m = C_{3v}$	Lithium niobate	LiNbO_3
$\bar{3}m = D_{3d}$	Corundum	Al_2O_3
$4 = C_4$	Iodosuccinimide	$\text{C}_4\text{H}_4\text{INO}_2$
$\bar{4} = S_4$	Boron phosphate	BPO_4
$4/m = C_{4h}$	Scheelite	CaWO_4
$422 = D_4$	Nickel sulfate	$\text{NiSO}_4 \cdot 6\text{H}_2\text{O}$
$4mm = C_{4v}$	Barium titanate	BaTiO_3
$\bar{4}2m = D_{2d}$	Potassium dihydrogen phosphate	KH_2PO_4
$4/mmm = D_{4h}$	Rutile	TiO_2
$6 = C_6$	Nepheline	$\text{NaAlSi}_3\text{O}_8$
$\bar{6} = C_{3h}$	Lead germanate	$\text{Pb}_5\text{Ge}_3\text{O}_{11}$
$6/m = C_{6h}$	Apatite	$\text{Ca}_5(\text{PO}_4)_3\text{F}$
$622 = D_6$	High-quartz	SiO_2
$6mm = C_{6v}$	Zincite	ZnO
$\bar{6}m2 = D_{3h}$	Benitoite	$\text{BaTiSi}_3\text{O}_9$
$6/mmm = D_{6h}$	Beryl	$\text{Be}_3\text{Al}_2\text{Si}_6\text{O}_{18}$
$23 = T$	Sodium chlorate	NaClO_3
$m3 = T_h$	Pyrite	FeS_2
$432 = O$	Manganese	$\beta\text{-Mn}$
$\bar{4}3m = T_d$	Zincblende	ZnS
$m3m = O_h$	Rocksalt	NaCl

Příklady Bodové symetrie

	I	O
1	0.67%	1.24%
$\bar{1}$	13.87	19.18
2	2.21	6.70
<i>m</i>	1.30	1.46
<i>2/m</i>	34.63	44.81
222	3.56	10.13
<i>mm2</i>	3.32	3.31
<i>mmm</i>	12.07	7.84
3	0.36	0.32
$\bar{3}$	1.21	0.58
32	0.54	0.22
<i>3m</i>	0.74	0.22
$\bar{3}m$	3.18	0.25
4	0.19	0.25
$\bar{4}$	0.25	0.18
<i>4/m</i>	1.17	0.67

	I	O
422	0.40%	0.48%
<i>4mm</i>	0.30	0.09
$\bar{4}2m$	0.82	0.34
<i>4/mmm</i>	4.53	0.69
6	0.41	0.22
$\bar{6}$	0.07	0.01
<i>6/m</i>	0.82	0.17
622	0.24	0.05
<i>6mm</i>	0.45	0.03
$\bar{6}m2$	0.41	0.02
<i>6/mmm</i>	2.82	0.05
23	0.44	0.09
<i>m3</i>	0.84	0.15
432	0.13	0.01
$\bar{4}3m$	1.42	0.11
<i>m3m</i>	6.66	0.12

I ... anorganické

72 % a, m, o

O... Organické

94 % a, m, o

I ... anorganické

82 % centrosymetrické

O... Organické

75 % centrosymetrické

Populace bodových grup ve vyskytujících se strukturách

Látky, které mohou být

Piezoelektrické 22 %
Pyroelektrické 12 %

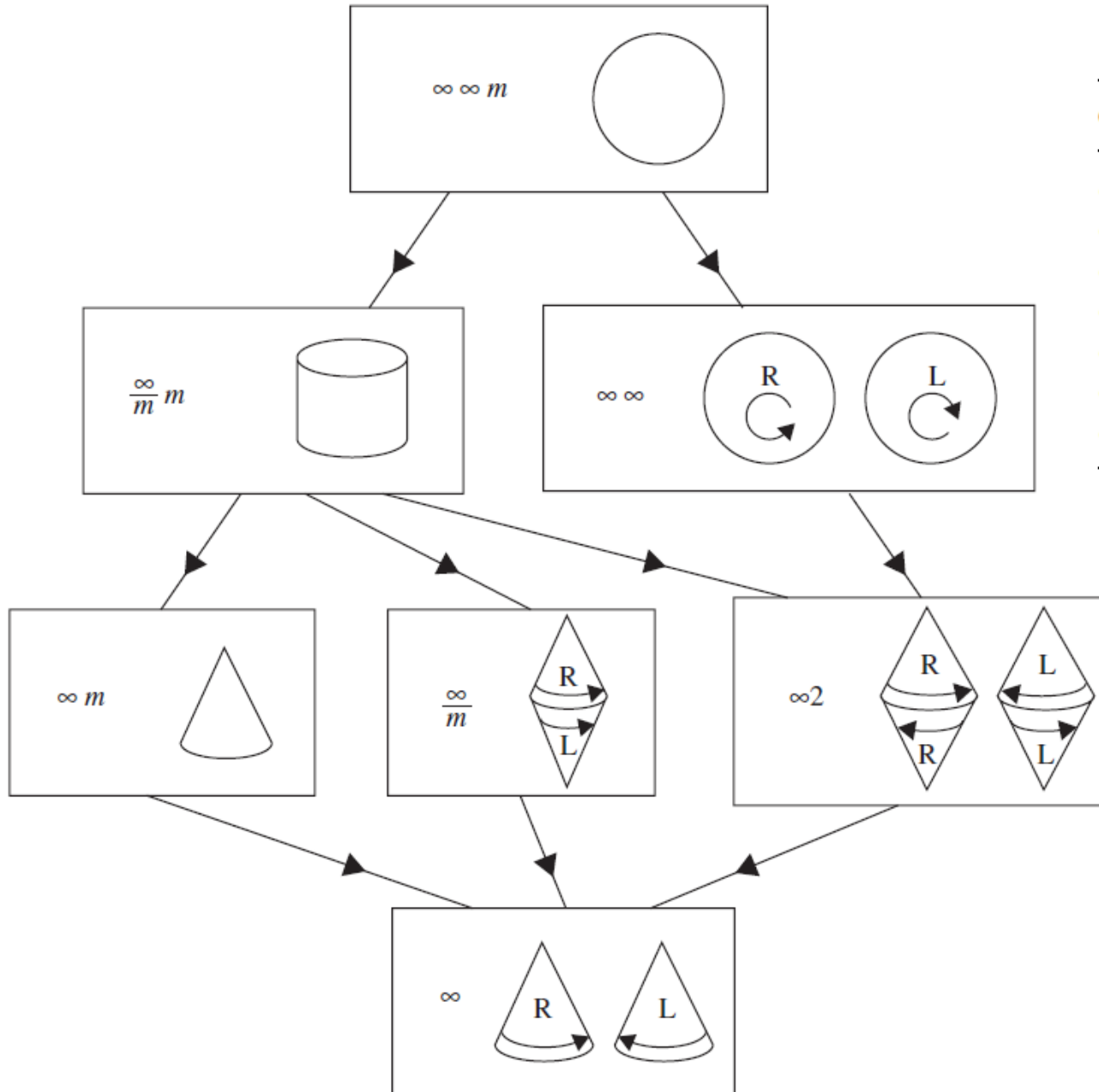
Dvojlom 95 %
Opticky dvojosé 87 %
Opticky jednosé 8 %
Opticky izotropní 5 %

Opticky aktivní (enantiomorfní) 15 %

Symetrie polykrystalických materiálů

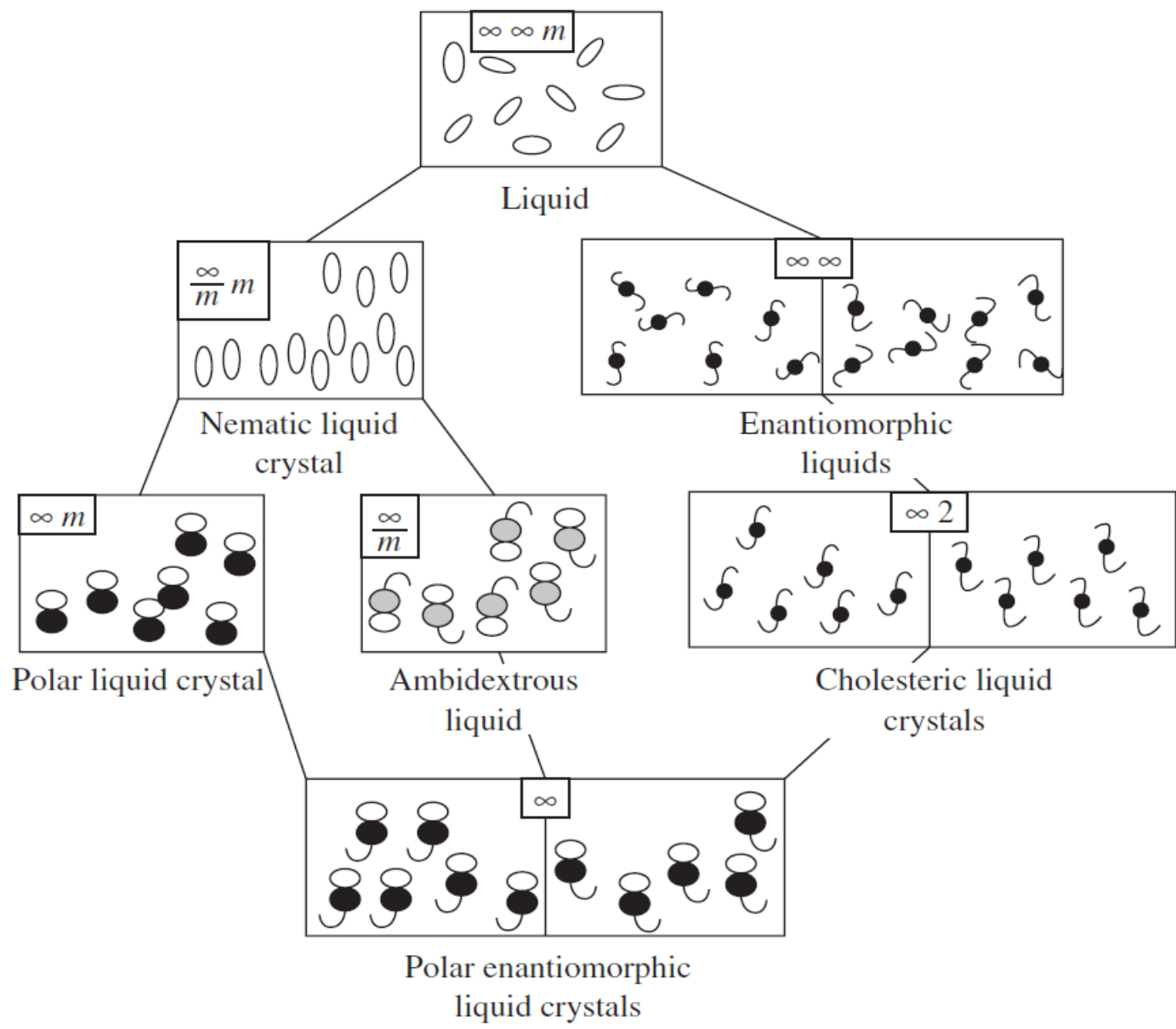
Curieovy grupy

Curie group	Symmetry operators
∞	$\infty \parallel Z_3$
∞m	$\infty \parallel Z_3, m \perp Z_1$
$\infty 2$	$\infty \parallel Z_3, 2 \parallel Z_1$
∞/m	$\infty \parallel Z_3, m \perp Z_3$
∞/mmm	$\infty \parallel Z_3, m \perp Z_3, m \perp Z_1$
$\infty\infty$	$\infty \parallel Z_3, \infty \parallel Z_1$
$\infty\infty m$	$\infty \parallel Z_3, \infty \parallel Z_1, m \perp Z_1$

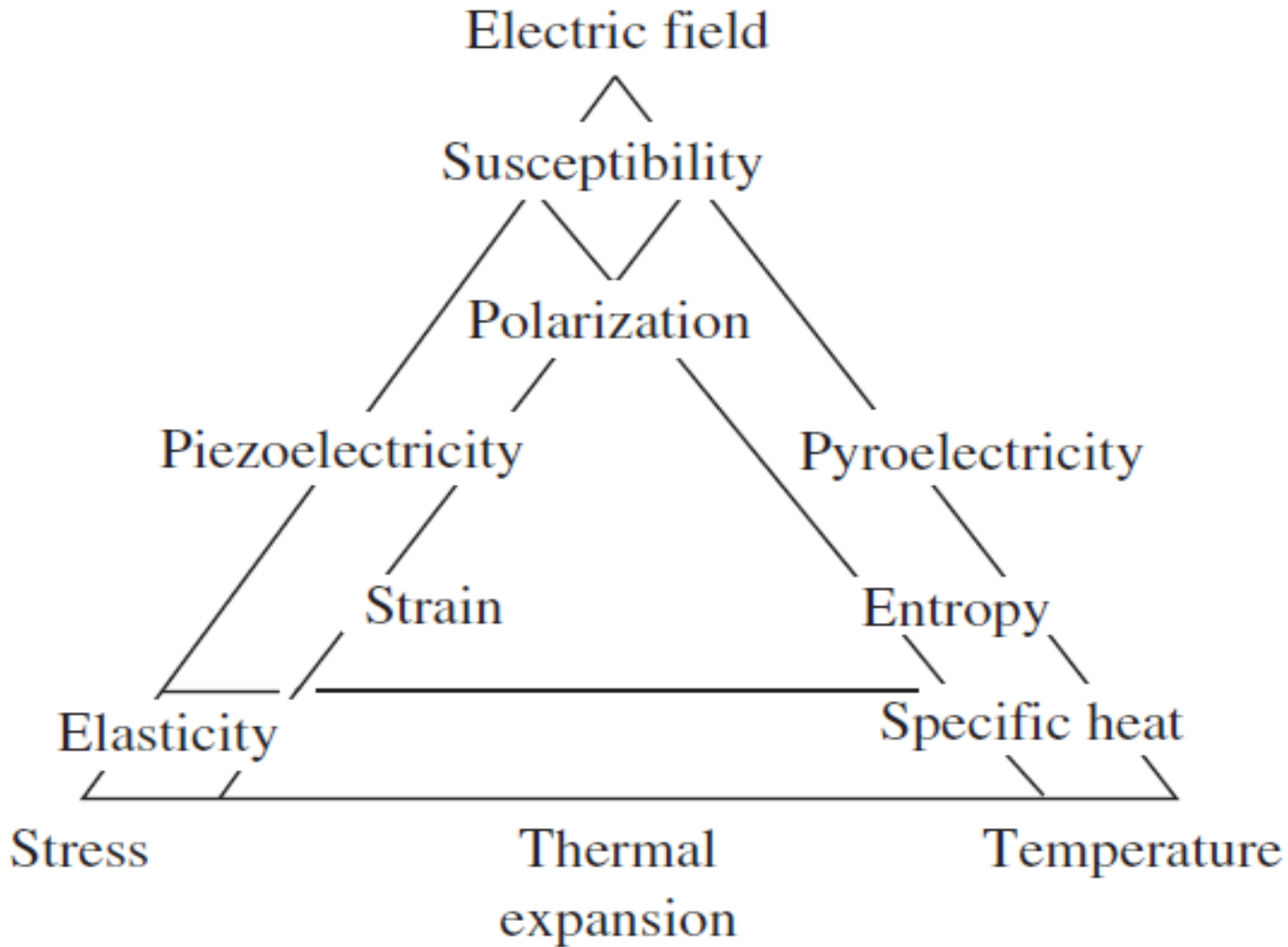


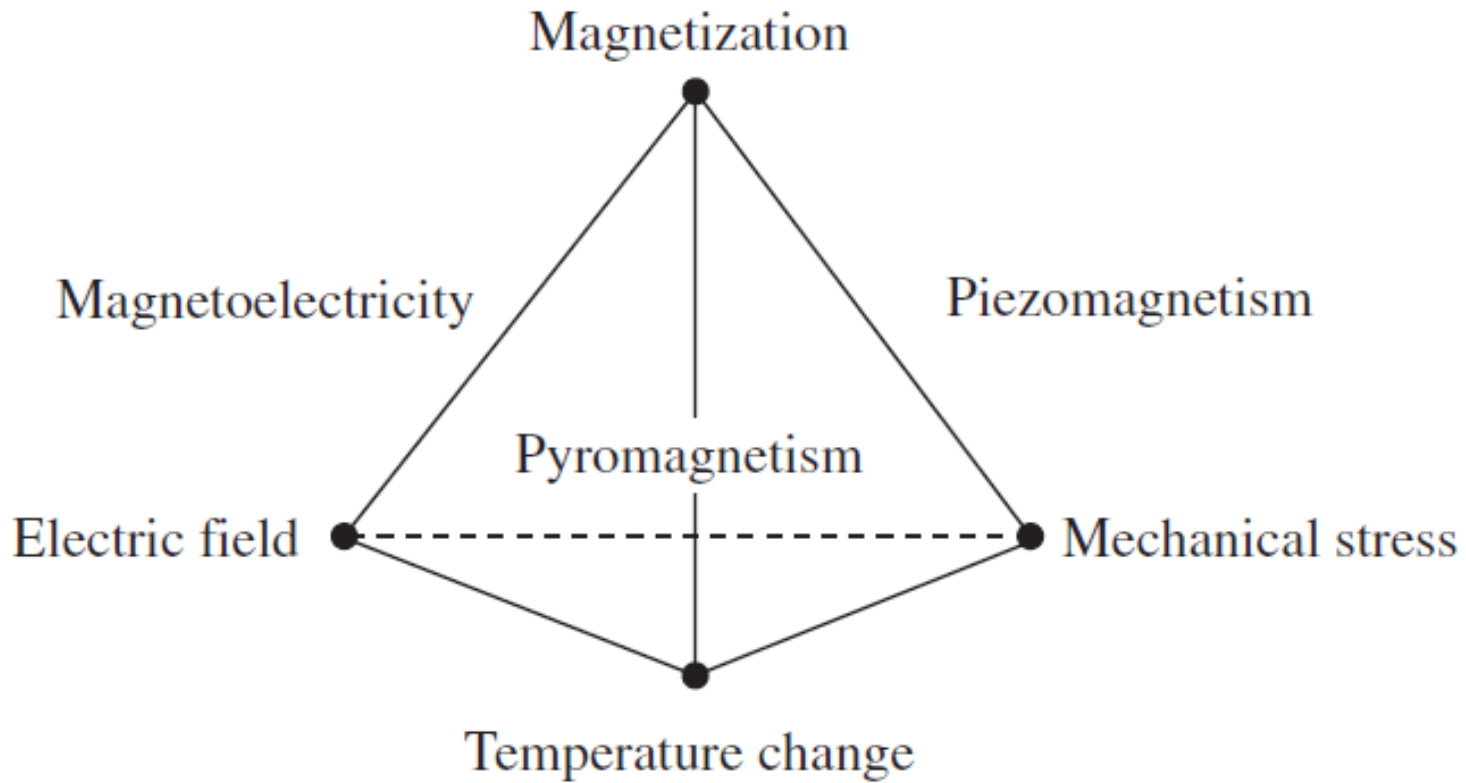
**Minimální
symetrie**

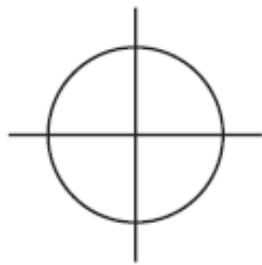
Symetrie kapalin



Heckmannův diagram

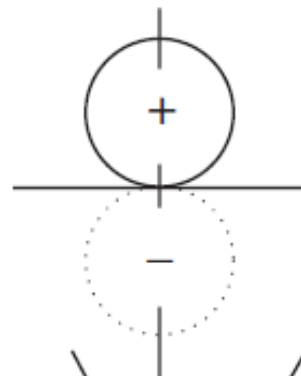






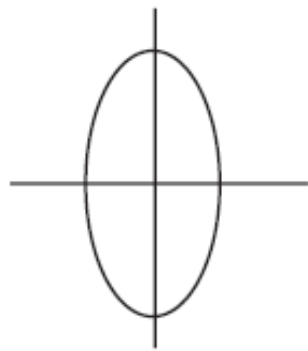
Zero rank (scalar)

Density



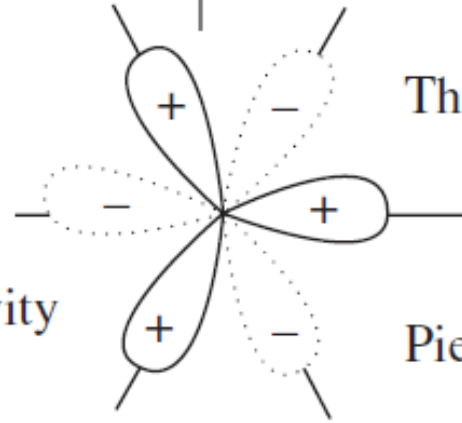
First rank (vector)

Pyroelectricity



Second rank tensor

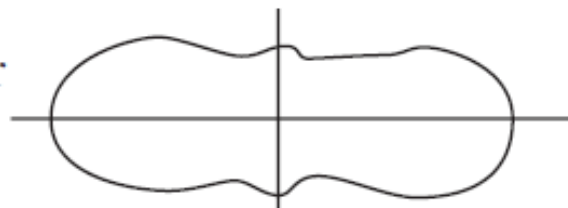
Thermal conductivity



Third rank tensor

Piezoelectricity

Fourth rank tensor
elasticity



0

$$T' = T$$

Sphere

1

$$T'_i = a_{ij}T_j$$

Vector

2

$$T'_{ij} = a_{ik}a_{jl}T_{kl}$$

Quadric

3

$$T'_{ijk} = a_{il}a_{jm}a_{kn}T_{lmn}$$

Cubic

4

$$T'_{ijkl} = a_{im}a_{jn}a_{ko}a_{lp}T_{mnop}$$

Quartic

Pyroelektřina – změna polarizace při změně teploty

$$P_i = D_i = p_i \delta T \text{ [C/m}^2\text{]}$$

$$D'_i = a_{ij} D_j = a_{ij} p_j \delta T = a_{ij} p_j \delta T' = p'_i \delta T'$$

$$p'_i = a_{ij} p_j$$

Tenzor 1. řádu

Pyroelektricitá nemůže být v centrosymetických materiálech (10 grup)

$$(p') = \begin{pmatrix} p'_1 \\ p'_2 \\ p'_3 \end{pmatrix} = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \begin{pmatrix} p_1 \\ p_2 \\ p_3 \end{pmatrix} = \begin{pmatrix} -p_1 \\ -p_2 \\ -p_3 \end{pmatrix} = -(p)$$

