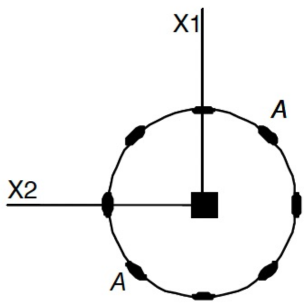
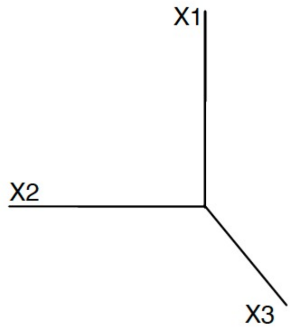
Test: problem 1





2-fold axis A-A is the only symmetry element:

What to do:
Write down the K-tensor in its general form, then use the Neumann principle

Vector component transformation:

$$x_1' = -x_2,\ x_2' = -x_1,\ x_3' = -x_3.$$

$$K_{11}' \sim p_1'p_1' = (-p_2)(-p_2) = p_2p_2 \sim K_{22}$$
$$K_{22}' \sim p_2'p_2' = (-p_1)(-p_1) = p_1p_1 \sim K_{11}$$
$$K_{33}' \sim p_3'p_3' = (-p_3)(-p_3) = p_3p_3 \sim K_{33}$$
$$K_{12}' \sim p_1'p_2' = (-p_2)(-p_1) = p_1p_2 \sim K_{12}$$
$$K_{13}' \sim p_1'p_3' = (-p_2)(-p_3) = p_2p_3 \sim K_{23}$$
$$K_{23}' \sim p_2'p_3' = (-p_1)(-p_3) = p_1p_3 \sim K_{13}$$

$$K_{ij}' = K_{ij}$$

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

$$K_{ij} = \begin{pmatrix} K_{11} & K_{12} & K_{13} \\ K_{12} & K_{11} & K_{13} \\ K_{13} & K_{13} & K_{33} \end{pmatrix}$$

Finally, it is known from tables of the course, that in point group 2 the symmetry of the dielectric response is *mmm*

Test: problem 2

$$D_1 = \varepsilon_0 K_{12} E_2 + \varepsilon_0 K_{13} E_3 + d_{11}\sigma_1 + p_1 \delta T$$

material of symmetry 32 is not pyroelectric

Exercises – Series 9, cross-coupled effects, thermoelectromechanics

Use of constitutive equations: tips and recommendations

$$D_i = \varepsilon_0 K_{ij} E_j + d_{in}\sigma_n + p_i \delta T$$

$$\varepsilon_n = d_{in} E_i + s_{nm}\sigma_m + \alpha_n \delta T$$

$$\delta S = p_i E_i + \alpha_m \sigma_m + \frac{C}{T}\delta T$$

- **What do you need to find?**
- **What are the boundary conditions?**
- **what input data are relevant, what are redundant? (some effects are not permitted because of symmetry…)**

Select the right set of equations (consider the boundary conditions)

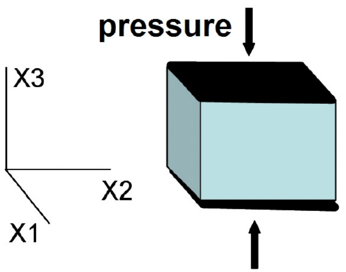
Exercises – Series 9, cross-coupled effects, thermoelectromechanics: solutions and comments

In all the exercises, the material used is $BaTiO_3$ in its tetragonal phase $4mm$. The 4-fold axis is always directed along the x_3 axis. You may use the table of values for $BaTiO_3$ given below if needed.

s_{11}	8.05×10^{-12} m^2/N	d_{15}	392×10^{-12} C/N
s_{12}	-2.35×10^{-12} m^2/N	d_{31}	-35×10^{-12} C/N
s_{13}	-5.24×10^{-12} m^2/N	d_{33}	86×10^{-12} C/N
s_{33}	15.7×10^{-12} m^2/N	K_{33}	150
C	$2.42 \times 10^6\ J/(m^3 \cdot K)$	p_3	$-5 \times 10^{-4}\ C/(m^2 \cdot K)$
α_3	$3.5 \times 10^{-5}\ 1/K$		

Some data are usable, others maybe redundant or irrelevant…

Problem 3



3. The piezocaloric effect is measured in a sample of $BaTiO_3$ (symmetry $4mm$, the 4-fold axis is directed along x_3 direction). The experimental setup is shown in Fig.3. The surfaces of the sample are under open circuit condition, the sample can freely expand in x_1 and x_2 directions, there is no heat exchange with the environment. Initial temperature of the sample is 300 K.

