Exercises N6 25.03.2025 Piezoelectricity - Solutions

6.1

Since the material is mechanically free along the X1 and X2 directions, but not along the X3 direction, we have

$$\sigma_1 = \sigma_2 = \sigma_4 = \sigma_5 = \sigma_6 = 0$$
$$\sigma_3 \neq 0 \quad .$$

The device shown in the figure measures the variation of the charge on the plates of the capacitor under the application of the force. The charge per unit area of the plate is equal to the normal component of the electric displacement , D_3 in our case.

Since the galvanometer short-circuits the plates, the electric field in the capacitor is zero and

$$D_3 = P_3 = d_{33}\sigma_3 \, .$$

For a material of the point symmetry $\bar{4}3m$ $d_{33} = 0$. It is possible to prove that $d_{33} = 0$ using the Neumann principle. Consider the $180°$ rotation along Ox_2 axis, which is a symmetry element of $\bar{4}3m$:

$$\begin{cases} 1 \to -1 \\ 2 \to 2 \\ 3 \to -3 \end{cases}$$

Under this operation the tensor component $d_{33} \equiv d_{333}$ transforms as

$$d'_{333} = (-1)(-1)(-1)d_{333} = -d_{333}$$

From Neumann principle, applying an operation of symmetry of the group should not change the components of the tensor: $d'_{333} = d_{333}$. Therefore, $d_{333} = -d_{333} = 0$. The material will show no piezoelectric response.

6.2

For a material of symmetry 23, all components of the piezoelectric tensor are zero except

$$d_{14} = d_{25} = d_{36} = 2d_{123} = 2d_{213} = 2d_{312} = d \ .$$

Group 432 contains all the symmetry operations of 23, therefore all restrictions for group 23 are valid for 432 as well. In addition to symmetry elements of 23, 432 contains four-fold symmetry axes, which may impose new restrictions on the piezoelectric tensor. The 4 rotation about Ox_1 transforms the Cartesian coordinates as

$$\begin{cases} 1 \to 1 \\ 2 \to 3 \\ 3 \to -2 \end{cases} .$$

Under this symmetry operation the non-zero components of the piezoelectric tensor transforms as

$$\begin{cases} d_{123}' = -d_{132} = -d_{123} \\ d_{213}' = -d_{312} = -d_{213} \\ d_{312}' = -d_{213} = -d_{312} \end{cases} .$$

The Neumann principle ($d'_{123} = d_{123}$,..) leads to

$$d = 2d_{123} = 2d_{213} = 2d_{312} = 0 .$$

Thus, although the group 432 is non-centrosymmetric it is not compatible with the piezoelectricity.

6.3

The group considered in the exercise **6.2**, 432, although being non-centrosymmetric, is not piezoelectric. Since the $\infty\infty$ group has higher symmetry than 432 (it contains all possible rotations), the relationships between the components of the piezoelectric tensor derived for lower symmetry remain valid. Thus, the symmetry $\infty\infty$ is not compatible with the piezoelectricity.

6.4

$\varepsilon_n = d_{in}E_i$ – converse piezoelectric effect.

The piezoelectric tensor for $BaTiO_3$, a perovskite structure with $4mm$ symmetry, for the reference frame described in the problem, is (see Symmetry Tables):

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

The relative variation of volume can be found as: $\frac{\Delta V}{V} = \varepsilon_{11} + \varepsilon_{22} + \varepsilon_{33} = \varepsilon_1 + \varepsilon_2 + \varepsilon_3$.

The converse piezoelectric effect gives:

$\varepsilon_1 = d_{i1}E_i = d_{11}E_1 + d_{21}E_2 + d_{31}E_3 = d_{31}E_3$ ($d_{11} = d_{21} = 0$ in the considered symmetry)

$$\varepsilon_2 = d_{i2}E_i = d_{32}E_3 = d_{31}E_3, \qquad \varepsilon_3 = d_{i3}E_i = d_{33}E_3.$$

$$\frac{\Delta V}{V} = \varepsilon_1 + \varepsilon_2 + \varepsilon_3 = d_{31}E_3 + d_{31}E_3 + d_{33}E_3 = (2d_{31} + d_{33})E_3.$$

Thus, change in volume is defined only by the E_3 component of the applied electric field.

(a) If the field is directed along the [111], $\vec{E} = \frac{E}{\sqrt{3}}(1,1,1)$, hence

$$\frac{\Delta V}{V} = (2d_{31} + d_{33})\frac{E}{\sqrt{3}} = \frac{E}{\sqrt{3}} \cdot 16\,\frac{\text{pC}}{\text{N}} > 0$$

Thus, the volume increases.

(b) If the field is directed along the $[11\bar{1}]$, $\vec{E} = \frac{E}{\sqrt{3}}(1,1,-1)$, and

$$\frac{\Delta V}{V} = -(2d_{31} + d_{33})\frac{E}{\sqrt{3}} = -\frac{E}{\sqrt{3}} \cdot 16\,\frac{\text{pC}}{\text{N}} < 0.$$

In this case, the volume decreases.

6.5 *Discussion in class*: paper “Induced giant piezoelectricity in centrosymmetric oxides”: Explanation of the mechanism of piezoelectric response in a centrosymmetric material (where it is normally forbidden)