Střed symetrie

Neumannův (Voigtův) princip

$$\begin{pmatrix} -p_1 \\ -p_2 \\ -p_3 \end{pmatrix} = \begin{pmatrix} p_1 \\ p_2 \\ p_3 \end{pmatrix} \longrightarrow p_1 = p_2 = p_3 = 0$$

Grupa 32 (např. křemen)

Neumann

$$\begin{pmatrix} p'_1 \\ p'_2 \\ p'_3 \end{pmatrix} = \begin{pmatrix} -1/2 & \sqrt{3}/2 & 0 \\ -\sqrt{3}/2 & -1/2 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} p_1 \\ p_2 \\ p_3 \end{pmatrix} = \begin{pmatrix} -p_1/2 + \sqrt{3}p_2/2 \\ -\sqrt{3}p_1/2 - p_2/2 \\ p_3 \end{pmatrix} = \begin{pmatrix} p_1 \\ p_2 \\ p_3 \end{pmatrix}$$

Trojčetné otočení

$p_1 = p_2 = 0.$

$$\begin{pmatrix} p'_1 \\ p'_2 \\ p'_3 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \begin{pmatrix} p_1 \\ p_2 \\ p_3 \end{pmatrix} = \begin{pmatrix} p_1 \\ -p_2 \\ -p_3 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ p_3 \end{pmatrix}$$

Dvojčetné otočení

$p_1 = p_2 = p_3 = 0$

Grupa 3m (např. turmalín)

Neumann

$$\begin{pmatrix} p'_1 \\ p'_2 \\ p'_3 \end{pmatrix} = \begin{pmatrix} -1/2 & \sqrt{3}/2 & 0 \\ -\sqrt{3}/2 & -1/2 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} p_1 \\ p_2 \\ p_3 \end{pmatrix} = \begin{pmatrix} -p_1/2 + \sqrt{3}p_2/2 \\ -\sqrt{3}p_1/2 - p_2/2 \\ p_3 \end{pmatrix} = \begin{pmatrix} p_1 \\ p_2 \\ p_3 \end{pmatrix}$$

Trojčetné otočení

$p_1 = p_2 = 0.$

$$\begin{pmatrix} p'_1 \\ p'_2 \\ p'_3 \end{pmatrix} = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} p_1 \\ p_2 \\ p_3 \end{pmatrix} = \begin{pmatrix} -p_1 \\ p_2 \\ p_3 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ p_3 \end{pmatrix}$$

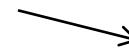
Zrcadlení

Grupa ∞m (feroelektrické keramiky)

$$\begin{pmatrix} p'_1 \\ p'_2 \\ p'_3 \end{pmatrix} = \begin{pmatrix} \cos \theta & -\sin \theta & 0 \\ \sin \theta & \cos \theta & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} p_1 \\ p_2 \\ p_3 \end{pmatrix}$$

$$= \begin{pmatrix} p_1 \cos \theta - p_2 \sin \theta \\ p_1 \sin \theta + p_2 \cos \theta \\ p_3 \end{pmatrix} = \begin{pmatrix} p_1 \\ p_2 \\ p_3 \end{pmatrix}$$

Pro všechna θ



$$p_1 = p_2 = 0.$$

$$\begin{pmatrix} p'_1 \\ p'_2 \\ p'_3 \end{pmatrix} = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} p_1 \\ p_2 \\ p_3 \end{pmatrix} = \begin{pmatrix} -p_1 \\ p_2 \\ p_3 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ p_3 \end{pmatrix}$$

Zrcadlení

Pyroelektrické třídy

10 tříd

Point group 1

$$\begin{pmatrix} p_1 \\ p_2 \\ p_3 \end{pmatrix}$$

Point group 2

$$\begin{pmatrix} 0 \\ p_2 \\ 0 \end{pmatrix}$$

Point group m

$$\begin{pmatrix} p_1 \\ 0 \\ p_3 \end{pmatrix}$$

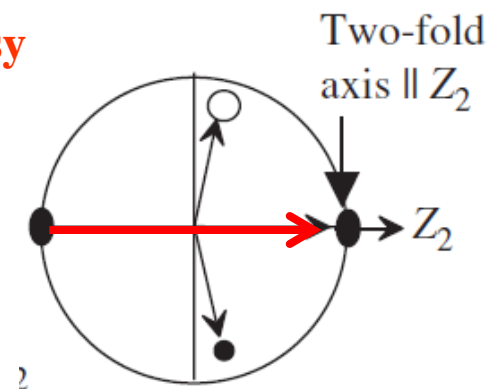
Point groups $mm2, 3, 3m, 4, 4mm, 6, 6mm, \infty, \infty m$

$$\begin{pmatrix} 0 \\ 0 \\ p_3 \end{pmatrix}$$

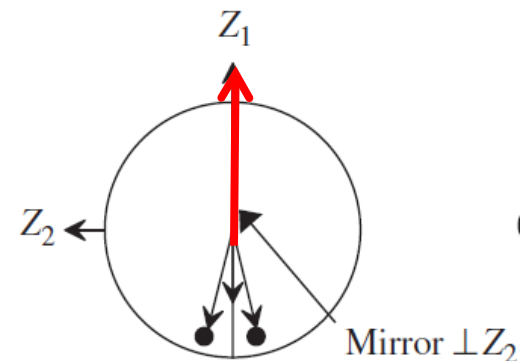
Polární osy

Vektory do ekvivalentních bodů

Point group 2

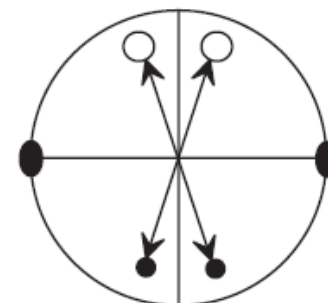


Point group m



Point group $2/m$

Nulový efekt



	Experimented value (p^X)	Secondary effect ($p^X - p^x$)	Primary effect (p_n^x)
	<i>Ferroelectrics</i>	Změna rozměrů buňky	Přeuspořádání polarizačních nábojů
Poled ceramic (∞m)			
BaTiO ₃	-200	+60	-260
PbZr _{0.95} Ti _{0.05} O ₃	-268	+37.7	-305.7
Crystal			
LiNbO ₃ (3 <i>m</i>)	-83	+12.8	-95.8
LiTaO ₃ (3 <i>m</i>)	-176	-1	-175
Pb ₅ Ge ₃ O ₁₁ (3)	-95	+15.5	-110.5
Ba ₂ NaNb ₅ O ₁₅ (<i>mm</i> 2)	-100	+41.7	-141.7
Sr _{0.5} Ba _{0.5} Nb ₂ O ₆ (4 <i>mm</i>)	-550	-48	-502
(CH ₂ CF ₂) _n (<i>mm</i> 2)	-27	-13	-14
TGS (2)	-270	-330	+60
	<i>Nonferroelectrics</i>		
Crystal			
CdSe (6 <i>mm</i>)	-3.5	-0.56	-2.94
CdS (6 <i>mm</i>)	-4.0	-1.0	-3.0
ZnO (6 <i>mm</i>)	-9.4	-2.5	-6.9
Tourmaline (3 <i>m</i>)	+4.0	-3.52	-0.48
Li ₂ SO ₄ · 2H ₂ O (2)	+86.3	+26.1	+60.2

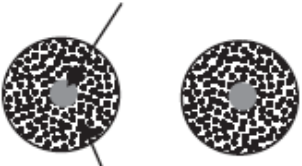
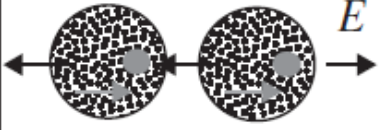
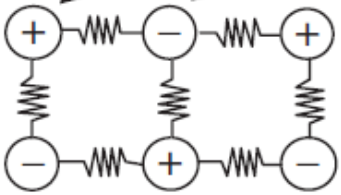
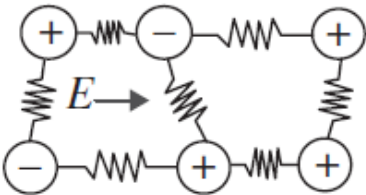
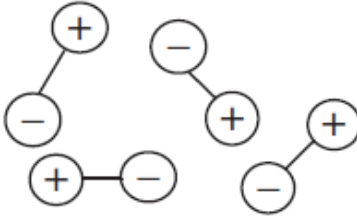
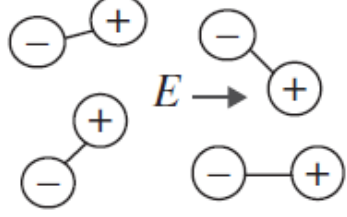
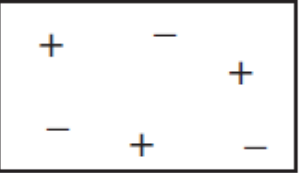
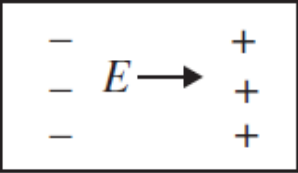
Dielektrické konstanty

$$K = \varepsilon / \varepsilon_0$$

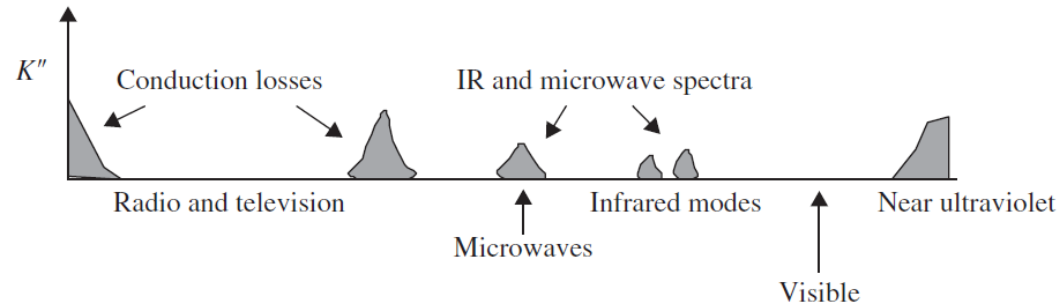
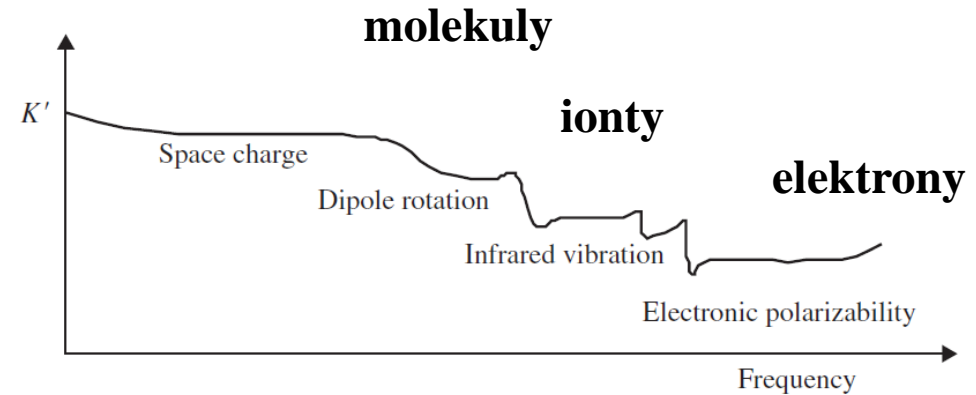
$$D = \varepsilon E$$

Mechanismy polarizace

[C/m²] [F/m] [V/m]

<p>Nucleus</p>  <p>Electron cloud</p>	<p>Electronic</p>  <p>Cloud shifts</p>
<p>Cation Anion</p> 	<p>Ionic motion</p> 
<p>Molecules</p> 	<p>Orientalional</p> 
<p>Mobile charges</p> 	<p>Space charge</p> 

$$D_i = \varepsilon_{ij} E_j$$



Transformace souřadnic v tenzorovém značení

Tenzor 2. řádu

$$D'_i = a_{ij}D_j = a_{ij}\varepsilon_{jk}E_k = a_{ij}\varepsilon_{jk}a_{lk}E'_l$$

$$D'_i = \varepsilon'_{il}E'_l.$$

$$\varepsilon'_{il} = a_{ij}a_{lk}\varepsilon_{jk}$$

$$K'_{il} = \frac{\varepsilon'_{il}}{\varepsilon_0} = a_{ij}a_{lk}K_{jk}$$

Transformace souřadnic v maticovém značení

$$\begin{aligned} \begin{matrix} 3 \times 1 \\ (D') \end{matrix} &= \begin{matrix} 3 \times 3 \\ (a) \end{matrix} \begin{matrix} 3 \times 1 \\ (D) \end{matrix} = \begin{matrix} 3 \times 3 \\ (a) \end{matrix} \begin{matrix} 3 \times 3 \\ (\varepsilon) \end{matrix} \begin{matrix} 3 \times 1 \\ (E) \end{matrix} \\ &= \begin{matrix} 3 \times 3 \\ (a) \end{matrix} \begin{matrix} 3 \times 3 \\ (\varepsilon) \end{matrix} \begin{matrix} 3 \times 3 \\ (a)^{-1} \end{matrix} \begin{matrix} 3 \times 1 \\ (E') \end{matrix} = \begin{matrix} 3 \times 3 \\ (\varepsilon') \end{matrix} \begin{matrix} 3 \times 1 \\ (E') \end{matrix} \end{aligned}$$



Směrové kosiny

$$(K') = (a)(K)(a)_t$$

Zachování energie

$$\varepsilon_{ij} = \varepsilon_{ji}$$

$$K_{ij} = K_{ji}$$

Změna energie při aplikaci pole

$$dU = E_i dD_i = \varepsilon_{ij} E_i dE_j$$

$$dU = \varepsilon_{11} E_1 dE_1 + \varepsilon_{12} E_1 dE_2 + \varepsilon_{21} E_2 dE_1 + \dots$$

$$\frac{\partial U}{\partial E_1} = \varepsilon_{11} E_1 + \varepsilon_{21} E_2 + \varepsilon_{31} E_3$$

$$\frac{\partial U}{\partial E_2} = \varepsilon_{12} E_1 + \varepsilon_{22} E_2 + \varepsilon_{32} E_3$$

$$\frac{\partial^2 U}{\partial E_1 \partial E_2} = \varepsilon_{21}$$

$$\frac{\partial^2 U}{\partial E_2 \partial E_1} = \varepsilon_{12}$$

Uložená energie nezávisí na pořadí aplikace složek pole

Uložená energie na jednotkový objem musí být kladná

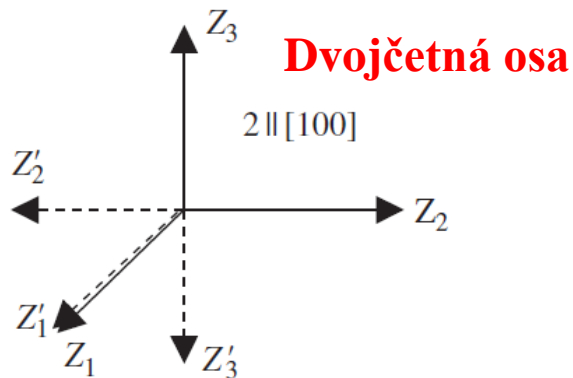
$$\begin{aligned}\int_0^E \varepsilon_{ij} E_i dE_j &= \frac{1}{2} \varepsilon_{ij} E_i E_j > 0 \\ &= \frac{1}{2} \varepsilon_{11} E_1^2 + \frac{1}{2} \varepsilon_{22} E_2^2 + \frac{1}{2} \varepsilon_{33} E_3^2 + \varepsilon_{12} E_1 E_2 + \varepsilon_{13} E_1 E_3 \\ &\quad + \varepsilon_{23} E_2 E_3 > 0.\end{aligned}$$


$$\mathbf{K}_{\mathbf{ii}} > \mathbf{0}$$

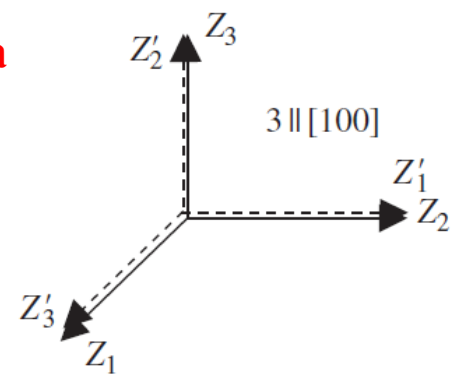
$$K_{11} + K_{22} > |2K_{12}|$$

Nediagonální prvky jsou
menší než diagonální

Příklad – minimální symetrie
v kubických krystalech – **grupa 32**



$$(a) = \begin{pmatrix} +1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$



$$(a) = \begin{pmatrix} 0 & +1 & 0 \\ 0 & 0 & +1 \\ +1 & 0 & 0 \end{pmatrix}$$

$$(K') = (a)(K)(a)_t$$

$$= \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \begin{pmatrix} K_{11} & K_{12} & K_{13} \\ K_{21} & K_{22} & K_{23} \\ K_{31} & K_{32} & K_{33} \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

$$= \begin{pmatrix} K_{11} & -K_{12} & -K_{13} \\ -K_{21} & K_{22} & K_{23} \\ -K_{31} & K_{32} & K_{33} \end{pmatrix} = \begin{pmatrix} K_{11} & K_{12} & K_{13} \\ K_{21} & K_{22} & K_{23} \\ K_{31} & K_{32} & K_{33} \end{pmatrix}.$$

Neumannův princip

$$K_{12} = K_{13} = K_{21} = K_{31} = 0$$

$$(K') = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix} \begin{pmatrix} K_{11} & 0 & 0 \\ 0 & K_{22} & K_{23} \\ 0 & K_{32} & K_{33} \end{pmatrix} \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}$$

$$= \begin{pmatrix} K_{22} & K_{23} & 0 \\ K_{32} & K_{33} & 0 \\ 0 & 0 & K_{11} \end{pmatrix} = \begin{pmatrix} K_{11} & 0 & 0 \\ 0 & K_{22} & K_{23} \\ 0 & K_{32} & K_{33} \end{pmatrix}.$$

$$K_{11} = K_{22} = K_{33} \quad K_{23} = K_{32} = 0$$

$$(K) = \begin{pmatrix} K_{11} & 0 & 0 \\ 0 & K_{11} & 0 \\ 0 & 0 & K_{11} \end{pmatrix}$$

Zjednodušené odvození

Dvojčetná osa
podél Z_1

$$Z_1 \rightarrow Z_1, Z_2 \rightarrow -Z_2, Z_3 \rightarrow -Z_3$$

$$1 \rightarrow 1, 2 \rightarrow -2, 3 \rightarrow -3.$$

$$K_{11} \quad 11 \rightarrow 11 = 11$$

$$K_{12} \quad 12 \rightarrow -12 = 12 \quad \therefore K_{12} = 0$$

$$K_{13} \quad 13 \rightarrow -13 = 13 \quad \therefore K_{13} = 0$$

⋮

Trojčetná osa
podél [111]

$$1 \rightarrow 2, 2 \rightarrow 3, 3 \rightarrow 1.$$

$$K_{11} \quad 11 \rightarrow 22 = 11 \quad \therefore K_{11} = K_{22}$$

⋮

Triclinic crystals
 Classes 1 and $\bar{1}$
 Six coefficients

$$\begin{pmatrix} K_{11} & K_{12} & K_{13} \\ K_{12} & K_{22} & K_{23} \\ K_{13} & K_{23} & K_{33} \end{pmatrix}$$

Monoclinic crystals
 Classes 2, m , and $2/m$
 Four coefficients

$$\begin{pmatrix} K_{11} & 0 & K_{13} \\ 0 & K_{22} & 0 \\ K_{13} & 0 & K_{33} \end{pmatrix}$$

Orthorhombic crystals
 Classes 222 , $mm2$, and mmm
 Three coefficients

$$\begin{pmatrix} K_{11} & 0 & 0 \\ 0 & K_{22} & 0 \\ 0 & 0 & K_{33} \end{pmatrix}$$

Uniaxial crystals
 Classes 3 , $\bar{3}$, 32 , $3m$, $\bar{3}m$, 4 , $\bar{4}$, $4/m$, 422 ,
 $4mm$, $\bar{4}2m$, $4/mmm$, 6 , $\bar{6}$, $6/m$, 622 ,
 $6mm$, $\bar{6}m2$, and $6/mmm$
 Curie groups ∞ , ∞m , ∞/m , $\infty 2$, and ∞/mm
 Two coefficients

$$\begin{pmatrix} K_{11} & 0 & 0 \\ 0 & K_{11} & 0 \\ 0 & 0 & K_{33} \end{pmatrix}$$