Determine the change of the temperature at application of pressure 100 MPa

$$D_i = \varepsilon_0 K_{ij} E_j + d_{ij}\sigma_j + p_i \delta T$$
$$\frac{\delta Q}{T} = p_i E_i + \alpha_i \sigma_i + \frac{C}{T}\delta T$$

(first equation exploits the electrical boundary conditions, second one – to calculate the change of temperature

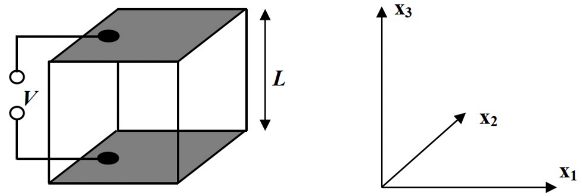
$$D_3 = \varepsilon_0 K_{13} E_1 + \varepsilon_0 K_{23} E_2 + \varepsilon_0 K_{33} E_3 + d_{33}\sigma_3 + p_3 \delta T = 0$$
$$\frac{\delta Q}{T} = p_1 E_1 + p_2 E_2 + p_3 E_3 + \alpha_3 \sigma_3 + \frac{C}{T}\delta T = 0$$

4mm symmetry:
$K_{13}=K_{23}=0$
$p_1=p_2=0$

$$E_3 = -\frac{d_{33}}{\varepsilon_0 K_{33}}\sigma_3 - \frac{p_3}{\varepsilon_0 K_{33}}\delta T \qquad \frac{\delta Q}{T} = p_3\left(-\frac{d_{33}}{\varepsilon_0 K_{33}}\sigma_3 - \frac{p_3}{\varepsilon_0 K_{33}}\delta T\right) + \alpha_3\sigma_3 + \frac{C}{T}\delta T = 0$$

$$\delta T = -\frac{\alpha_3 - \dfrac{p_3 d_{33}}{\varepsilon_0 K_{33}}}{\dfrac{C}{T} - \dfrac{p_3^2}{\varepsilon_0 K_{33}}}\sigma_3 \qquad \delta T = 0.86\text{K}$$

Problem 4. The impact of mechanical conditions on the electro-caloric effect is investigated. The voltage is applied along the polar axis; the sample temperature is measured.



$$\varepsilon_i = d_{ji}E_j + s_{ij}\sigma_j + \alpha_i \delta T,$$
$$\delta Q = T p_i E_i + T\alpha_i \sigma_i + C\delta T = 0$$

In case **(a)**, the sample is mechanically free, implying all $\sigma_i = 0$. Then,

$$\delta Q = T p_1 E_1 + T p_2 E_2 + T p_3 E_3 + C\delta T = 0$$

For geometry $4mm$ with 4-fold axis directed along x_3, symmetry restrictions impose $p_1 = p_2 = 0$, $p_3 \neq 0$. Therefore,

$$T p_3 E_3 + C\delta T = 0$$
$$\delta T_{(a)} = -T E_3 \frac{p_3}{C} = -T \frac{V}{L}\frac{p_3}{C}.$$

In case **(b)**, the sample is kept mechanically free in x_1 and x_2 directions, implying $\sigma_1 = \sigma_2 = \sigma_4 = \sigma_5 = \sigma_6 = 0$, and $\sigma_3 \neq 0$. The constitutive equation for δQ is then simplified into:

$$\delta Q = T p_3 E_3 + T\alpha_3\sigma_3 + C\delta T = 0.$$

$$\varepsilon_3 = d_{13}E_1 + d_{23}E_2 + d_{33}E_3 + s_{33}\sigma_3 + \alpha_3\delta T.$$

$$\varepsilon_3 = d_{33}E_3 + s_{33}\sigma_3 + \alpha_3\delta T = 0 \quad \Rightarrow \quad \sigma_3 = -\frac{d_{33}}{s_{33}}E_3 - \frac{\alpha_3}{s_{33}}\delta T$$

$$\delta T_{(b)} = -T E_3 \frac{p_3 - \frac{\alpha_3 d_{33}}{s_{33}}}{C - T\frac{\alpha_3^2}{s_{33}}} \approx -T E_3 \frac{p_3 - \frac{\alpha_3 d_{33}}{s_{33}}}{C} = -T\frac{V}{L}\frac{p_3 - \frac{\alpha_3 d_{33}}{s_{33}}}{C} \qquad \frac{\alpha_3 d_{33}}{s_{33}} > 0, \text{ and } p_3 < 0$$

the change of temperature is larger in case (b)