Exercises N5 18.03.2025 - Solutions

5.1 The anisotropy of the tensor can be understood with the ellipsoid "Representation quadric". To find the relation between axes of the ellipsoid, we should first diagonalize the tensor. To do this we should find its principle values, i.e. to solve the equation:

$$\begin{vmatrix} 2-\lambda & 1 & 0 \\ 1 & 2-\lambda & 0 \\ 0 & 0 & 2-\lambda \end{vmatrix} = 0$$

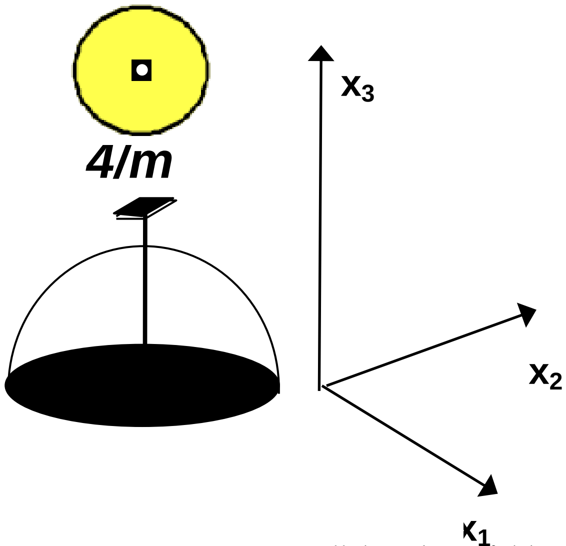
$$(2-\lambda)[(2-\lambda)^2 - 1] = 0$$

This equation has three roots: $\lambda_1 = 1,\ \lambda_2 = 2,\ \lambda_3 = 3$. Thus the diagonalized tensor has the form:

$$T' = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 3 & 0 \\ 0 & 0 & 2 \end{pmatrix}.$$

We obtain the tensor where all diagonal components are different. From the table we see that the group with the highest symmetry corresponding to this tensor is *mmm*. The symmetry of the property described by this tensor is also *mmm*.

It is possible (optional) to find the coordinate system where tensor T_{ij} has its diagonal form: the axes of this reference frame are directed along $[\bar{1}10]$, [110], [001]. Thus, the fullest set of the symmetry elements that do not change the tensor T_{ij} is: inversion, three two-fold axes $[\bar{1}10]$, [110], [001], and three mirror planes $(\bar{1}10)$, (110), (001).



5.2 Consider the reference frame where OX3 is parallel to the 4-fold axis

To find the structure of the K_{ij} tensor invariant with respect to the *4/m* symmetry operation, it is sufficient to check its invariance with respect to the 90-degree rotation about the 4-fold axis and the inversion, since the remaining mirror plane operation can be found as a combination of these two symmetry operations.

a) Inversion

All even-rank tensors are invariant with respect to the operation of inversion.

b) 4-fold axis

Rotation around 4-fold axis parallel to Ox_3 direction leads to the following relationships between vector components in new and old reference frames:

$$\begin{cases} p_1' = p_2 \\ p_2' = -p_1 \\ p_3' = p_3 \end{cases}$$

Using the component product method, the tensor

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

can be transformed to the new reference frame where it has the form

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

The Neumann principle requires that the dielectric constant tensor remain unchanged upon this transformation, i.e.

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

Consequently, $K_{11} = K_{22}$, $K_{23} = K_{13}$, $-K_{13} = K_{23}$, $K_{12} = -K_{12}$, i.e.

$$K_{12} = K_{13} = K_{23} = 0, \quad K_{11} = K_{22}$$

This implies the following structure of the tensor in the material of the *4/m* symmetry:

$$\begin{pmatrix} K_1 & 0 & 0 \\ & K_1 & 0 \\ & & K_3 \end{pmatrix}$$

To show that the symmetry of the property is $\frac{\infty}{m}m$, we can verify that OX_3 is the ∞ axis. Let's apply rotation for an arbitrary angle θ to the reference frame, with following direction cosine matrix:

$$a_{ij} = \begin{pmatrix} \cos\theta & \sin\theta & 0 \\ -\sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