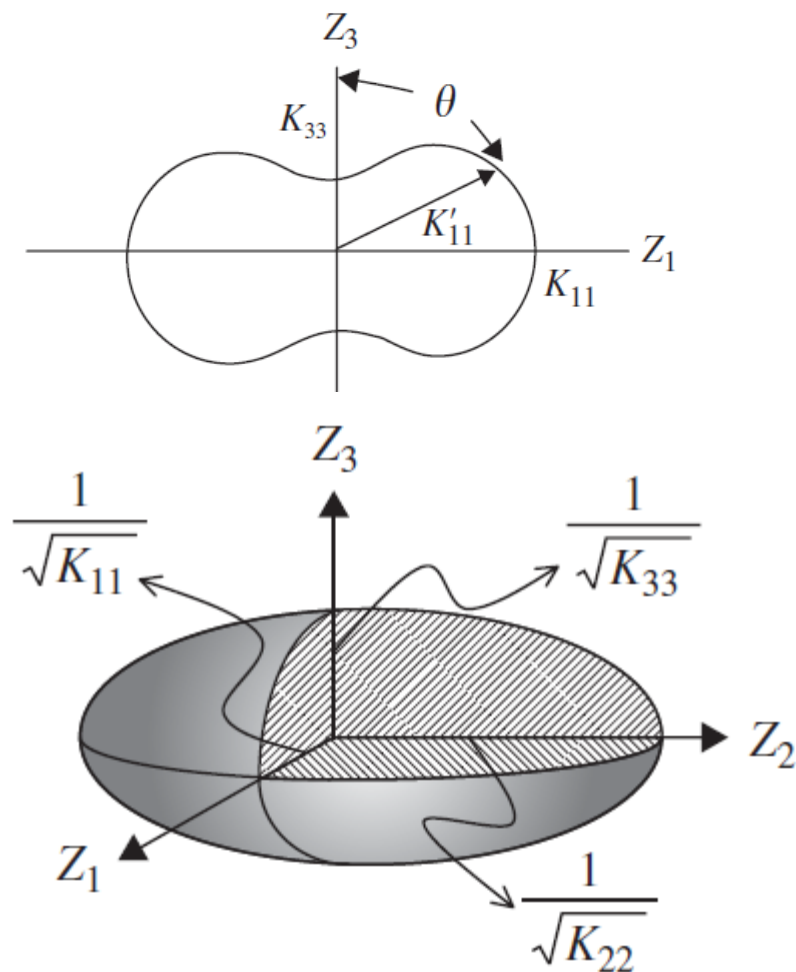
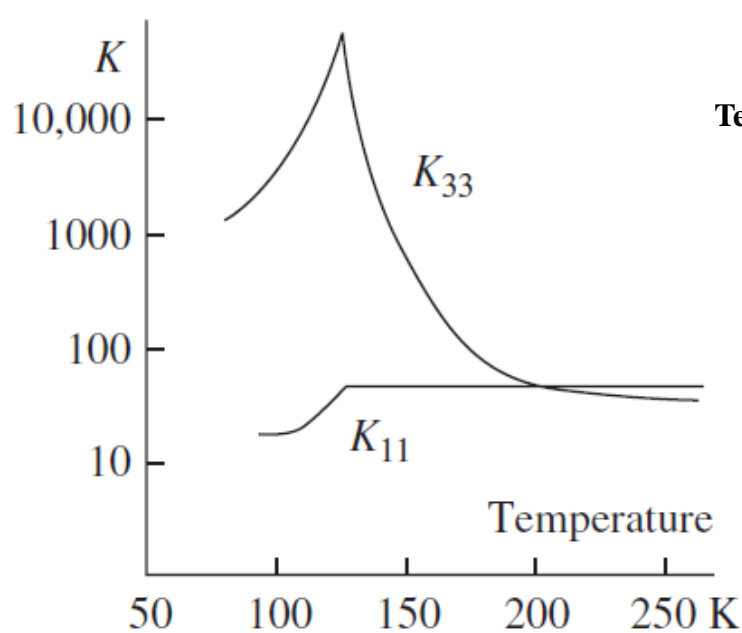
Cubic crystals
 Classes 23 , $m\bar{3}$, 432 , $\bar{4}3m$ and $m\bar{3}m$
 Curie groups $\infty\infty$ and $\infty\infty m$
 One coefficient

$$\begin{pmatrix} K_{11} & 0 & 0 \\ 0 & K_{11} & 0 \\ 0 & 0 & K_{11} \end{pmatrix}$$

$$K'_{11} = a_{11}^2 K_{11} + a_{12}^2 K_{22} + a_{13}^2 K_{33}.$$

Ve sférických souřadnicích

$$K'_{11} = K_{11} \cos^2 \phi \sin^2 \theta + K_{22} \sin^2 \phi \sin^2 \theta + K_{33} \cos^2 \theta$$



Silně anizotropní a teplotně závislá permitivita

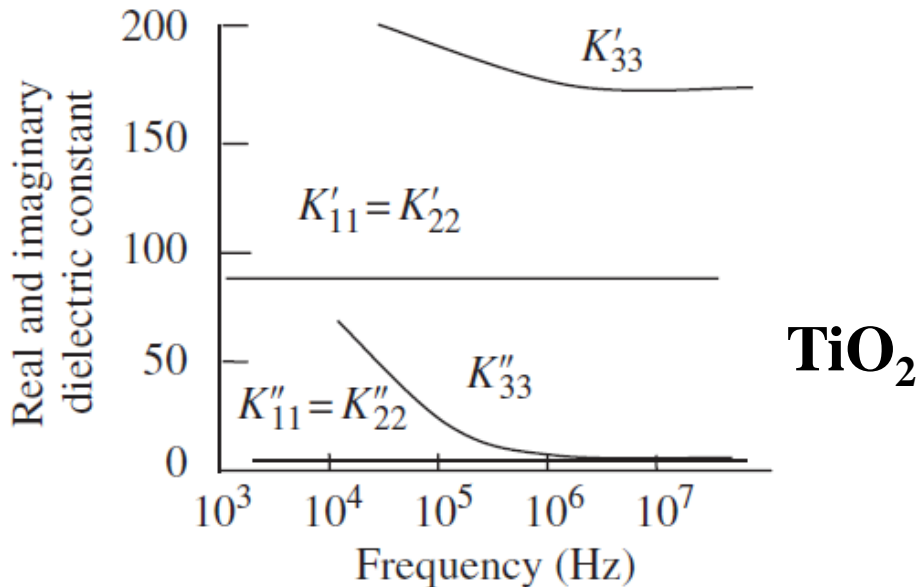
Polykrystalická dielektrika

$$\langle K'_{11} \rangle = \frac{1}{3}(K_{11} + K_{22} + K_{33})$$

$$\langle K'_{11} \rangle = K_{11} \langle a_{11}^2 \rangle + K_{22} \langle a_{12}^2 \rangle + K_{33} \langle a_{13}^2 \rangle$$

Středování směrových kosinů
přes všechny úhly

$$\langle a_{11}^2 \rangle = \frac{\int_{-1}^{+1} a_{11}^2 da_{11}}{\int_{-1}^{+1} da_{11}} = \frac{1}{3} = \langle a_{12}^2 \rangle = \langle a_{13}^2 \rangle.$$

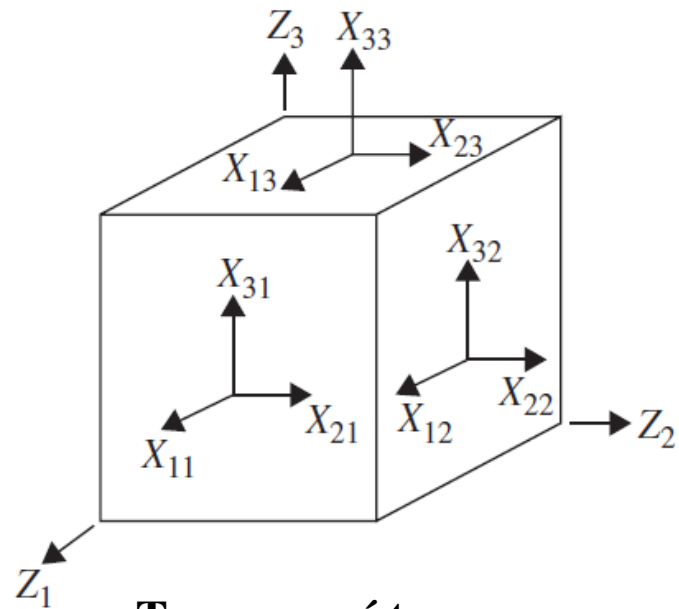


Napětí a deformace

$$(X_{ij}) = \begin{pmatrix} X_{11} & X_{12} & X_{13} \\ X_{12} & X_{22} & X_{23} \\ X_{13} & X_{23} & X_{33} \end{pmatrix} \quad [\text{N/m}^2]$$

Směr síly

Normála k ploše



**Tenzor není tenzorem
vlastnosti!!!**

Statická rovnováha – absence rotace – symetrický tenzor

$$\begin{pmatrix} X'_{11} & X'_{12} & X'_{13} \\ X'_{12} & X'_{22} & X'_{23} \\ X'_{13} & X'_{23} & X'_{33} \end{pmatrix} = \begin{pmatrix} X'_1 = X'_{11} \\ X'_2 = X'_{22} \\ X'_3 = X'_{33} \\ X'_4 = X'_{23} \\ X'_5 = X'_{13} \\ X'_6 = X'_{12} \end{pmatrix}$$

Tahové složky podél Z'_1, Z'_2, Z'_3

V hlavních osách tenzoru

$$\begin{pmatrix} X_{11} & 0 & 0 \\ 0 & X_{22} & 0 \\ 0 & 0 & X_{33} \end{pmatrix} = \begin{pmatrix} X_1 = X_{11} \\ X_2 = X_{22} \\ X_3 = X_{33} \\ 0 \\ 0 \\ 0 \end{pmatrix}$$

Smykové složky podél Z'_1, Z'_2, Z'_3

Transformace tenzoru napětí

$$X'_{ij} = a_{ik}a_{jl}X_{kl} \quad \begin{pmatrix} X'_1 \\ X'_2 \\ X'_3 \\ X'_4 \\ X'_5 \\ X'_6 \end{pmatrix} = \begin{pmatrix} \alpha_{11} & \alpha_{12} & \alpha_{13} & \alpha_{14} & \alpha_{15} & \alpha_{16} \\ \alpha_{21} & \alpha_{22} & \alpha_{23} & \alpha_{24} & \alpha_{25} & \alpha_{26} \\ \alpha_{31} & \alpha_{32} & \alpha_{33} & \alpha_{34} & \alpha_{35} & \alpha_{36} \\ \alpha_{41} & \alpha_{42} & \alpha_{43} & \alpha_{44} & \alpha_{45} & \alpha_{46} \\ \alpha_{51} & \alpha_{52} & \alpha_{53} & \alpha_{54} & \alpha_{55} & \alpha_{56} \\ \alpha_{61} & \alpha_{62} & \alpha_{63} & \alpha_{64} & \alpha_{65} & \alpha_{66} \end{pmatrix} \begin{pmatrix} X_1 \\ X_2 \\ X_3 \\ X_4 \\ X_5 \\ X_6 \end{pmatrix}$$

$$X'_1 = \alpha_{11}X_1 + \alpha_{12}X_2 + \dots + \alpha_{16}X_6$$

$$X'_{11} = a_{11}^2X_{11} + a_{11}a_{12}aX_{12} + a_{12}a_{11}X_{21} + \dots + a_{12}^2X_{22} + \dots$$



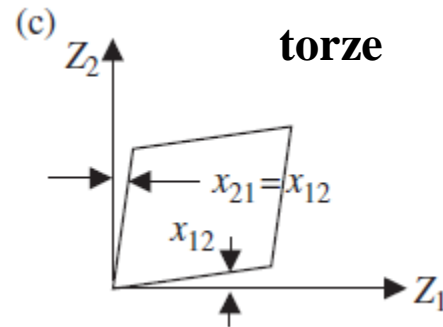
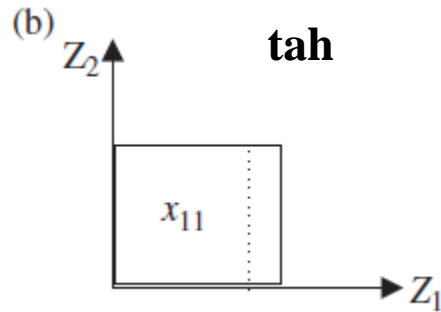
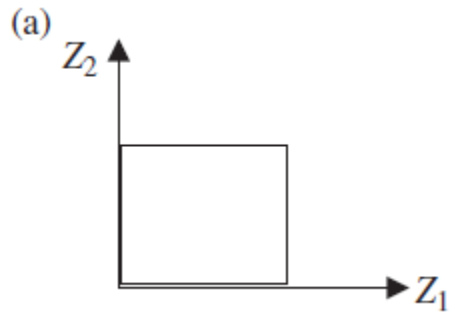
$$\alpha_{11} = a_{11}^2, \alpha_{12} = a_{12}^2, \alpha_{16} = 2a_{11}a_{12}$$

$$\begin{aligned}
(\alpha) & \begin{pmatrix} (a_{11}^2) & (a_{12}^2) & (a_{13}^2) & (2a_{12}a_{13}) & (2a_{13}a_{11}) & (2a_{11}a_{12}) \\ (a_{21}^2) & (a_{22}^2) & (a_{23}^2) & (2a_{22}a_{23}) & (2a_{23}a_{21}) & (2a_{21}a_{22}) \\ (a_{31}^2) & (a_{32}^2) & (a_{33}^2) & (2a_{32}a_{33}) & (2a_{33}a_{31}) & (2a_{31}a_{32}) \\ (a_{21}a_{31}) & (a_{22}a_{32}) & (a_{23}a_{33}) & (a_{22}a_{33} + a_{23}a_{32}) & (a_{21}a_{33} + a_{23}a_{31}) & (a_{22}a_{31} + a_{21}a_{32}) \\ (a_{31}a_{11}) & (a_{32}a_{12}) & (a_{33}a_{13}) & (a_{12}a_{33} + a_{13}a_{32}) & (a_{13}a_{31} + a_{11}a_{33}) & (a_{11}a_{32} + a_{12}a_{31}) \\ (a_{11}a_{21}) & (a_{12}a_{22}) & (a_{13}a_{23}) & (a_{12}a_{23} + a_{13}a_{22}) & (a_{13}a_{21} + a_{11}a_{23}) & (a_{11}a_{22} + a_{12}a_{21}) \end{pmatrix} \\
(\alpha^{-1}) & \begin{pmatrix} (a_{11}^2) & (a_{21}^2) & (a_{31}^2) & (2a_{21}a_{31}) & (2a_{31}a_{11}) & (2a_{11}a_{21}) \\ (a_{12}^2) & (a_{22}^2) & (a_{32}^2) & (2a_{22}a_{32}) & (2a_{32}a_{12}) & (2a_{12}a_{22}) \\ (a_{13}^2) & (a_{23}^2) & (a_{33}^2) & (2a_{23}a_{33}) & (2a_{33}a_{13}) & (2a_{13}a_{23}) \\ (a_{12}a_{13}) & (a_{22}a_{23}) & (a_{32}a_{33}) & (a_{22}a_{33} + a_{32}a_{23}) & (a_{12}a_{33} + a_{32}a_{13}) & (a_{22}a_{13} + a_{12}a_{23}) \\ (a_{13}a_{11}) & (a_{23}a_{21}) & (a_{33}a_{31}) & (a_{21}a_{33} + a_{31}a_{23}) & (a_{31}a_{13} + a_{11}a_{33}) & (a_{11}a_{23} + a_{21}a_{13}) \\ (a_{11}a_{12}) & (a_{21}a_{22}) & (a_{31}a_{32}) & (a_{21}a_{32} + a_{31}a_{22}) & (a_{31}a_{12} + a_{11}a_{32}) & (a_{11}a_{22} + a_{21}a_{12}) \end{pmatrix}
\end{aligned}$$

$$\alpha_{mn} = \alpha_{ijkl} = a_{ik}a_{jl} + (1 - \delta_{kl})a_{il}a_{jk}$$

$$\alpha_{mn}^{-1} = \alpha_{ijkl}^{-1} = a_{ki}a_{lj} + (1 - \delta_{kl})a_{kj}a_{li}.$$

Tensor deformace

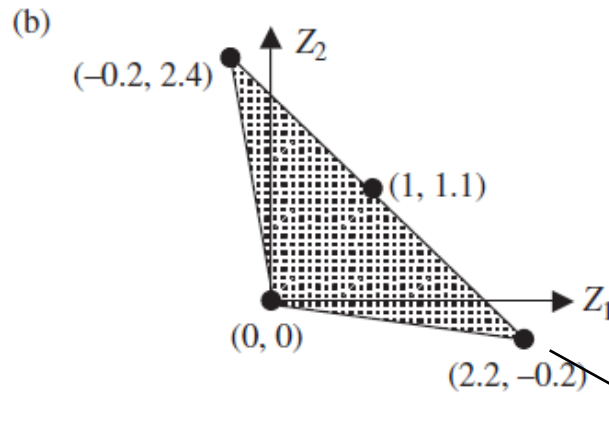
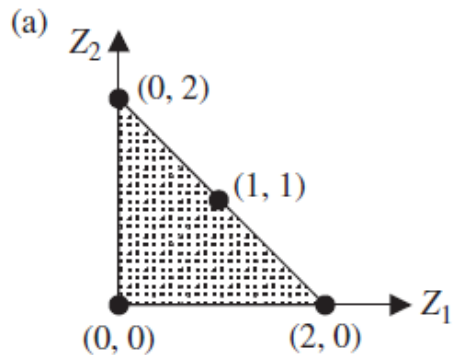


Symetrický tenzor

Příklad

$$(x_{ij}) = \begin{pmatrix} 0.1 & -0.1 & 0 \\ -0.1 & 0.2 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

$$(x_{ij}) = \frac{\delta u_i}{\delta Z_j} = \begin{pmatrix} x_{11} & x_{12} & x_{13} \\ x_{12} & x_{22} & x_{23} \\ x_{13} & x_{23} & x_{33} \end{pmatrix}$$



$$u_i = x_{ij}Z_j$$

$$u_1 = 0.1(2) - 0.1(0)$$

$$u_2 = -0.1(2) + 0.2(0)$$

$$\begin{pmatrix} x'_{11} & x'_{12} & x'_{13} \\ x'_{12} & x'_{22} & x'_{23} \\ x'_{13} & x'_{23} & x'_{33} \end{pmatrix} = \begin{pmatrix} x'_1 = x'_{11} \\ x'_2 = x'_{22} \\ x'_3 = x'_{33} \\ x'_4 = 2x'_{23} \\ x'_5 = 2x'_{13} \\ x'_6 = 2x'_{12} \end{pmatrix}$$

$$x'_6 = x'_{12} + x'_{21} = 2x'_{12}.$$

Změna objemu jednotkové krychle

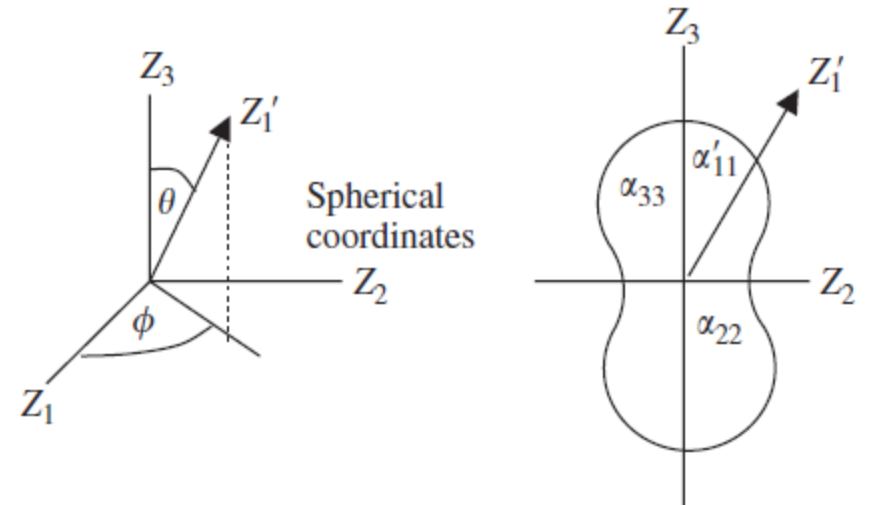
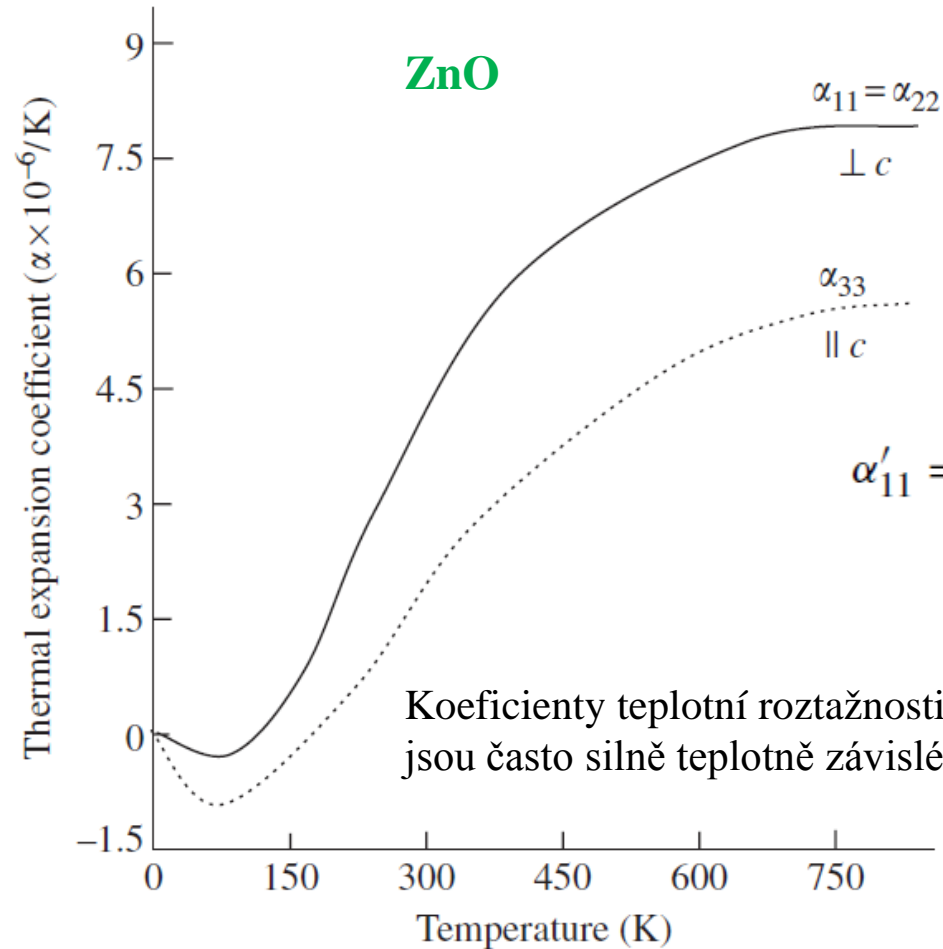
$$\frac{\Delta V}{V} = x_{11} + x_{22} + x_{33}$$

Teplotní roztažnost

$$x_{ij} = \alpha_{ij} \Delta T$$

Symetrický tenzor
2. řádu

strain



$$\alpha'_{11} = \alpha_{11} \cos^2 \phi \sin^2 \theta + \alpha_{22} \sin^2 \phi \sin^2 \theta + \alpha_{33} \cos^2 \theta$$

Pro krystaly s nízkou symetrií

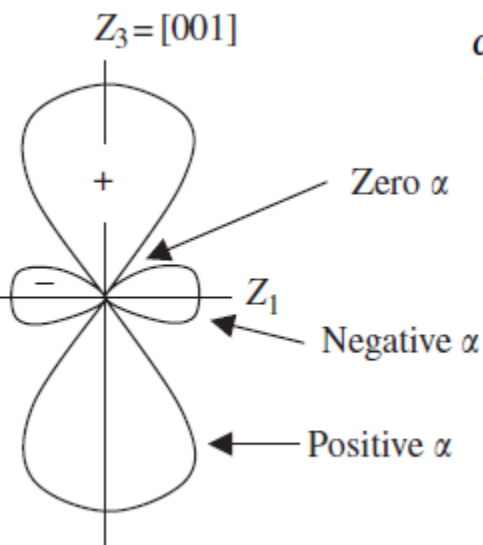
Stejný typ tenzoru jako
dielektrická konstanta

Koeficienty mohou být
kladné i záporné

Trigonální, hexagonální, tetragonální

kalцит

$$\alpha'_{11} = 0 = \alpha_{11} \sin^2 \theta + \alpha_{33} \cos^2 \theta$$



$$\alpha_{11} = \alpha_{22} = -5.6 \times 10^{-6}/K$$

$$\alpha_{33} = +25 \times 10^{-6}/K$$

<i>Cubic crystals</i>	α ($10^{-6}K$)
-----------------------	-------------------------

Diamond (C)	1.4
Silicon (Si)	4.2
Germanium (Ge)	5.9
Copper (Cu)	17
Silver (Ag)	20
Gold (Au)	15
Iron (Fe)	12
Platinum (Pt)	8.3
Tungsten (W)	4.3

<i>Trigonal crystals</i>	α_{11}	α_{33}
--------------------------	---------------	---------------

Calcium Carbonate (CaCO ₃)	-3.8	21
Sodium Nitrate (NaNO ₃)	11	120
Tellurium (Te)	28	-1.7
Antimony (Sb)	8.2	16
Aluminum Oxide (Al ₂ O ₃)	5.4	6.6

<i>Orthorhombic crystals</i>	α_{11}	α_{22}	α_{33}
------------------------------	---------------	---------------	---------------

Iodine (I ₂)	133	95	35
Lead Chloride (PbCl ₂)	34	39	17

<i>Hexagonal crystals</i>	α_{11}	α_{33}
---------------------------	---------------	---------------

Magnesium (Mg)	27	28
Zinc (Zn)	14	61
Cadmium (Cd)	19	48
Magnesium Hydroxide (Mg(OH) ₂)	11	45

<i>Tetragonal crystals</i>	α_{11}	α_{33}
----------------------------	---------------	---------------

Tin (Sn)	46	22
Titanium Oxide (TiO ₂)	7.1	9.2

Piezolektrina

Piezo – tlak, mechanická síla

$$P_j = d_{jkl} X_{kl}$$

polarizace

napětí

$$P'_i = a_{ij} P_j = a_{ij} d_{jkl} X_{kl}$$

$$P'_i = a_{ij} d_{jkl} a_{mk} a_{nl} X'_{mn} = d'_{imn} X'_{mn}$$

Tenzor 3. řádu

$$d'_{imn} = a_{ij} a_{mk} a_{nl} d_{jkl}$$

Symetrický – 18 koeficientů

$$\begin{pmatrix} P_1 \\ P_2 \\ P_3 \end{pmatrix} = \begin{pmatrix} d_{11} & d_{12} & d_{13} & d_{14} & d_{15} & d_{16} \\ d_{21} & d_{22} & d_{23} & d_{24} & d_{25} & d_{26} \\ d_{31} & d_{32} & d_{33} & d_{34} & d_{35} & d_{36} \end{pmatrix}$$

$$\begin{pmatrix} X_1 \\ X_2 \\ X_3 \\ X_4 \\ X_5 \\ X_6 \end{pmatrix}$$

$$X_{11} = X_1, \quad X_{22} = X_2, \quad X_{33} = X_3, \quad X_{12} = X_{21} = X_6,$$

$$X_{13} = X_{31} = X_5, \quad \text{and} \quad X_{23} = X_{32} = X_4.$$

$$d_{111} = d_{11}, \quad d_{122} = d_{12}, \quad d_{133} = d_{13}, \quad d_{123} + d_{132} = 2d_{123} = d_{14},$$

$$d_{131} + d_{113} = 2d_{113} = d_{15}, \quad d_{112} + d_{121} = 2d_{112} = d_{16}.$$

$$x_{ij} = d_{ijk}E_k$$

Inverzni piezoelektrický jev

$$\begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \\ x_5 \\ x_6 \end{pmatrix} = \begin{pmatrix} d_{11} & d_{21} & d_{31} \\ d_{12} & d_{22} & d_{32} \\ d_{13} & d_{23} & d_{33} \\ d_{14} & d_{24} & d_{34} \\ d_{15} & d_{25} & d_{35} \\ d_{16} & d_{26} & d_{36} \end{pmatrix} \begin{pmatrix} E_1 \\ E_2 \\ E_3 \end{pmatrix}$$

Příklad

Bodová grupa 2

Dvojčetná osa $\parallel Z_2$

$$(a) = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

V maticové formě

Neumannův princip

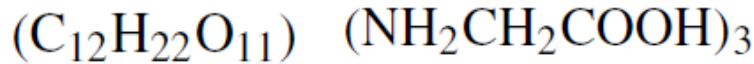
$$(d') = (a)(d)(\alpha)^{-1}$$

$$(d') = (a) \begin{pmatrix} d_{11} & d_{12} & d_{13} & d_{14} & d_{15} & d_{16} \\ d_{21} & d_{22} & d_{23} & d_{24} & d_{25} & d_{26} \\ d_{31} & d_{32} & d_{33} & d_{34} & d_{35} & d_{36} \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 \end{pmatrix}$$

$$(d') = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \begin{pmatrix} d_{11} & d_{12} & d_{13} & -d_{14} & d_{15} & -d_{16} \\ d_{21} & d_{22} & d_{23} & -d_{24} & d_{25} & -d_{26} \\ d_{31} & d_{32} & d_{33} & -d_{34} & d_{35} & -d_{36} \end{pmatrix}$$

8 různých nenulových koeficientů

$$= \begin{pmatrix} -d_{11} & -d_{12} & -d_{13} & +d_{14} & -d_{15} & +d_{16} \\ +d_{21} & +d_{22} & +d_{23} & -d_{24} & +d_{25} & -d_{26} \\ -d_{31} & -d_{32} & -d_{33} & +d_{34} & -d_{35} & +d_{36} \end{pmatrix}.$$



Coefficient	Sucrose	Triglycine sulfate	
d_{21}	1.48	23.6	feroelektrikum
d_{22}	-3.42	7.9	
d_{23}	0.74	25.3	
d_{14}	1.25	2.8	
d_{16}	-2.42	-4.6	
d_{25}	-0.87	24.3	
d_{34}	-4.22	-3.2	
d_{36}	0.42	2.8	

Pro keramiku

∞m

$$\begin{pmatrix} 0 & 0 & 0 & 0 & d_{15} & 0 \\ 0 & 0 & 0 & d_{15} & 0 & 0 \\ d_{31} & d_{31} & d_{33} & 0 & 0 & 0 \end{pmatrix}$$

v pC/N

Poled ceramics (<i>∞m</i>)	d_{31}	d_{33}	d_{15}
BaTiO ₃	-78	190	260
Pb(Zr, Ti)O ₃			
PZT-5H	-274	593	741
PZT-8	-27	225	330
K _{0.5} Na _{0.5} NbO ₃	-51	127	306

Point groups $\bar{1}$, $2/m$, mmm , $\bar{3}$, $\bar{3}m$, $4/m$,
 $4/mmm$, $6/m$, $6/mmm$, $m\bar{3}$, 432 ,
 $m\bar{3}m$, ∞/m , ∞/mmm , $\infty\infty$, $\infty\infty m$

$$\begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

Point group 1

$$\begin{pmatrix} d_{11} & d_{12} & d_{13} & d_{14} & d_{15} & d_{16} \\ d_{21} & d_{22} & d_{23} & d_{24} & d_{25} & d_{26} \\ d_{31} & d_{32} & d_{33} & d_{34} & d_{35} & d_{36} \end{pmatrix} \quad (18)$$

Point group 2

$$\begin{pmatrix} 0 & 0 & 0 & d_{14} & 0 & d_{16} \\ d_{21} & d_{22} & d_{23} & 0 & d_{25} & 0 \\ 0 & 0 & 0 & d_{34} & 0 & d_{36} \end{pmatrix} \quad (8)$$

Point group 4, 6, ∞

$$\begin{pmatrix} 0 & 0 & 0 & d_{14} & d_{15} & 0 \\ 0 & 0 & 0 & d_{15} & -d_{14} & 0 \\ d_{31} & d_{31} & d_{33} & 0 & 0 & 0 \end{pmatrix} \quad (4)$$

Point group $\bar{4}$

$$\begin{pmatrix} 0 & 0 & 0 & d_{14} & -d_{15} & 0 \\ 0 & 0 & 0 & d_{25} & d_{14} & 0 \\ d_{31} & -d_{31} & 0 & 0 & 0 & d_{36} \end{pmatrix} \quad (3)$$

Point group $4mm$, $6mm$, ∞m

$$\begin{pmatrix} 0 & 0 & 0 & 0 & d_{15} & 0 \\ 0 & 0 & 0 & d_{15} & 0 & 0 \\ d_{31} & d_{31} & d_{33} & 0 & 0 & 0 \end{pmatrix} \quad (3)$$

Point group $\bar{6}$

$$\begin{pmatrix} d_{11} & -d_{11} & 0 & 0 & 0 & -2d_{22} \\ -d_{22} & d_{22} & 0 & 0 & 0 & -2d_{11} \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

(2)

Point group $\bar{6}m2$

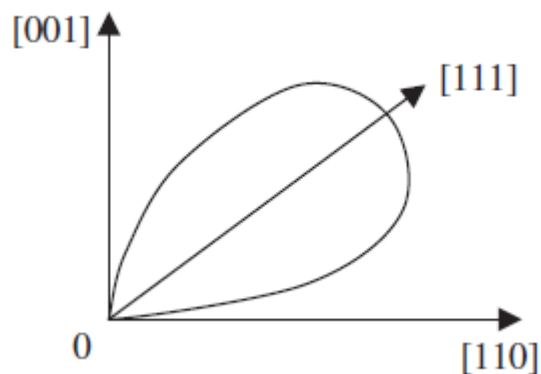
$$\begin{pmatrix} 0 & 0 & 0 & 0 & 0 & -2d_{22} \\ -d_{22} & d_{22} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

(1)

$\bar{4}3m, 23$

$$\begin{pmatrix} 0 & 0 & 0 & d_{14} & 0 & 0 \\ 0 & 0 & 0 & 0 & d_{14} & 0 \\ 0 & 0 & 0 & 0 & 0 & d_{14} \end{pmatrix}$$

(1)



Řez piezoelektrickým povrchem

Cubic ($\bar{4}3m$)

d_{14} (pC/N)

Bi ₁₂ SiO ₂₀	40
NaClO ₃	1.7
GaAs	2.6
ZnS	3.2

Hexagonal ($6mm$)

d_{31}	d_{33}	d_{15}
ZnO	12.4	-8.3
CdS	10.3	-14.0
AlN	5.0	4.0

Tetragonal ($4mm$)

d_{31}	d_{33}	d_{15}
BaTiO ₃	85.6	392
PbTiO ₃	117	62

Tetragonal ($\bar{4}2m$)

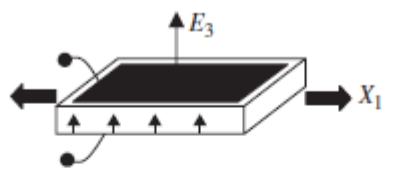
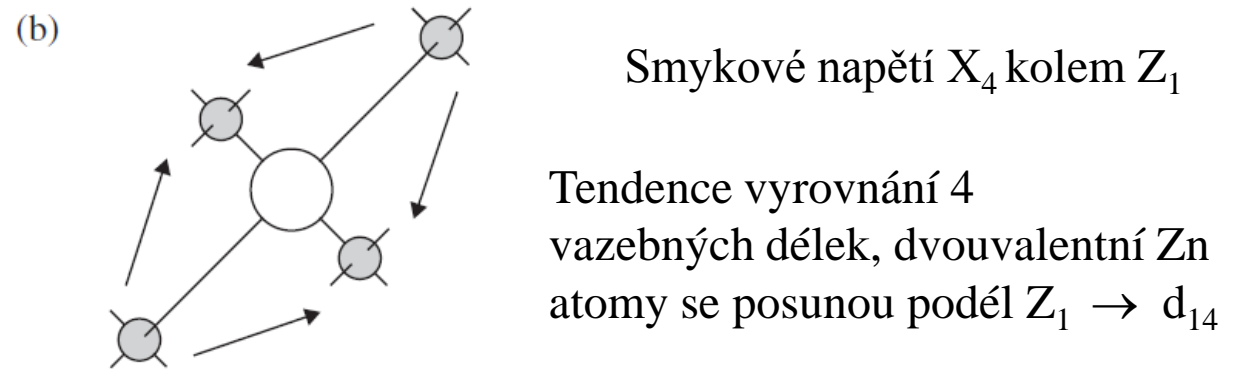
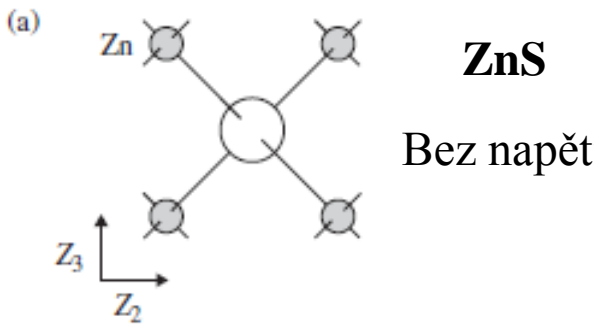
d_{14}	d_{36}
KH ₂ PO ₄	21
NH ₄ H ₂ PO ₄	48

Tetragonal (422)

d_{14}	
TeO ₂	8.1

Trigonal ($3m$)

d_{31}	d_{22}	d_{33}	d_{15}
LiNbO ₃	21	16	74
LiTaO ₃	9.0	9.0	26
Tourmaline	-0.3	-1.8	-3.6

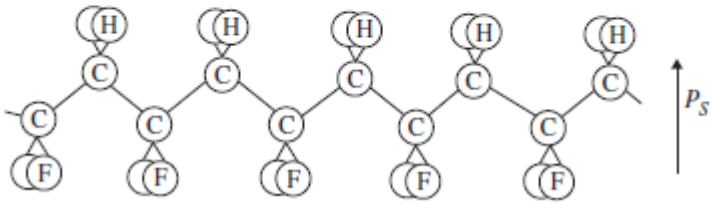


Elektrické pole $\propto m$ Tahové napětí \propto/mm

Curieův zákon

Společné prvky: m kolmo k Z_1, Z_2 a 2 podél Z_3

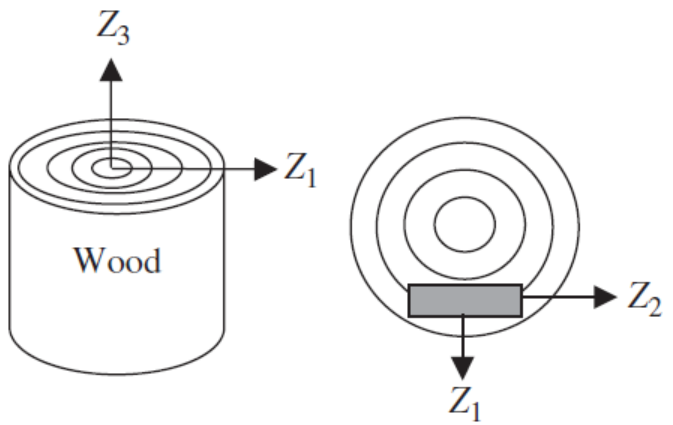
Ortorombická grupa $mm2$



PVDF = $(CH_2CF_2)_n$
polyvinylidene fluoride

$d_{31} = 20 \text{ pC/N}$ $d_{32} = 2$, $d_{33} = -30$

další malé



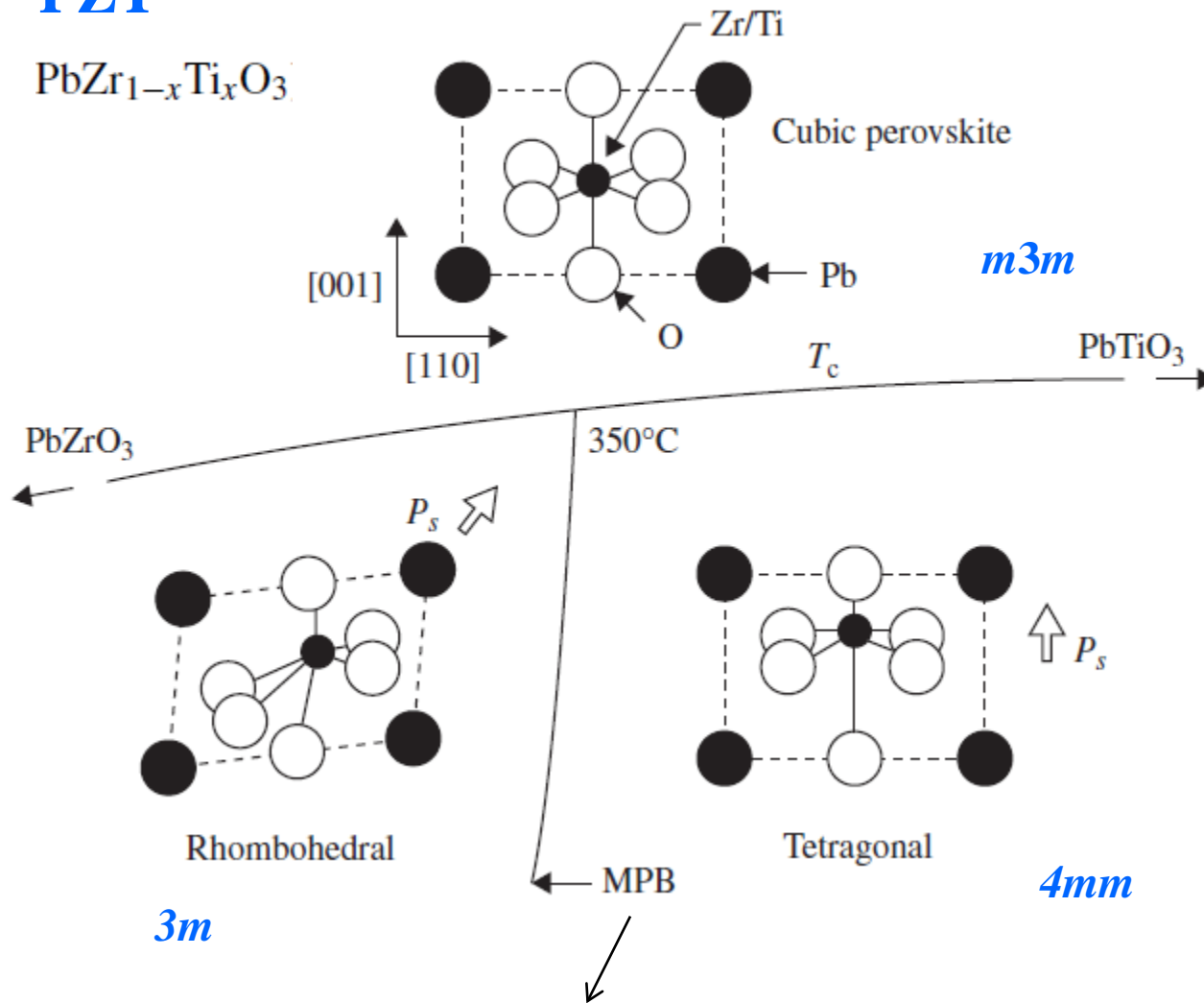
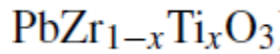
Dřevo grupa 222