Applying the 2-rank tensor transformation rule, $K' = aKa^T$, we obtain:

$$K' = \begin{pmatrix} \cos\theta & \sin\theta & 0 \\ -\sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} K_1 & 0 & 0 \\ 0 & K_1 & 0 \\ 0 & 0 & K_3 \end{pmatrix} \begin{pmatrix} \cos\theta & -\sin\theta & 0 \\ \sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix} =$$

$$= \begin{pmatrix} K_1\cos\theta & K_1\sin\theta & 0 \\ -K_1\sin\theta & K_1\cos\theta & 0 \\ 0 & 0 & K_3 \end{pmatrix} \begin{pmatrix} \cos\theta & -\sin\theta & 0 \\ \sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} K_1 & 0 & 0 \\ 0 & K_1 & 0 \\ 0 & 0 & K_3 \end{pmatrix}$$

Thus, the tensor is invariant with respect to rotation by an arbitrary angle around the axis parallel to Ox_3

As for remaining symmetry of the property, that is the mirror plane lying not perpendicular but along Ox_3 axis, it is enough to show invariance for reflection by (100) mirror plane. The vector transformation law for this operation reads

$$\begin{cases} p_1' = -p_1 \\ p_2' = p_2 \\ p_3' = p_3 \end{cases}$$

One readily checks that the tensor is invariant with respect to this.

Thus, the symmetry of the dielectric response of a material of symmetry $4/m$ is ∞/mm.

5.3

a)

The relation between c_{61} and c_{62} can be found by applying the Neumann principle. First we pass from the Voight to tensor notations: $c_{61} = c_{1211}$ and $c_{62} = c_{1222}$.

For a *4-fold* inversion axis ($\bar{4}$), the axes transform as follows:

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

Applying this symmetry operation to the stiffness tensor, we obtain

$$c'_{1211} = -c_{2122}$$

Thus, for this symmetry operation the Neumann equation reads:

$$c_{1211} = c'_{1211} = -c_{2122}$$

Back to the two-suffix notation, we find that in class $\bar{4}$

$$c_{61} = c'_{61} = -c_{62}$$

b)

The relation between c_{61} and c_{62} can also be found with the Neumann principle. First we recollect that $c_{61}=c_{1211}$ and $c_{62}=c_{1222}$.

The *422* class includes a four-fold rotation axis, which we take to be parallel to Ox_3 [001], along with two-fold rotation axes about the directions parallel to Ox_1 [100] and Ox_2 [010], and another two-fold rotation axes parallel to [110] and [$\bar{1}10$] directions.

For example, the *2-fold* rotation about Ox_1 transforms the reference frame as

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

The considered tensor components transform under this operation as

$$c'_{1211} = -c_{1211}, \qquad c'_{1222} = -c_{1222}$$

i.e. they change their sings. Thus they are equal to zero.

5.4

We start by rewriting the relation $c_{66} = \frac{c_{11} - c_{12}}{2}$, valid for hexagonal systems, in the four-index tensor notation:

$$c_{1212} = \frac{c_{1111} - c_{1122}}{2}$$

Since this relationship follows from the Neumann's equation for the fourth-rank stiffness tensor, having its specific suffix-permutation symmetry, it must be applicable to the compliance tensor, which have the same rank and the same suffix-permutation symmetry:

$$c_{1212} = \frac{c_{1111} - c_{1122}}{2} \quad \leftrightarrow \quad s_{1212} = \frac{s_{1111} - s_{1122}}{2}$$

Using the conventions for the transformation between the four-suffix and two-suffix notations,

$$s_{1212} = \frac{s_{66}}{4}, \quad s_{1111} = s_{11}, \quad s_{1122} = s_{12}$$

we can rewrite the relation for compliance tensor as:

$$s_{66} = 4\frac{s_{11} - s_{22}}{2} = 2(s_{11} - s_{12})$$

5.5

Matrix *C* is inverse to *S* i.e. *CS=I*, where *I* is the identity matrix, from this relation one can obtain the necessary equations. Considering that for the cubic crystal there are only 3 independent coefficients c_{11}, c_{12} and c_{44} (or s_{11}, s_{12} and s_{44}), and s_{44} is not needed, only two equations are required :

$c_{11}s_{11} + c_{12}s_{12} + c_{12}s_{12} = 1$
$c_{11}s_{12} + c_{12}s_{11} + c_{12}s_{12} = 0$

From these equations one readily finds :

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