Malé koeficienty

bříza

$d_{14} = -0.18$, $d_{25} = 0.30$, $d_{36} = 0.07 \text{ pC/N}$

PZT

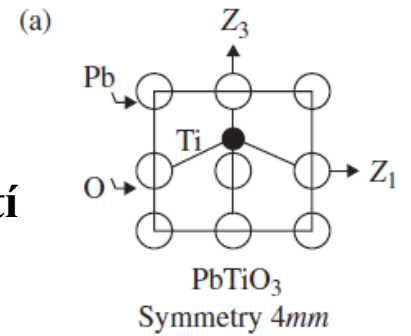


14 možných orientací polární osy

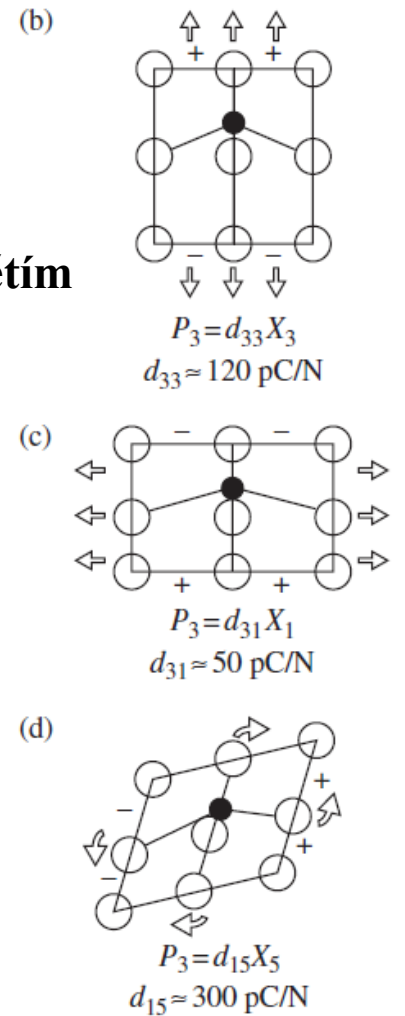
8 $\langle 111 \rangle$

6 $\langle 100 \rangle$

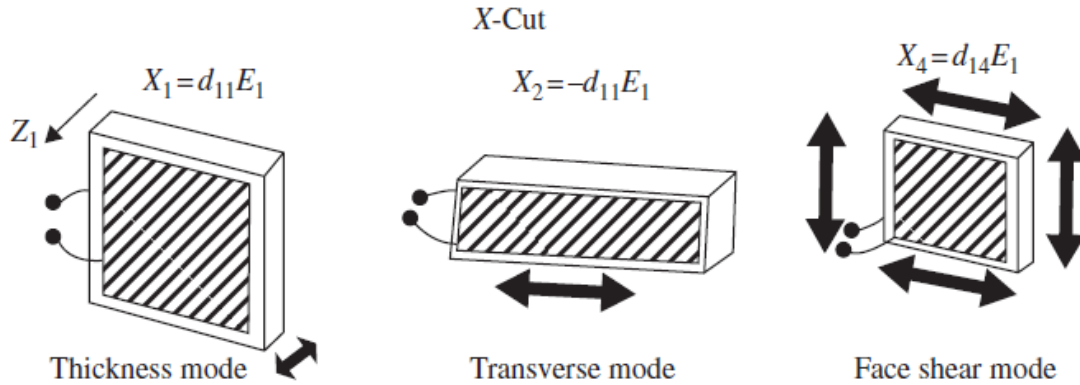
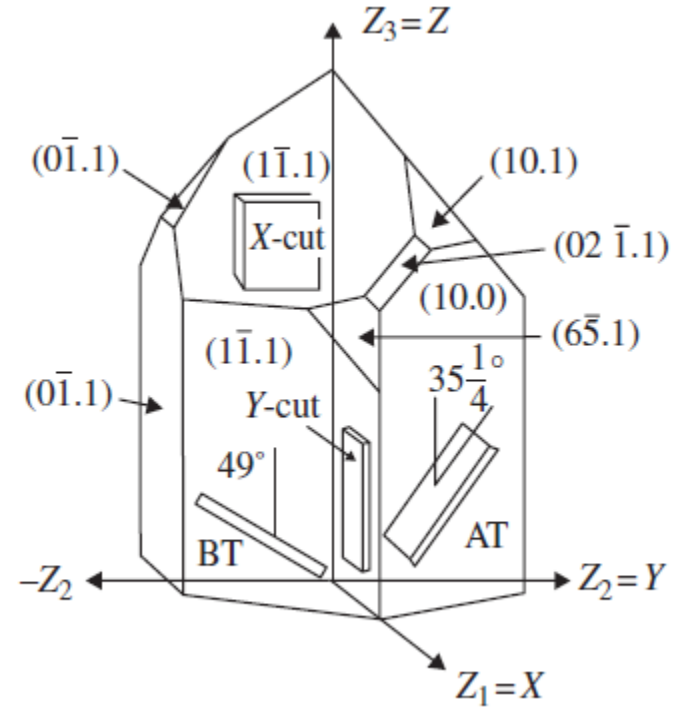
Bez
napětí



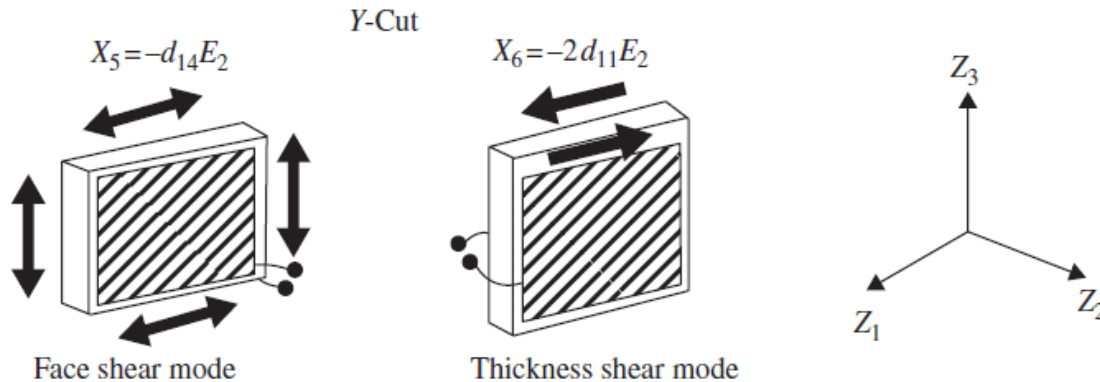
Pod
napětím



$$\begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \\ x_5 \\ x_6 \end{pmatrix} = \begin{pmatrix} d_{11} & 0 & 0 \\ -d_{11} & 0 & 0 \\ 0 & 0 & 0 \\ d_{14} & 0 & 0 \\ 0 & -d_{14} & 0 \\ 0 & -2d_{11} & 0 \end{pmatrix} \begin{pmatrix} E_1 \\ E_2 \\ E_3 \end{pmatrix} \quad \begin{aligned} d_{11} &= 2.27 \\ d_{14} &= -0.67 \text{ pC/N} \end{aligned}$$



Různé řezy krystalu



Elasticita

$$X_{ij} = c_{ijkl}x_{kl}$$

2 směry pro specifikaci napětí (síla, normála k rovině)
2 směry pro specifikaci deformace (posunutí, orientace osy měření) → tenzor 4. řádu

$$X'_{ij} = a_{ik}a_{jl}X_{kl} = a_{ik}a_{jl}c_{klmn}x_{mn}$$

$$= a_{ik}a_{jl}c_{klmn}a_{om}a_{pn}x'_{op}$$

$$= c'_{ijop}x'_{op}$$

$$c'_{ijop} = a_{ik}a_{jl}a_{om}a_{pn}c_{klmn}$$

81 složek

$$\begin{pmatrix} X_1 \\ X_2 \\ X_3 \\ X_4 \\ X_5 \\ X_6 \end{pmatrix} = \begin{pmatrix} c_{11} & c_{12} & c_{13} & c_{14} & c_{15} & c_{16} \\ c_{21} & c_{22} & c_{23} & c_{24} & c_{25} & c_{26} \\ c_{31} & c_{32} & c_{33} & c_{34} & c_{35} & c_{36} \\ c_{41} & c_{42} & c_{43} & c_{44} & c_{45} & c_{46} \\ c_{51} & c_{52} & c_{53} & c_{54} & c_{55} & c_{56} \\ c_{61} & c_{62} & c_{63} & c_{64} & c_{65} & c_{66} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \\ x_5 \\ x_6 \end{pmatrix}$$

Symetrické tenzory → 36 složek

Uložená mechanická energie

$$\begin{aligned}dW &= X_i dx_i = c_{ij} x_j dx_i \\ &= c_{11} x_1 dx_1 + c_{12} x_2 dx_1 + c_{21} x_1 dx_2 + \dots\end{aligned}$$

$$\frac{\partial W}{\partial x_1} = c_{11} x_1 + c_{12} x_2 + \dots + c_{16} x_6$$

$$\frac{\partial W}{\partial x_2} = c_{21} x_1 + c_{22} x_2 + \dots + c_{26} x_6.$$

$$\frac{\partial^2 W}{\partial x_1 \partial x_2} = c_{12}$$

$$\frac{\partial^2 W}{\partial x_2 \partial x_1} = c_{21}$$

$$c_{12} = c_{21}.$$

$$c_{ij} = c_{ji}.$$

$$c_{ijkl} = c_{klmn} = \delta_{im} \delta_{jn}$$

21 potřebných složek

Pro kubické krystaly

$$c_{11} = (s_{11} + s_{12}) / (s_{11} - s_{12})(s_{11} + 2s_{12})$$

$$c_{12} = -s_{12} / (s_{11} - s_{12})(s_{11} + 2s_{12})$$

$$c_{44} = 1/s_{44}.$$

Pro hexagonální krystaly

$$c_{11} + c_{12} = s_{33}/S$$

$$c_{11} - c_{12} = 1/(s_{11} - s_{12})$$

$$c_{13} = -s_{13}/S$$

$$c_{33} = (s_{11} + s_{12})/S$$

$$c_{44} = 1/s_{44},$$

$$S = s_{33}(s_{11} + s_{12}) - 2s_{13}^2.$$

Příklad 4/m



$$4 \parallel Z_3$$



$$1 \rightarrow 2, 2 \rightarrow -1, 3 \rightarrow 3$$

$$\begin{pmatrix} s_{11} & s_{12} & s_{13} & 0 & 0 & s_{16} \\ s_{12} & s_{11} & s_{13} & 0 & 0 & -s_{16} \\ s_{13} & s_{13} & s_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & s_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & s_{44} & 0 \\ s_{16} & -s_{16} & 0 & 0 & 0 & s_{66} \end{pmatrix}$$

$$1111 \rightarrow 2222$$

$$2222 \rightarrow 1111$$

$$3333 \rightarrow 3333$$

$$1122 \rightarrow 2211$$

$$1133 \rightarrow 2233$$

$$1212 \rightarrow 2121$$

$$1313 \rightarrow 2323$$

$$1233 \rightarrow -2133$$

$$2321 \rightarrow 1312$$

$$1312 \rightarrow -2321$$

$$1112 \rightarrow -2221$$

⋮

$$(s_{11} = s_{22})$$

$$(s_{22} = s_{11})$$

$$(s_{33})$$

$$(s_{12} = s_{21})$$

$$(s_{13} = s_{23})$$

$$(s_{66})$$

$$(s_{55} = s_{44})$$

$$(s_{63} = -s_{63} = 0)$$

$$(s_{46} = s_{56})$$

$$(s_{56} = -s_{46} = -s_{56} = 0)$$

$$(s_{16} = -s_{26})$$

$$m \perp Z_3$$

$$1 \rightarrow \hat{1}, 2 \rightarrow \tilde{2}, \hat{3} \rightarrow -3$$

Žádná nová omezení

Příklady

Orthorhombic
222, $mm2$, mmm

$$\begin{pmatrix} c_{11} & c_{12} & c_{13} & 0 & 0 & 0 \\ c_{12} & c_{22} & c_{23} & 0 & 0 & 0 \\ c_{13} & c_{23} & c_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & c_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & c_{55} & 0 \\ 0 & 0 & 0 & 0 & 0 & c_{66} \end{pmatrix}$$

Tetragonal
 4 , $\bar{4}$, $4/m$

$$\begin{pmatrix} c_{11} & c_{12} & c_{13} & 0 & 0 & c_{16} \\ c_{12} & c_{11} & c_{13} & 0 & 0 & -c_{16} \\ c_{13} & c_{13} & c_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & c_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & c_{44} & 0 \\ c_{16} & -c_{16} & 0 & 0 & 0 & c_{66} \end{pmatrix}$$

Hexagonal

6 , $\bar{6}$, $6/m$, 622 , $6mm$, $\bar{6}m2$,
 $6/mmm$

Curie groups

∞ , ∞m , ∞/m , $\infty 2$, ∞/mm

$$\begin{pmatrix} c_{11} & c_{12} & c_{13} & 0 & 0 & 0 \\ c_{12} & c_{11} & c_{13} & 0 & 0 & 0 \\ c_{13} & c_{13} & c_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & c_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & c_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{2}(c_{11} - c_{12}) \end{pmatrix}$$

Cubic

23 , $m3$, 432 , $\bar{4}3m$, $m3m$

$$\begin{pmatrix} c_{11} & c_{12} & c_{12} & 0 & 0 & 0 \\ c_{12} & c_{11} & c_{12} & 0 & 0 & 0 \\ c_{12} & c_{12} & c_{11} & 0 & 0 & 0 \\ 0 & 0 & 0 & c_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & c_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & c_{44} \end{pmatrix}$$

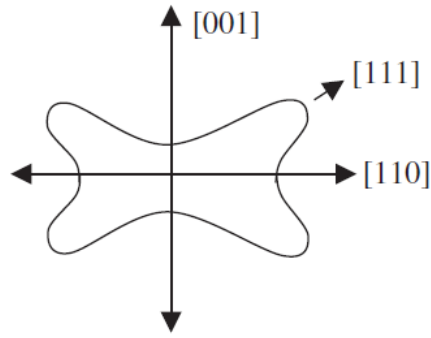
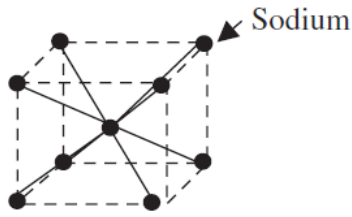
v 10^{11} N/m²

	c_{11}	c_{12}	c_{14}	A
<i>Alkali metals (body-centered cubic)</i>				
Li	0.135	0.114	0.088	8.4
Na	0.074	0.062	0.042	7.2
K	0.037	0.031	0.019	6.7
<i>Semiconductors (diamond structure)</i>				
C	10.20	2.50	4.92	1.3
Si	1.66	0.64	0.80	1.6
Ge	1.30	0.49	0.67	1.7
<i>Alkali halides (NaCl structure)</i>				
NaCl	0.485	0.125	0.127	0.7
KCl	0.405	0.066	0.063	0.37
RbCl	0.363	0.062	0.047	0.31

$$A = 2c_{44}/(c_{11} - c_{12})$$

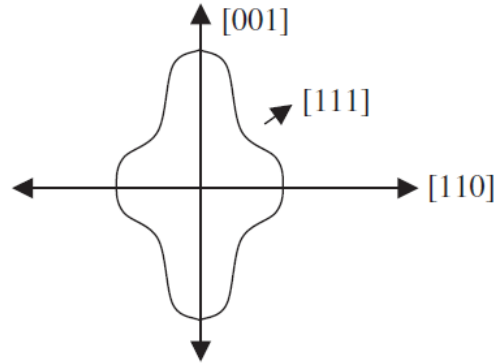
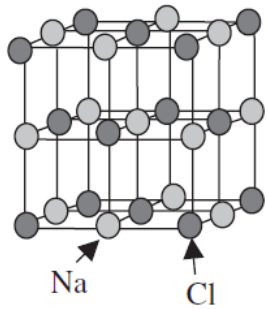
Anizotropie**A < 1 nejtvrdší podél <100>****A > 1 nejtvrdší podél <111>**

Na

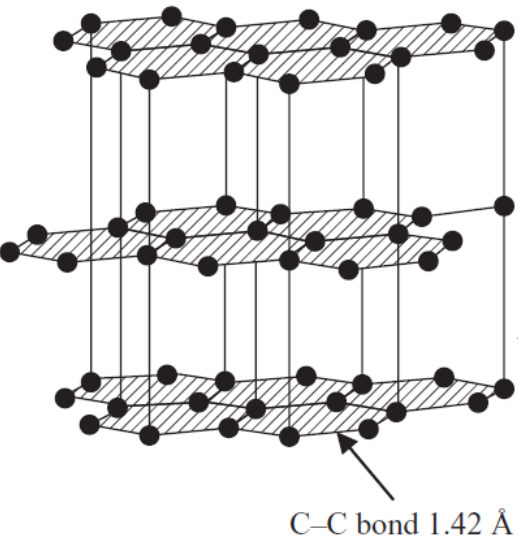


Stiffness (tuhost)

NaCl



grafit



$$\begin{pmatrix} 11.6 & 2.9 & 1.1 & 0 & 0 & 0 \\ 2.9 & 11.6 & 1.1 & 0 & 0 & 0 \\ 1.1 & 1.1 & 0.5 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0.02 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0.02 & 0 \\ 0 & 0 & 0 & 0 & 0 & 4.4 \end{pmatrix}$$

$c_{11} \gg c_{33}$

Metal	c_{11}	c_{33}	c_{33}/c_{11}	a	c	c/a
Be	2.92	3.36	1.16	2.29	3.58	1.56
Cd	1.16	0.51	0.44	2.98	5.62	1.89
Co	3.07	3.58	1.17	2.51	4.07	1.62
Hf	1.81	1.97	1.09	3.20	5.06	1.58
Mg	0.60	0.62	1.03	3.21	5.21	1.62
Re	6.13	6.83	1.12	2.76	4.46	1.62
Ti	1.62	1.81	1.12	2.95	4.69	1.59
Zn	1.61	0.61	0.38	2.66	4.95	1.86
Zr	1.43	1.65	1.15	3.23	5.15	1.59

Stlačitelnost

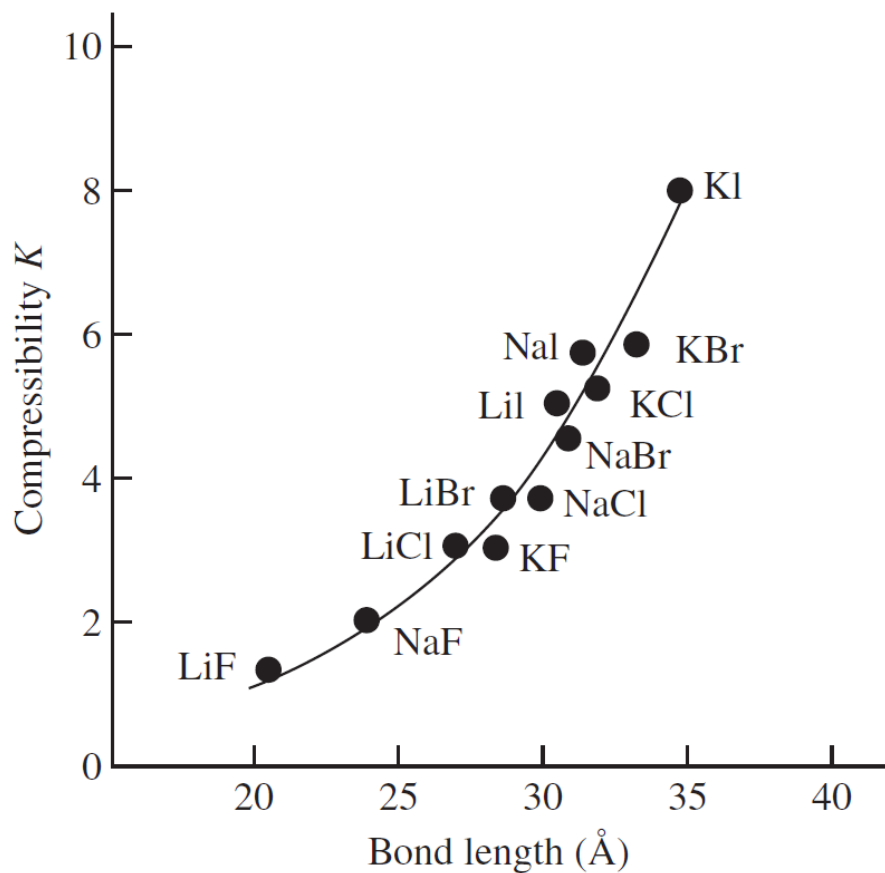
Změna objemu na jednotkový objem

$$x_{11} + x_{22} + x_{33}$$

$$K = -\frac{1}{V} \frac{dV}{dp}$$

$$x_{ii} = s_{iikl} X_{kl} = -s_{iikl} p \delta_{kl}$$

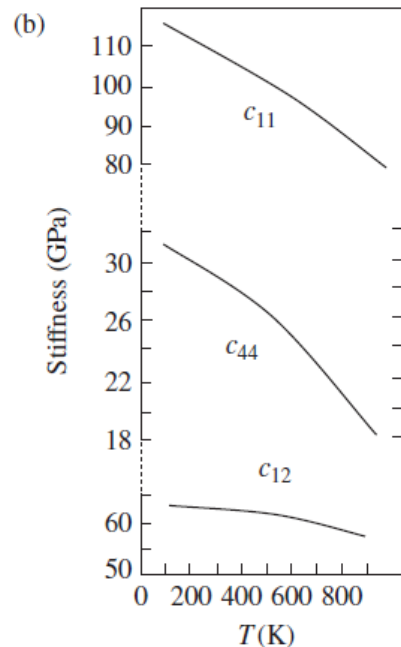
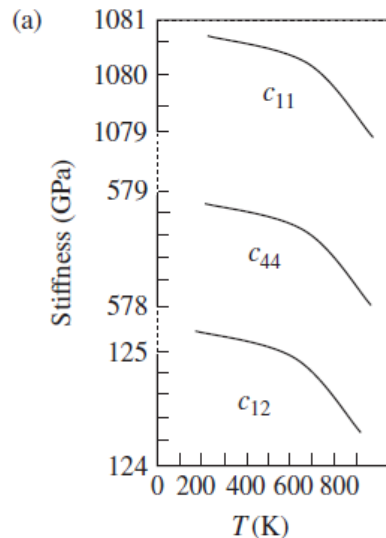
$$K = s_{iikk} = s_{1111} + s_{1122} + s_{1133} + s_{2211} + s_{2222} + s_{2233} \\ + s_{3311} + s_{3322} + s_{3333} \\ + s_{22} + s_{33} + 2s_{12} + 2s_{13} + 2s_{23}.$$



Krystaly s dlouhými vazbami jsou stlačitelnější

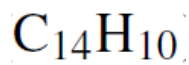
Teplotní závislost elastických konstant

diamant



hliník

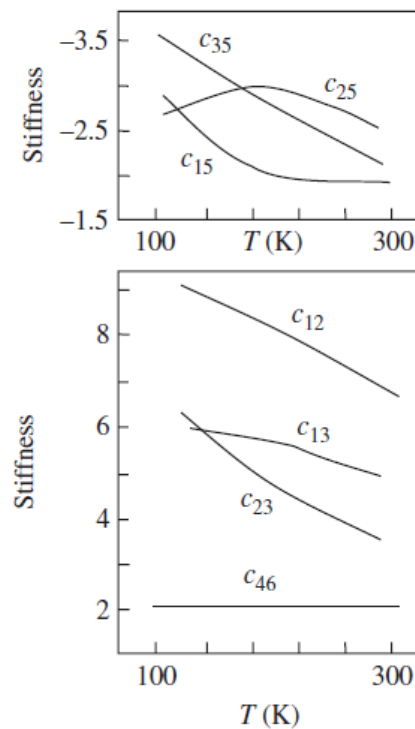
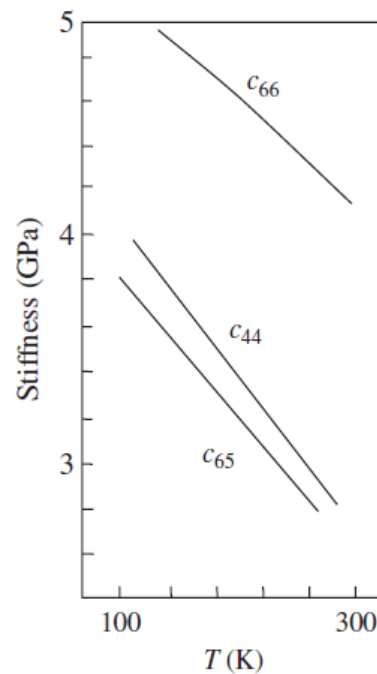
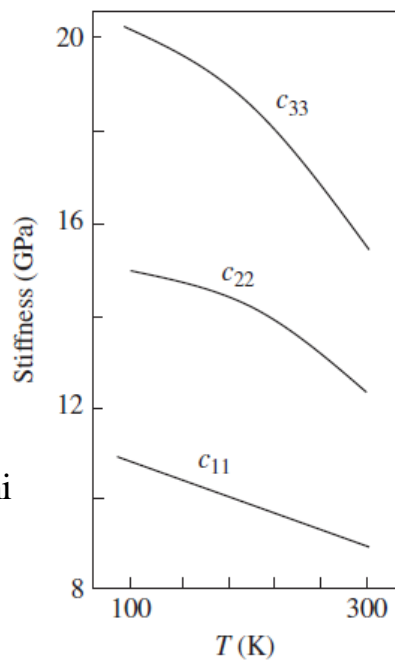
Antracen



$2/m$

Silná anizotropie
slabé vazby mezi molekulami

(c)



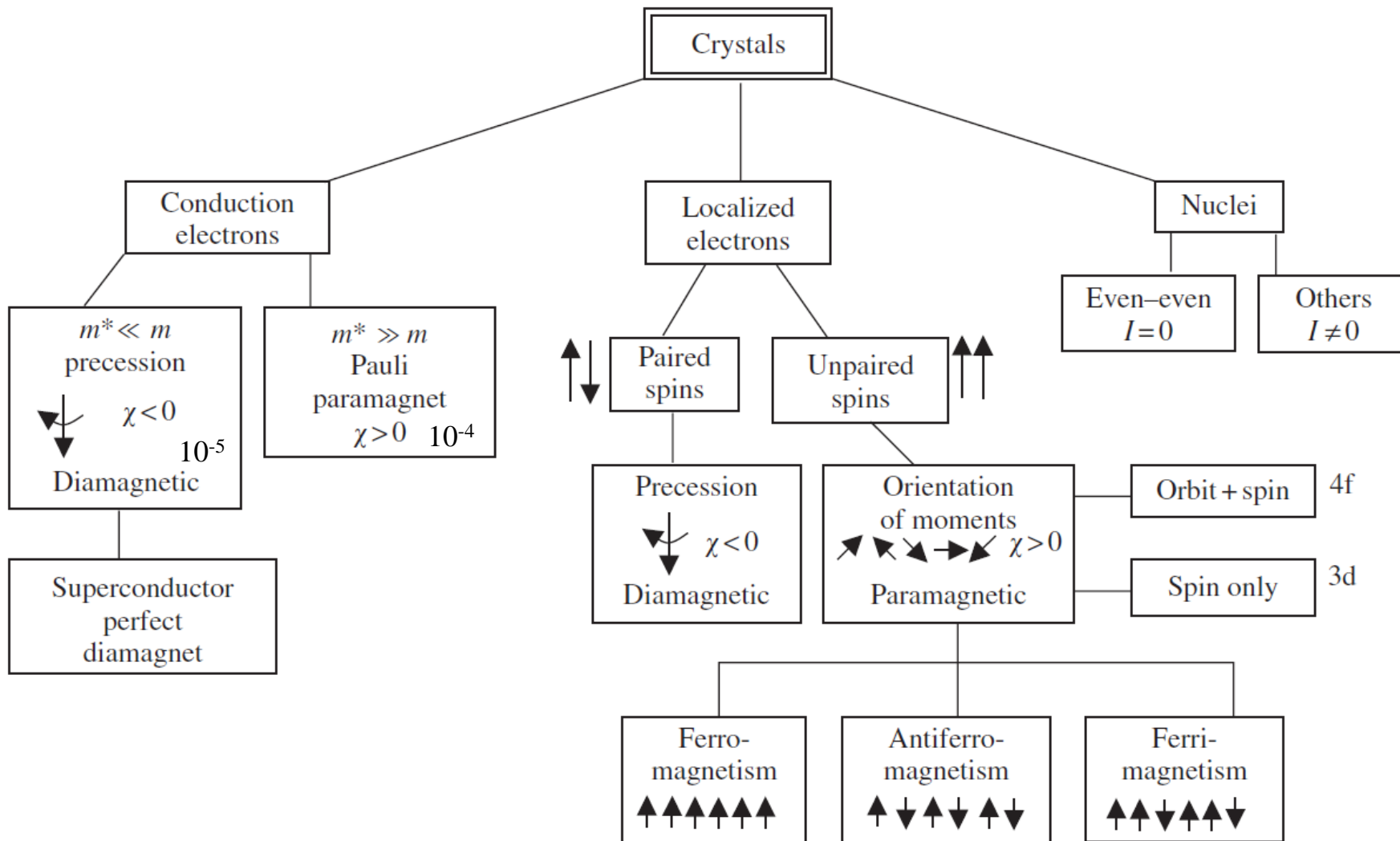
Magnetické vlastnosti

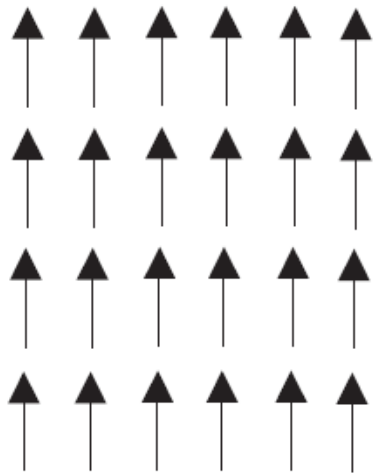
$$I = \chi H$$

Magnetizace
 ↓
 Magnetická susceptibilita

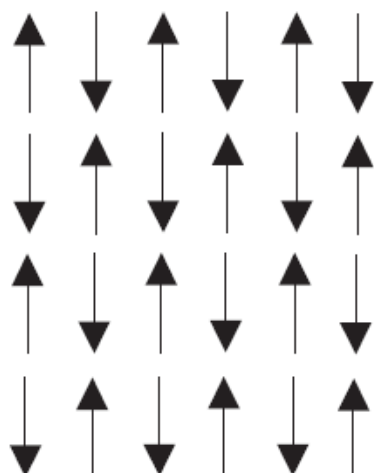
$$B = \mu H$$

↓
 Magnetická permeabilita

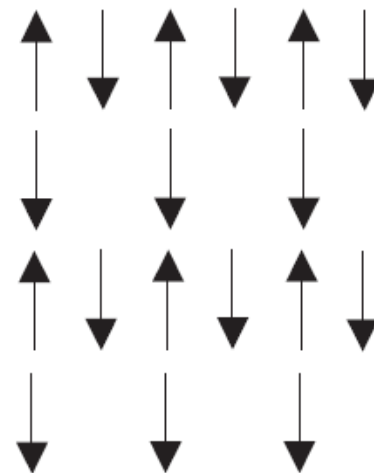




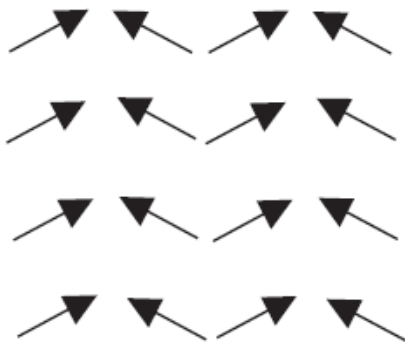
Collinear
ferromagnet



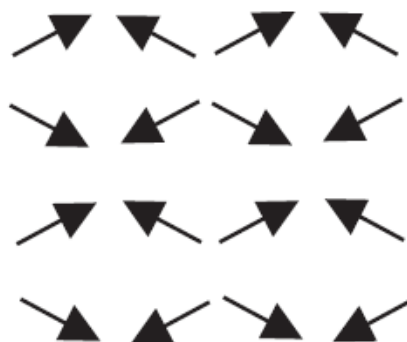
Collinear
antiferromagnet



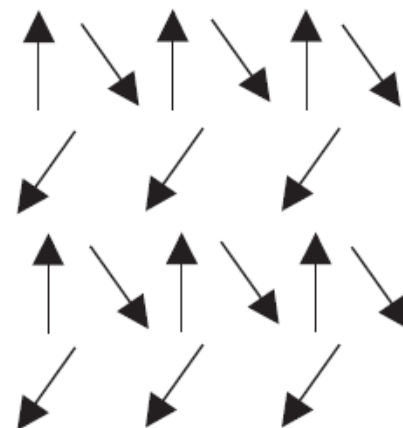
Collinear
ferrimagnet



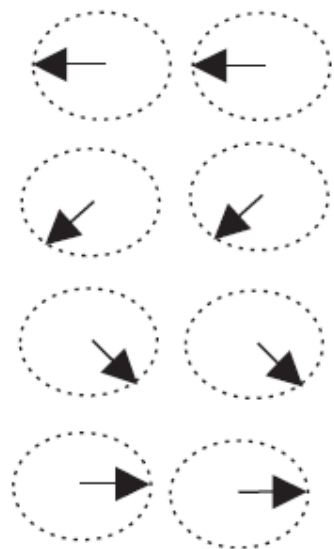
Non collinear
weak
ferromagnet



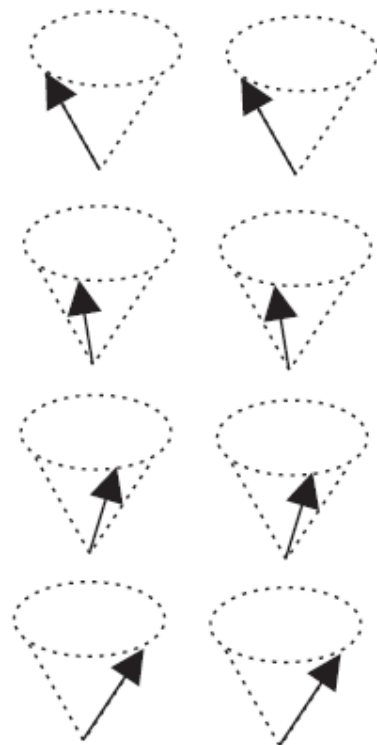
Non collinear
weak
antiferromagnet



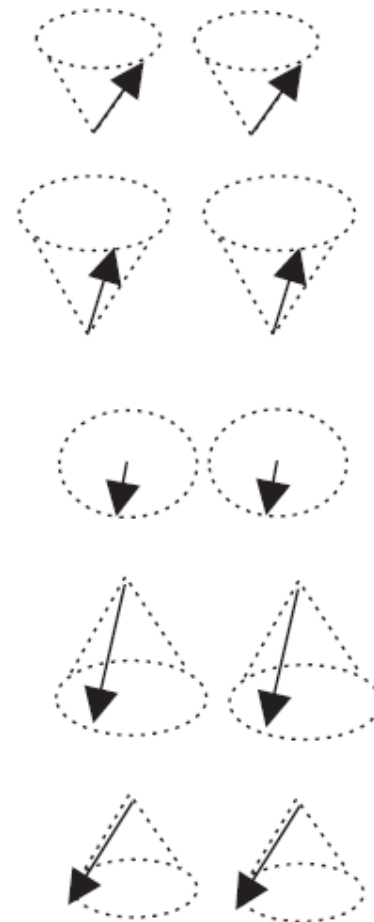
Strongly
canted
ferrimagnet



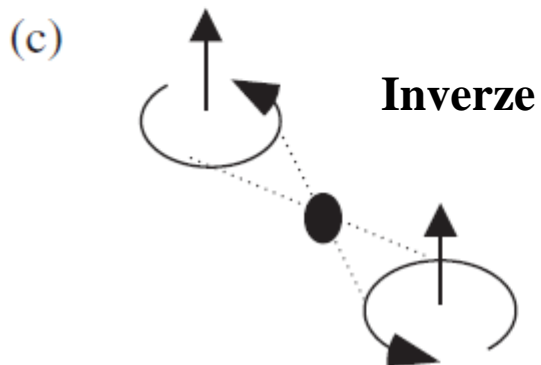
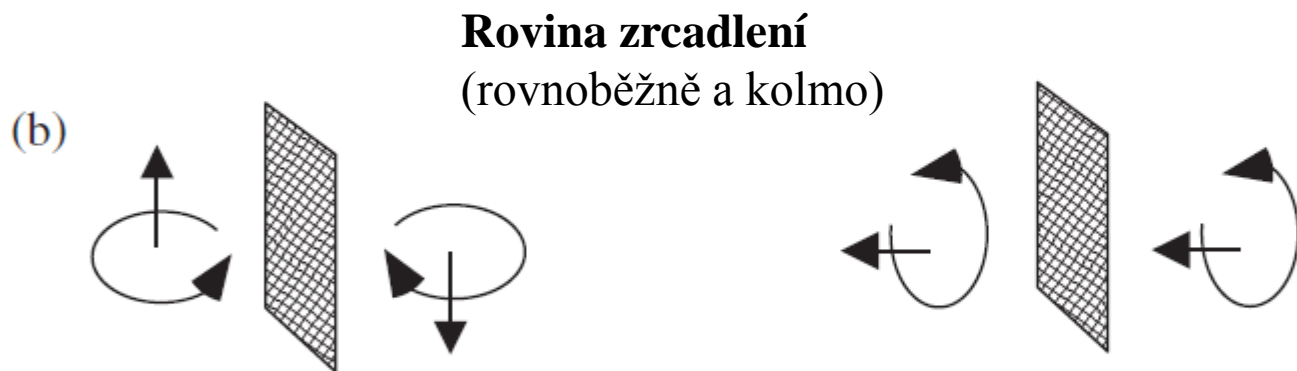
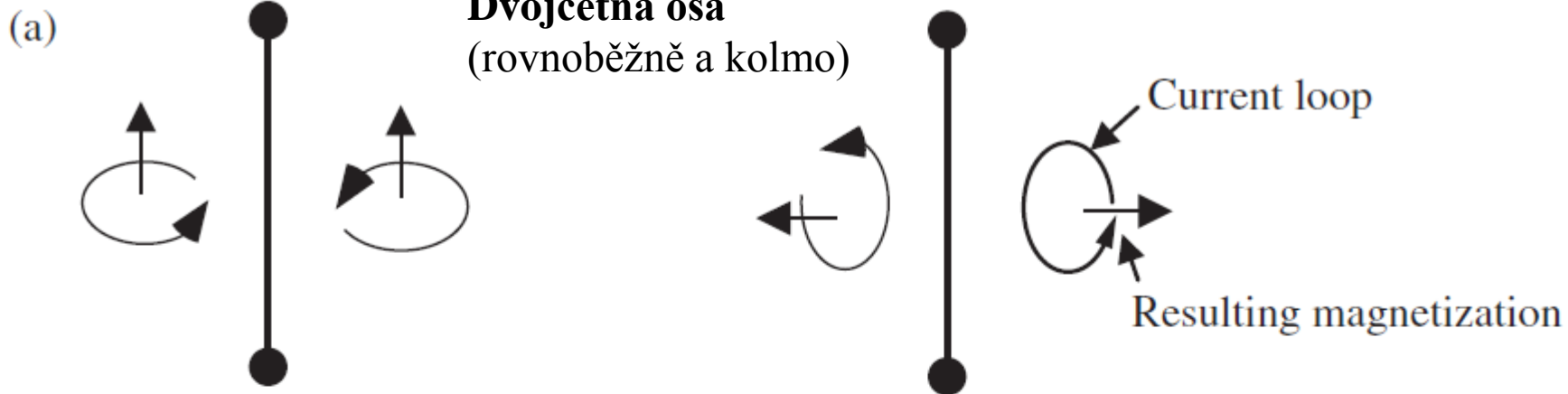
Antiferromagnetic
helicoid

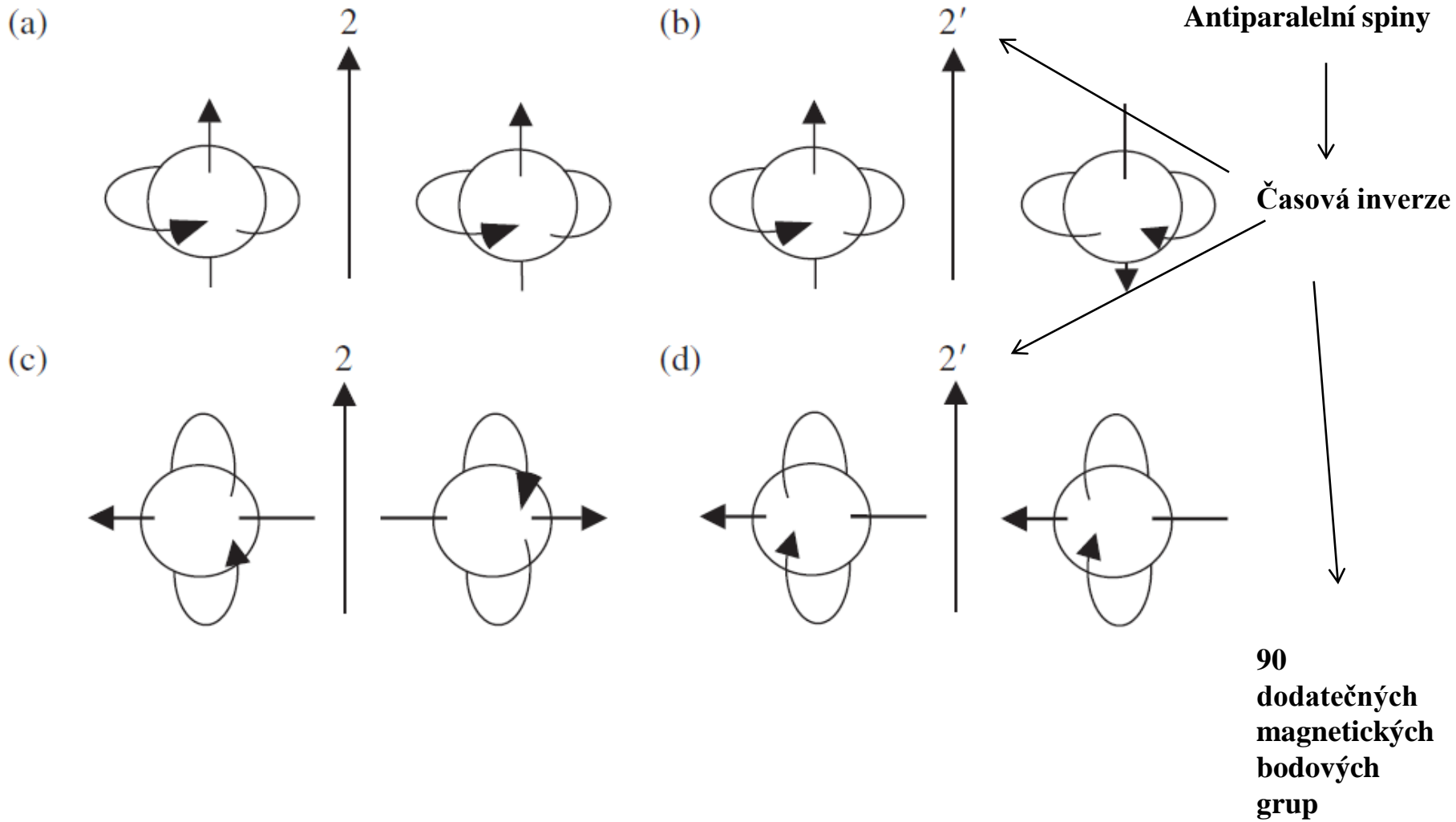


Ferromagnetic
helicoid



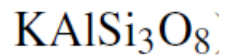
Cycloidal
antiferromagnet





Magnetické bodové grupy

$2/m$



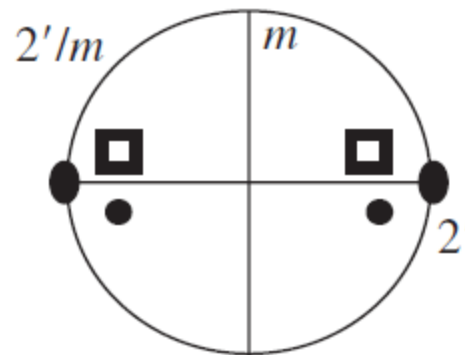
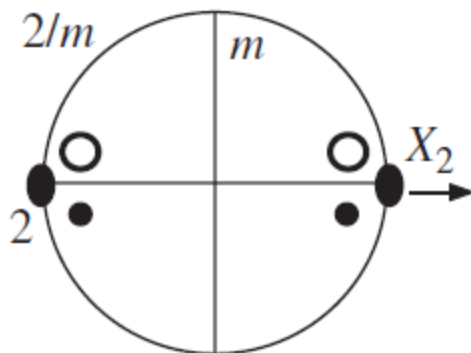
nemagnetické

$2, 2', m, m', -1$

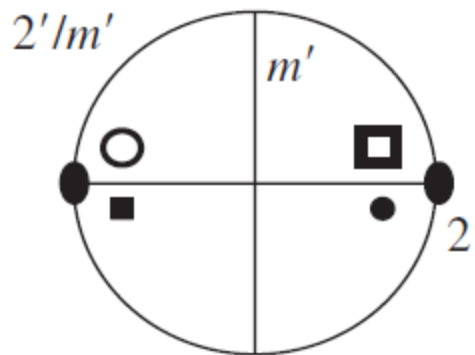
Krystalografická grupa (obsahuje obyčejné a časově převrácené prvky symetrie)

$2/m1'$ →

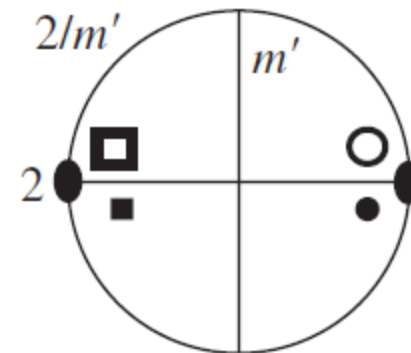
Čtyři magnetické grupy



ErOOH

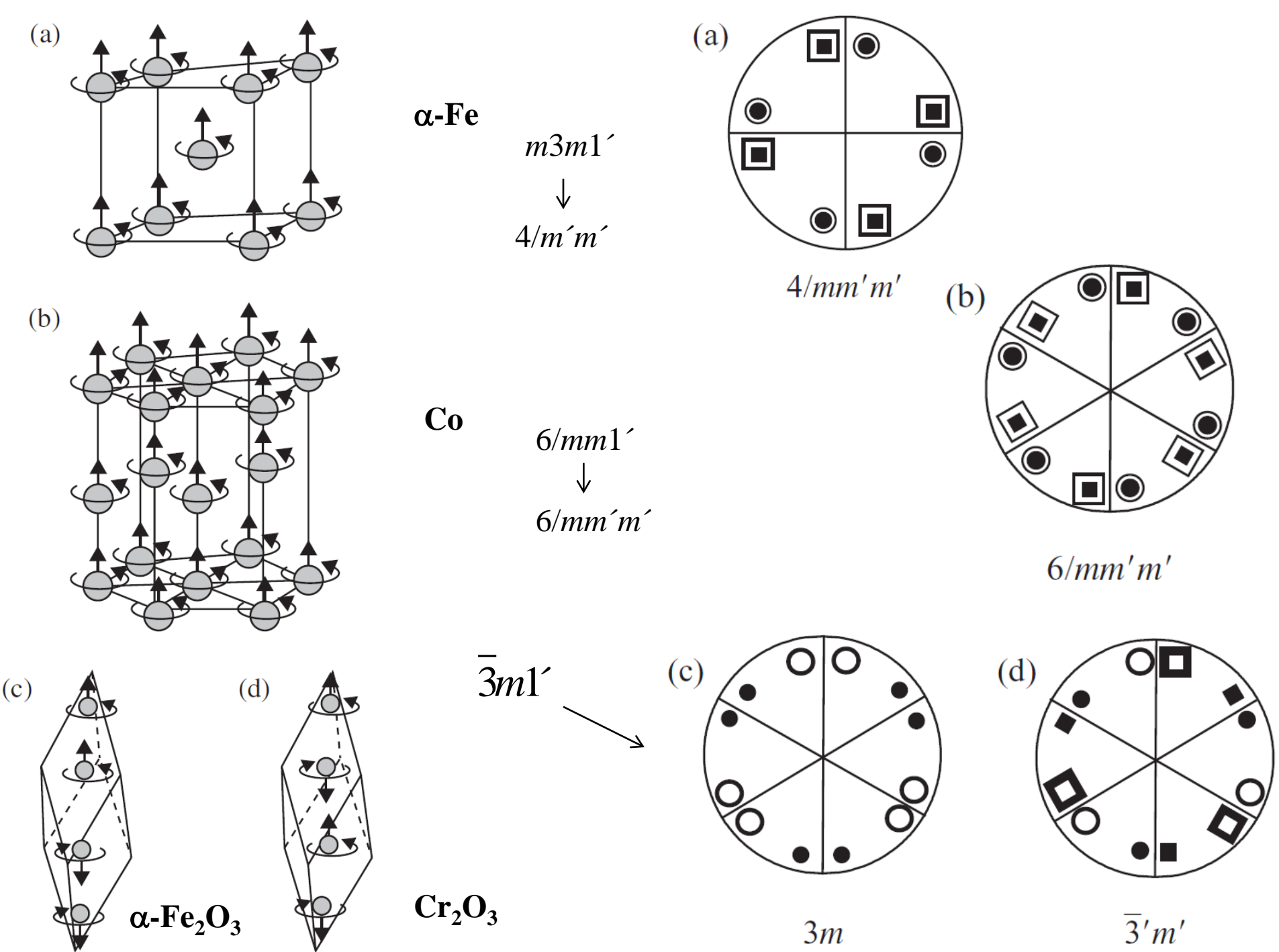


Fe_3Se_4



DyOOH

	Pyromagnetic	Magnetoelectric	Piezomagnetic	Generating elements
Tetragonal				
$4'/mmm'$	0	0	3(2)	$m \perp Z_1, m \perp Z_3, 4' \parallel Z_3$
$4/mm'm'$	1(1)	0	5(3)	$m' \perp Z_1, m \perp Z_3, 4 \parallel Z_3$
$4/m'm'm'$	0	3(2)	0	$m' \perp Z_1, m' \perp Z_3, 4 \parallel Z_3$
$4/m'mm$	0	2(1)	0	$m \perp Z_1, m' \perp Z_3, 4 \parallel Z_3$
$4'/m'mm'$	0	2(1)	0	$m \perp Z_1, m' \perp Z_3, 4' \parallel Z_3$
Cubic				
23	0	3(1)	3(1)	$2 \parallel Z_1, 3 \parallel [111]$
$m3$	0	0	3(1)	$m \perp Z_1, 3 \parallel [111]$
$m'3$	0	3(1)	0	$m' \perp Z_1, 3 \parallel [111]$
432	0	3(1)	0	$4 \parallel Z_1, 3 \parallel [111]$
$4'32$	0	0	3(1)	$4' \parallel Z_1, 3 \parallel [111]$
$\bar{4}3m$	0	0	0	$\bar{4} \parallel Z_1, 3 \parallel [111]$
$\bar{4}'3m'$	0	3(1)	3(1)	$\bar{4}' \parallel Z_1, 3 \parallel [111]$
$m3m$	0	0	0	$m \perp Z_1, 3 \parallel [111],$ $m \perp [100]$
$m3m'$	0	0	3(1)	$m \perp Z_1, 3 \parallel [111],$ $m' \perp [110]$
$m'3m'$	0	3(1)	0	$m' \perp Z_1, 3 \parallel [111],$ $m' \perp [110]$
$m'3m$	0	0	0	$m' \perp Z_1, 3 \parallel [111],$ $m \perp [110]$



Maxwellovy rovnice ve dvou formách

Vector form

Tensor form

$$\vec{\nabla} \times \vec{E} = -\frac{\partial \vec{B}}{\partial t}$$

$$\varepsilon_{ijk} \frac{\partial E_k}{\partial Z_j} = -\frac{\partial B_i}{\partial t}$$

$$\vec{\nabla} \times \vec{H} = \vec{J} + \frac{\partial \vec{D}}{\partial t}$$

$$\varepsilon_{ijk} \frac{\partial H_k}{\partial Z_j} = J_i + \frac{\partial D_i}{\partial t}$$

$$\vec{\nabla} \cdot \vec{B} = 0$$

$$\frac{\partial B_i}{\partial Z_i} = 0$$

$$\vec{\nabla} \cdot \vec{D} = \rho$$

$$\frac{\partial D_i}{\partial Z_i} = \rho$$

Pyromagnetismus

Spontánní magnetizace

$$\Delta I_s = Q \Delta T$$

Pyromagnetický koeficient

$$\begin{aligned} \Delta I'_i &= \pm |a| a_{ij} \Delta I_j = \pm |a| a_{ij} Q_j \Delta T \\ &= \pm |a| a_{ij} Q_j \Delta T' = Q'_i \Delta T'. \end{aligned}$$

$$Q'_i = \pm |a| a_{ij} Q_j$$

$$\begin{matrix} 3 \times 1 & & 3 \times 3 & 3 \times 1 \\ (Q') & = \pm |a| & (a) & (Q). \end{matrix}$$

Příklad: Co

$6/m\bar{m}'m'$

Generátory:

$6 \parallel Z_3, m \perp Z_3$
 $m' \perp Z_1$

$$(Q') = (+1)(-1) \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix} (Q) = \begin{pmatrix} -Q_1 \\ -Q_2 \\ Q_3 \end{pmatrix}$$

$$Q_1 = -Q_1 = 0, Q_2 = -Q_2 = 0, Q_3 = Q_3$$

$$(Q') = (-1)(-1) \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ Q_3 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ Q_3 \end{pmatrix}$$

Magnetic point groups

Pyromagnetic matrix

Pyromagnetické grupy

$1, \bar{1}$ (Q_1, Q_2, Q_3)

$2', m', 2'/m'$ $(Q_1, 0, Q_3)$

$2, m, 2/m$ $(0, Q_2, 0)$

$2'2'2, m'm'2, m'2'm,$ $(0, 0, Q_3)$

$m'm'm, 3, \bar{3}, 32', 3m',$

$\bar{3}m', 4, \bar{4}, 4/m, 42'2',$

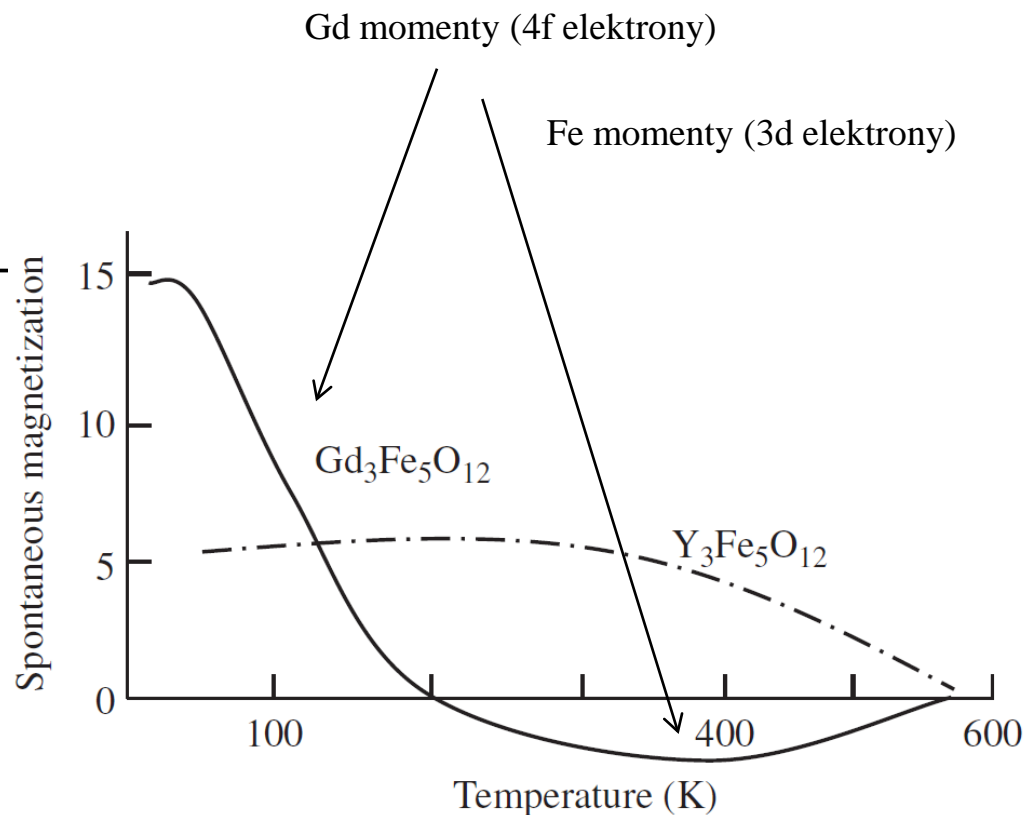
$4m'm', 42'm', 4/mm'm', 6$

$\bar{6}, 6/m, 62'2', 6m'm', \bar{6}m'2',$

$6/mm'm', \infty, \infty/m, \infty2', \infty m',$

∞/mm'

All others $(0, 0, 0)$



Magnetická susceptibilita, permeabilita

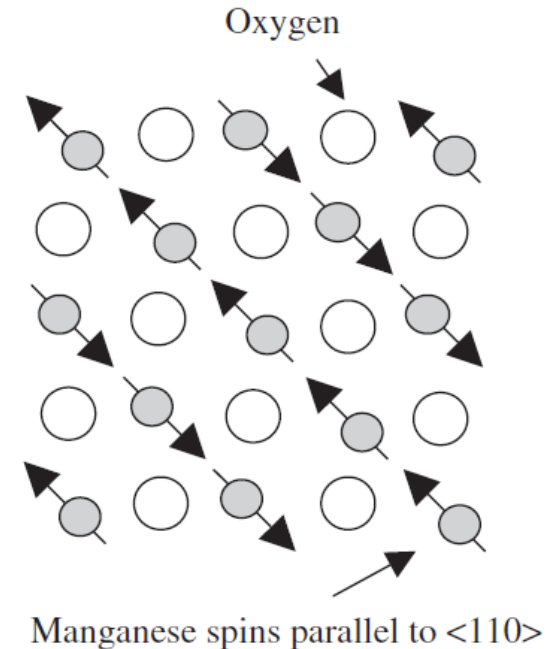
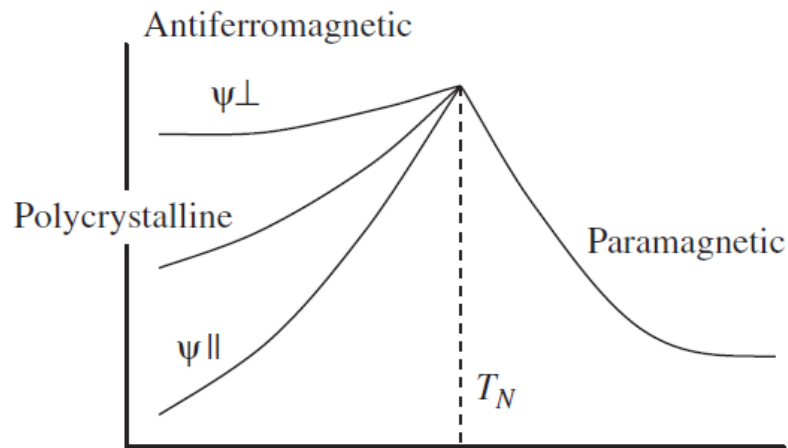
$$\chi'_{ij} = a_{ik}a_{il}\chi_{kl}$$

$$\mu'_{ij} = a_{ik}a_{jl}\mu_{kl} = \chi'_{ij} + \mu_0$$

Analogie s elektrickou permitivitou
a dielektrickou konstantou

Příklad:

Anizotropie magnetické susceptibilitity MnO



Magnetoelektrický jev

$$\begin{aligned}
 [Wb/m^2] \leftarrow I'_i &= \pm |a| a_{ij} I_j = \pm |a| a_{ij} Q_{jk} E_k \\
 &= \pm |a| a_{ij} Q_{jk} a_{lk} E'_l = Q'_{il} E'_l \\
 Q'_{il} &= \pm |a| a_{ij} a_{lk} Q_{jk}.
 \end{aligned}$$

$[Wb/V\ m]$
 $[V/m]$

$$\begin{aligned}
 \begin{matrix} 3 \times 1 \\ (I') \end{matrix} &= \pm |a| \begin{matrix} 3 \times 3 \\ (a) \end{matrix} \begin{matrix} 3 \times 1 \\ (I) \end{matrix} = \pm |a| \begin{matrix} 3 \times 3 \\ (a) \end{matrix} \begin{matrix} 3 \times 3 \\ (Q) \end{matrix} \begin{matrix} 3 \times 1 \\ (E) \end{matrix} \\
 &= \pm |a| \begin{matrix} 3 \times 3 \\ (a) \end{matrix} \begin{matrix} 3 \times 3 \\ (Q) \end{matrix} \begin{matrix} 3 \times 3 \\ (a)_t \end{matrix} \begin{matrix} 3 \times 1 \\ (E') \end{matrix} = \begin{matrix} 3 \times 3 \\ (Q') \end{matrix} \begin{matrix} 3 \times 1 \\ (E') \end{matrix} \\
 \begin{matrix} 3 \times 3 \\ (Q') \end{matrix} &= \pm |a| \begin{matrix} 3 \times 3 \\ (a) \end{matrix} \begin{matrix} 3 \times 3 \\ (Q) \end{matrix} \begin{matrix} 3 \times 3 \\ (a)_t \end{matrix}.
 \end{aligned}$$

Magnetoelektrický jev je nulový pro všechny grupy obsahující časovou i obyčejnou inverzi

$$(Q') = (-1)(+1)(+1)(Q)(+1) = (-Q) = (Q) = 0.$$

$$(Q') = (+1)(-1)(-1)(Q)(-1) = (-Q) = (Q) = 0.$$

Příklad: Cr_2O_3
 $\bar{3}'m'$ $m' \perp Z_1$

$$\begin{pmatrix} Q'_{11} & Q'_{12} & Q'_{13} \\ Q'_{21} & Q'_{22} & Q'_{23} \\ Q'_{31} & Q'_{32} & Q'_{33} \end{pmatrix} = (-1)(-1) \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} Q_{11} & Q_{12} & Q_{13} \\ Q_{21} & Q_{22} & Q_{23} \\ Q_{31} & Q_{32} & Q_{33} \end{pmatrix}$$

$$\times \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

Neumann

$$= \begin{pmatrix} Q_{11} & -Q_{12} & -Q_{13} \\ -Q_{21} & Q_{22} & Q_{23} \\ -Q_{31} & Q_{32} & Q_{33} \end{pmatrix} = \begin{pmatrix} Q_{11} & Q_{12} & Q_{13} \\ Q_{21} & Q_{22} & Q_{23} \\ Q_{31} & Q_{32} & Q_{33} \end{pmatrix}$$

$$Q_{12} = Q_{13} = Q_{21} = Q_{31} = 0$$

$\bar{3}' \parallel Z_3$

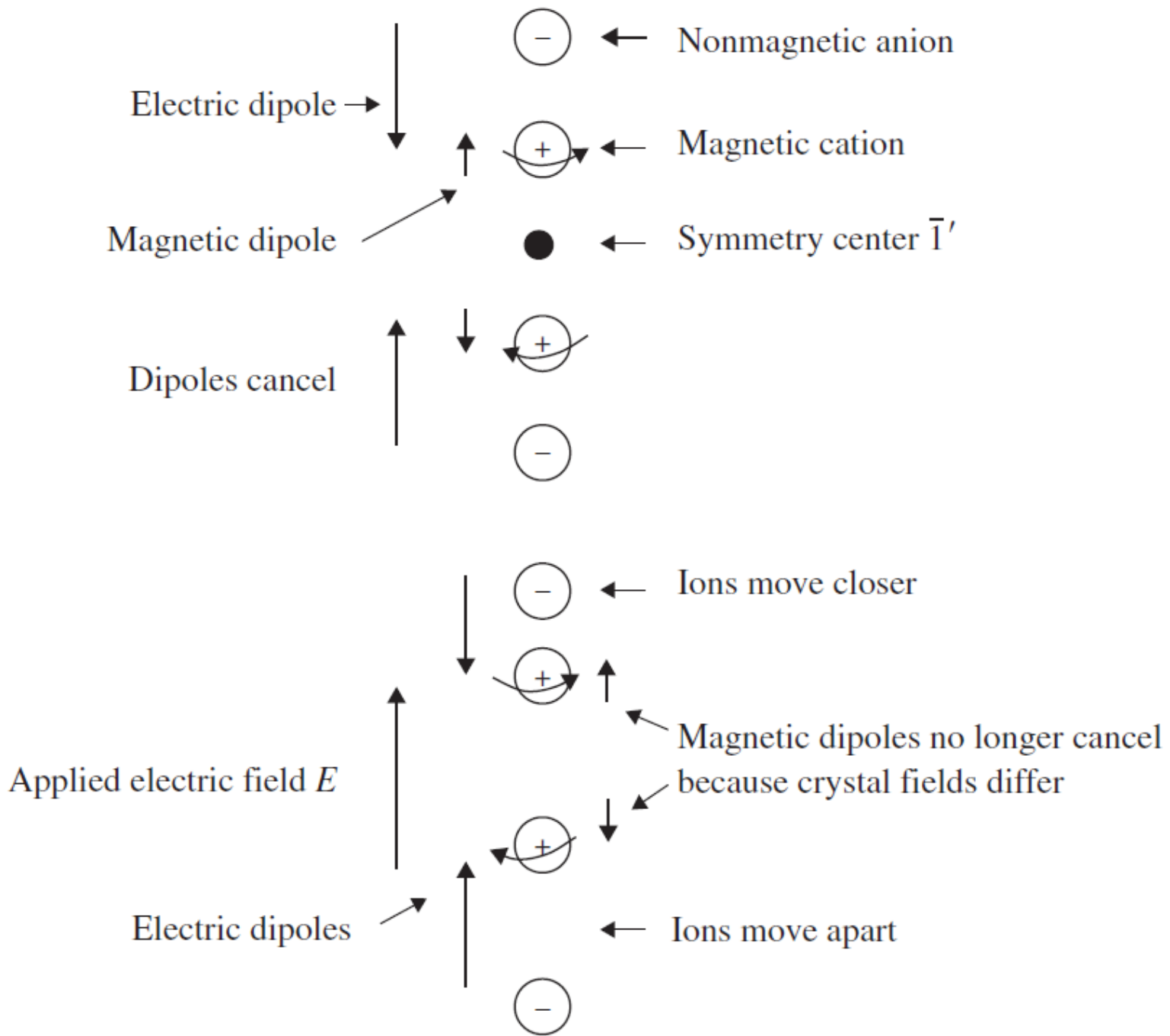
$$\begin{aligned}
\begin{pmatrix} Q'_{11} & Q'_{12} & Q'_{13} \\ Q'_{21} & Q'_{22} & Q'_{23} \\ Q'_{31} & Q'_{32} & Q'_{33} \end{pmatrix} &= (-1)(-1) \begin{pmatrix} \frac{1}{2} & -\frac{\sqrt{3}}{2} & 0 \\ \frac{\sqrt{3}}{2} & \frac{1}{2} & 0 \\ 0 & 0 & -1 \end{pmatrix} \begin{pmatrix} Q_{11} & 0 & 0 \\ 0 & Q_{22} & Q_{23} \\ 0 & Q_{32} & Q_{33} \end{pmatrix} \\
&\times \begin{pmatrix} \frac{1}{2} & \frac{\sqrt{3}}{2} & 0 \\ -\frac{\sqrt{3}}{2} & \frac{1}{2} & 0 \\ 0 & 0 & -1 \end{pmatrix} \\
&= \begin{pmatrix} (\frac{1}{4}Q_{11} + \frac{3}{4}Q_{22}) & (-\frac{\sqrt{3}}{4}Q_{11} + \frac{\sqrt{3}}{4}Q_{22}) & (\frac{\sqrt{3}}{2}Q_{23}) \\ (\frac{\sqrt{3}}{4}Q_{11} - \frac{\sqrt{3}}{4}Q_{22}) & (\frac{3}{4}Q_{11} + \frac{1}{4}Q_{22}) & (-\frac{1}{2}Q_{23}) \\ (\frac{\sqrt{3}}{2}Q_{32}) & (-\frac{1}{2}Q_{32}) & (Q_{33}) \end{pmatrix} \\
&= \begin{pmatrix} Q_{11} & 0 & 0 \\ 0 & Q_{22} & Q_{23} \\ 0 & Q_{32} & Q_{33} \end{pmatrix}
\end{aligned}$$

 $\bar{3}'m'$

$$Q_{11} = Q_{22} \quad Q_{23} = Q_{32} = 0$$

$$\begin{pmatrix} Q_{11} & 0 & 0 \\ 0 & Q_{11} & 0 \\ 0 & 0 & Q_{33} \end{pmatrix}$$

58 magnetoelektrických grup



Piezomagnetismus

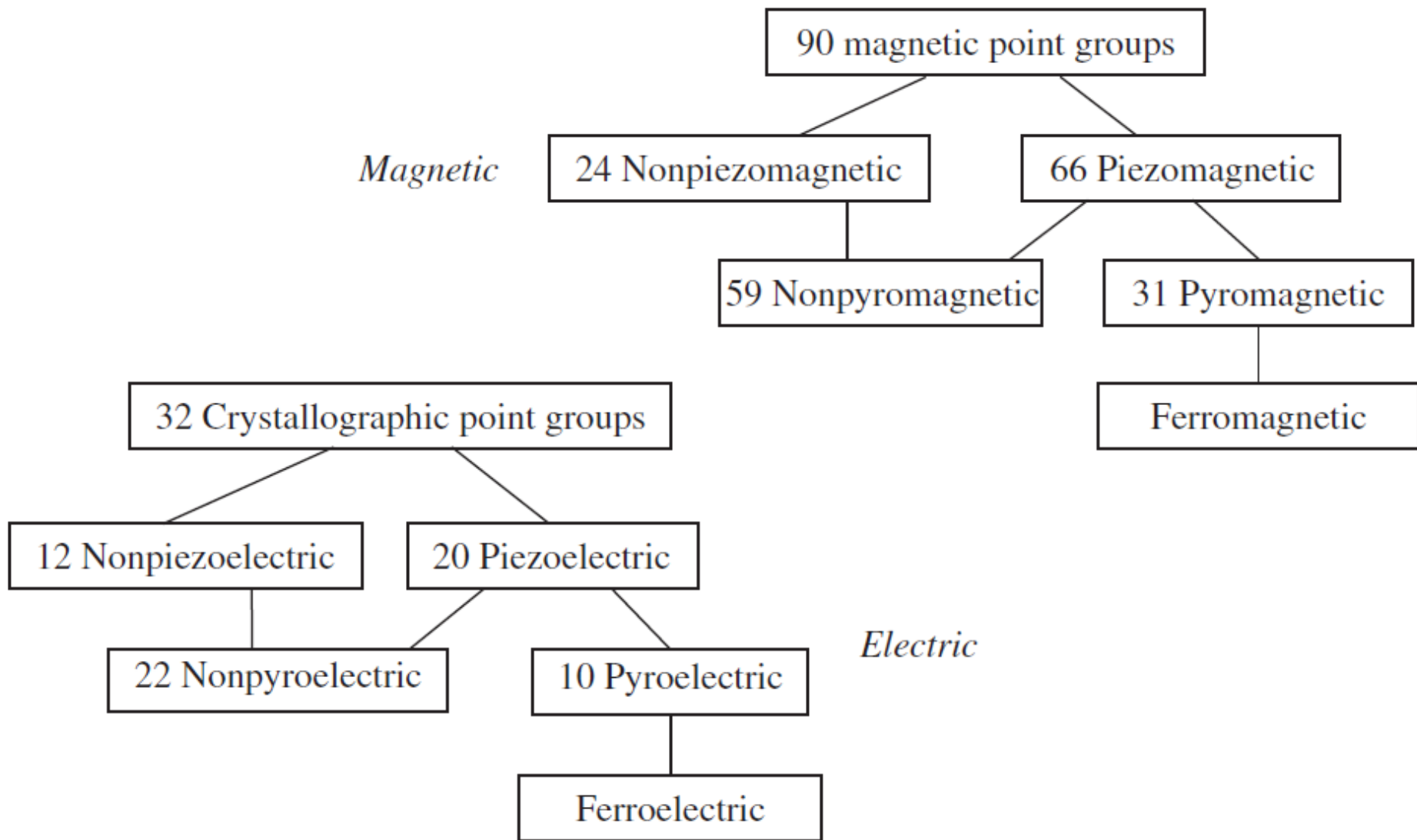
$$I_i \text{ [Wb/m}^2\text{]} = Q_{ijk} \text{ [Wb/N]} X_{jk} \text{ [N/m}^2\text{]}$$

$$I'_i = \pm |a| a_{ij} I_j = \pm |a| a_{ij} Q_{jkl} X_{kl}$$

$$= \pm |a| a_{ij} a_{mk} a_{nl} Q_{jkl} X'_{mn} = Q'_{imn} X'_{mn}$$

$$Q'_{imn} = \pm |a| a_{ij} a_{mk} a_{nl} Q_{jkl}.$$

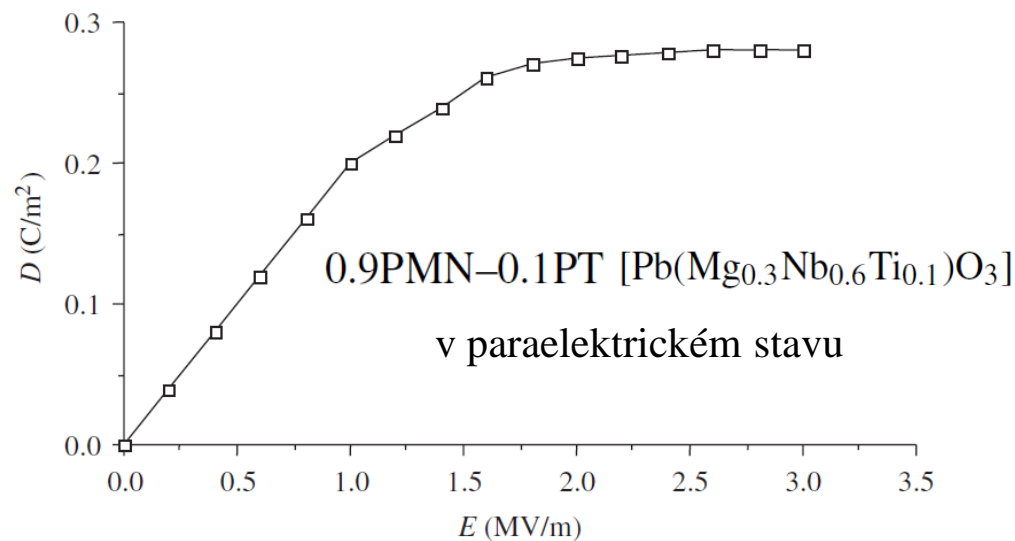
Tenzor 3. řádu



Nelineární jevy

Dielektrické vlastnosti

$$D_i = \varepsilon_{ij}E_j + \varepsilon_{ijk}E_jE_k + \varepsilon_{ijkl}E_jE_kE_l + \dots$$



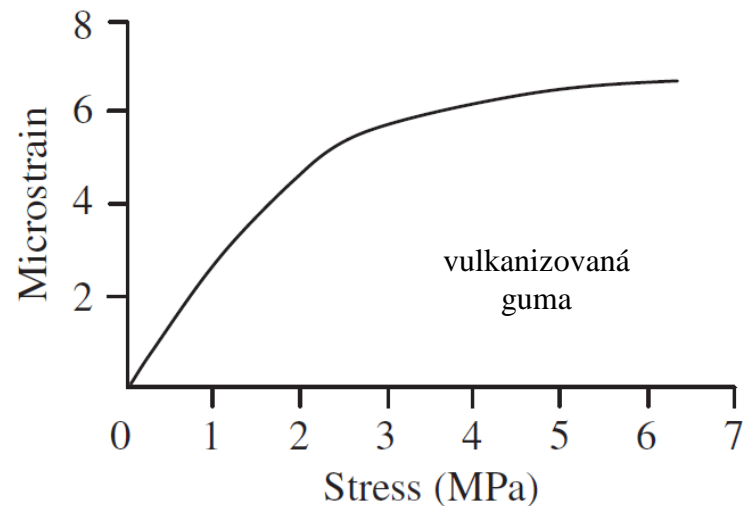
Elastické vlastnosti

napětí

deformace

$$X_{ij} = c_{ijkl}x_{kl} + c_{ijklmn}x_{kl}x_{mn} + \dots$$

$$c'_{ijklmn} = a_{io}a_{jp}a_{kq}a_{lr}a_{ms}a_{nt}c_{opqrst}$$



V maticové formě

$$X_i = c_{ij}x_j + c_{ijk}x_jx_k + \dots$$

Cubic crystals ($m\bar{3}m$)	c_{111}	c_{112}	c_{123}	c_{144}	c_{155}	c_{456}
NaCl	-8.43	-0.5	+0.46	+0.29	-0.6	+0.26
Ge	-7.20	-3.80	-0.3	-0.1	-3.05	-0.45
Cu	-13.50	-8.00	-1.2	+0.66	-7.20	-0.32
Hexagonal crystals ($6/mmm$)	c_{111}	c_{112}	c_{113}	c_{123}	c_{133}	
Mg	-6.63	-1.78	+0.30	-0.76	-0.86	
	c_{144}	c_{155}	c_{222}	c_{333}	c_{344}	
	-0.30	-0.58	-8.64	-7.26	-1.93	

U polymerů kladné

Symmetry	Second order	Third order
Triclinic ($1, \bar{1}$)	21	56
Monoclinic ($2, m, 2/m$)	13	32
Orthorhombic ($222, mm2, mmm$)	9	20
Trigonal ($3, \bar{3}$)	7	20
($32, 3m, \bar{3}m$)	6	14
Tetragonal ($4, \bar{4}, 4/m$)	7	16
($422, 4mm, \bar{4}2m, 4/mmm$)	6	12
Hexagonal ($6, \bar{6}, 6/m$)	5	12
($\bar{6}m2, 622, 6mm, 6/mmm$)	5	10
Cubic ($23, m\bar{3}$)	3	8
($432, \bar{4}3m, m\bar{3}m$)	3	6

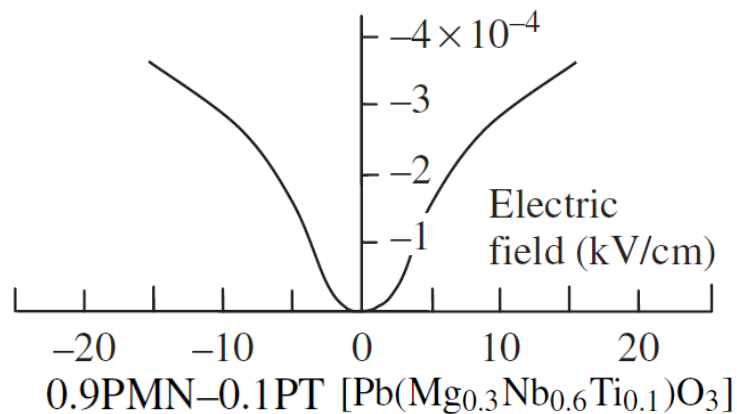
Počet nezávislých koeficientů

$$x_{ij} = d_{ijk}E_k + M_{ijkl}E_kE_l$$

$$x_{ij} = Q_{ijkl}P_kP_l$$

Tenzor 4. řádu, narušil od piezoelektrického jevu přítomen ve všech grupách

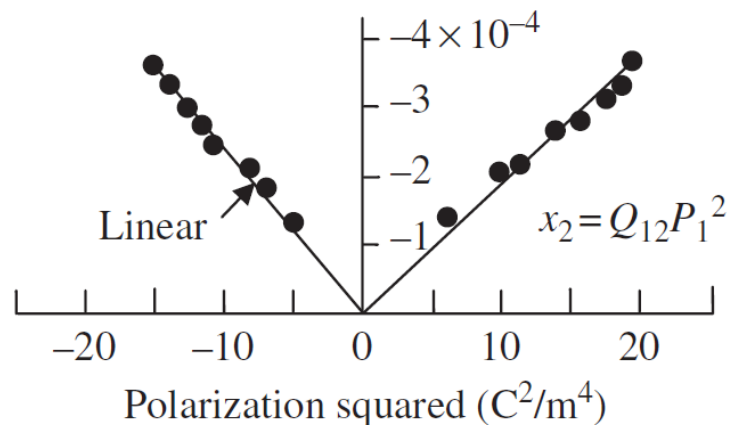
(a) Transverse strain



Pro kubické krystaly

$$\begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \\ x_5 \\ x_6 \end{pmatrix} = \begin{pmatrix} Q_{11} & Q_{12} & Q_{12} & 0 & 0 & 0 \\ Q_{12} & Q_{11} & Q_{12} & 0 & 0 & 0 \\ Q_{12} & Q_{12} & Q_{11} & 0 & 0 & 0 \\ 0 & 0 & 0 & Q_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & Q_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & Q_{44} \end{pmatrix} \begin{pmatrix} P_1^2 \\ P_2^2 \\ P_3^2 \\ P_2P_3 \\ P_3P_1 \\ P_1P_2 \end{pmatrix}$$

(b) Transverse strain

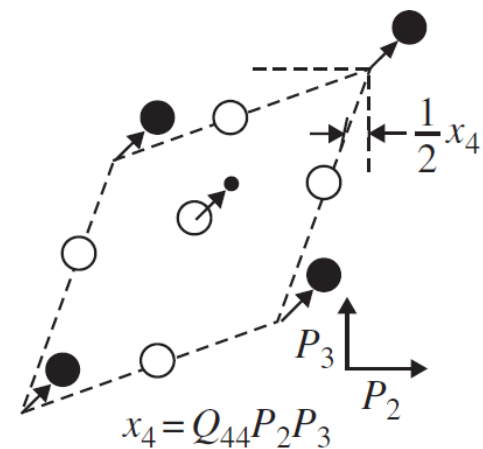
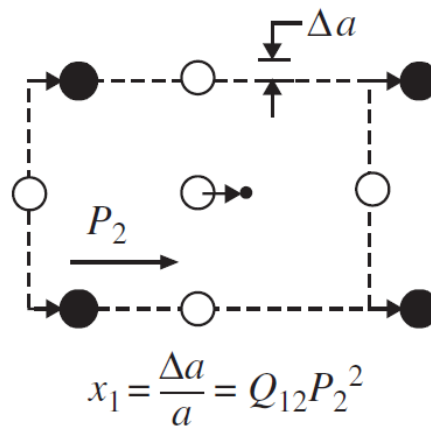
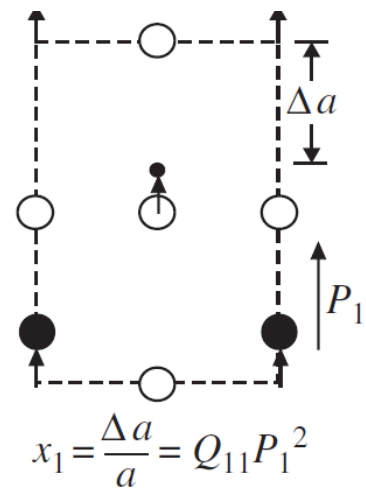
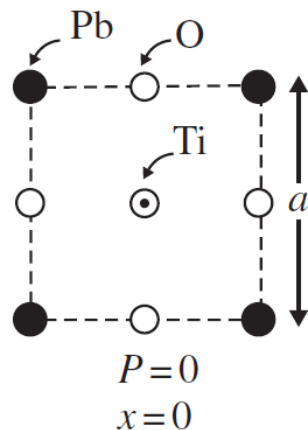


Mikroblasti s fluktuacemi polarizace

Částečné uspořádání
oktaedrických kationtů

Mg a Nb ionty mění polohy,
ale jen na vzdálenosti několika buněk

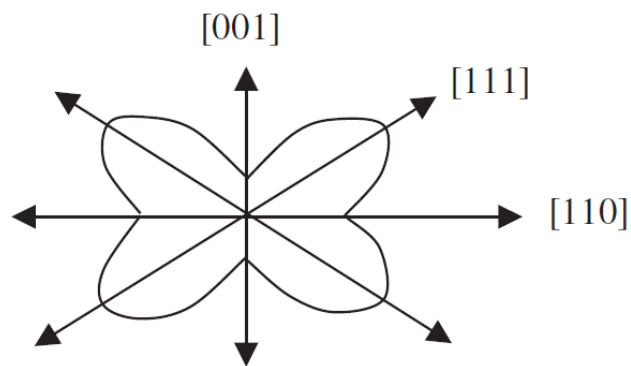
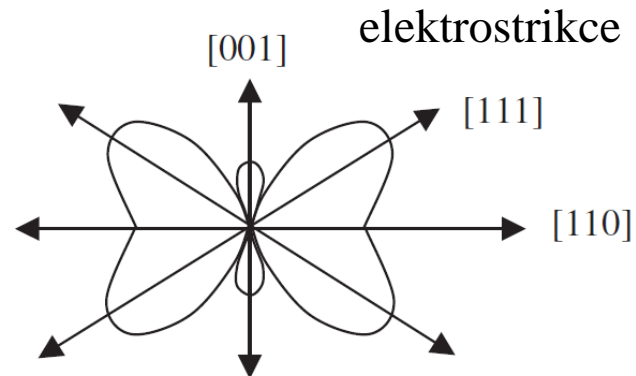
V těchto uspořádaných ostrůvcích
vznikají fluktuace dipólů,
které generují vysoké polarizace
a elektrostikční pohyby.



CaF₂

elektrostriktice

elasticita



$$x_{ij} = N_{ijkl} I_k I_l$$

Často silnější než
piezomagnetismus

$$\begin{aligned} x'_{ij} &= a_{ik} a_{jl} x_{kl} = a_{ik} a_{jl} N_{klmn} I_m I_n \\ &= a_{ik} a_{jl} N_{klmn} (\pm |a| a_{om} I'_o) (\pm |a| a_{pn} I'_p) \\ &= N'_{ijop} I'_o I'_p \end{aligned}$$

$$N'_{ijop} = a_{ik} a_{jl} a_{om} a_{pn} N_{klmn}.$$

$$\begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \\ x_5 \\ x_6 \end{pmatrix} = \begin{pmatrix} N_{11} & N_{12} & N_{13} & N_{14} & N_{15} & N_{16} \\ N_{21} & N_{22} & N_{23} & N_{24} & N_{25} & N_{26} \\ N_{31} & N_{32} & N_{33} & N_{34} & N_{35} & N_{36} \\ N_{41} & N_{42} & N_{43} & N_{44} & N_{45} & N_{46} \\ N_{51} & N_{52} & N_{53} & N_{54} & N_{55} & N_{56} \\ N_{61} & N_{62} & N_{63} & N_{64} & N_{65} & N_{66} \end{pmatrix} \begin{pmatrix} I_1^2 \\ I_2^2 \\ I_3^2 \\ I_2 I_3 \\ I_3 I_1 \\ I_1 I_2 \end{pmatrix}$$