Exercises N4 11.03.2025 - Solutions

1. The table of direction cosines is :

$$a_{ij} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1/\sqrt{2} & 1/\sqrt{2} \\ 0 & -1/\sqrt{2} & 1/\sqrt{2} \end{pmatrix}$$

Here we will solve this problem using both methods: full tensor calculus and vector components product method.

Full tensor calculus method

$e'_{113} = a_{1i}a_{1j}a_{3k}e_{ijk}$

$= a_{11}a_{12}a_{33}e_{123} + a_{12}a_{11}a_{33}e_{213} + a_{11}a_{13}a_{32}e_{132} + a_{13}a_{11}a_{32}e_{312} + a_{12}a_{13}a_{31}e_{231} +$

$a_{13}a_{12}a_{31}e_{321} = 0 + 0 + 0 + 0 + 0 + 0 = 0$

$e'_{123} = a_{1i}a_{2j}a_{3k}e_{ijk}$

$= a_{11}a_{22}a_{33}e_{123} + a_{12}a_{21}a_{33}e_{213} + a_{11}a_{23}a_{32}e_{132} + a_{13}a_{21}a_{32}e_{312} + a_{12}a_{23}a_{31}e_{231}$

$+ a_{13}a_{22}a_{31}e_{321} = \frac{d}{2} + 0 - \frac{d}{2} + 0 + 0 + 0 = 0$

$e'_{133} = a_{1i}a_{3j}a_{3k}e_{ijk}$

$= a_{11}a_{32}a_{33}e_{123} + a_{12}a_{31}a_{33}e_{213} + a_{11}a_{33}a_{32}e_{132} + a_{13}a_{31}a_{32}e_{312} + a_{12}a_{33}a_{31}e_{231}$

$+ a_{13}a_{32}a_{31}e_{321} = -\frac{d}{2} + 0 - \frac{d}{2} + 0 + 0 + 0 = -d$

Vector components product method

Tensor e_{ijk} transforms as $p_i q_j r_k$, with $p'_i = a_{ij}p_j$:

$p'_1 = p_1$

$p'_2 = \frac{1}{\sqrt{2}}(p_2 + p_3)$

$p'_3 = \frac{1}{\sqrt{2}}(p_3 - p_2)$

Same transformation law is valid for the other two vectors $\boldsymbol{q}$ and $\boldsymbol{r}$, specifically for components q_1, q_2, q_3 and r_1, r_2, r_3

Using this property, we transform e_{ijk} as follows:

$e'_{113} \sim p'_1 q'_1 r'_3 = \frac{1}{\sqrt{2}} p_1 q_1 (r_3 - r_2) \sim \frac{1}{\sqrt{2}}(e_{113} - e_{112}) \Rightarrow e'_{113} = 0$

$e'_{123} \sim p'_1 q'_2 r'_3 = \frac{1}{2} p_1 (q_2 + q_3)(r_3 - r_2) \sim \frac{1}{2}(e_{123} + e_{133} - e_{122} - e_{132}) \Rightarrow e'_{123} = 0$

$e'_{133} \sim p'_1 q'_3 r'_3 = \frac{1}{2} p_1 (q_3 - q_2)(r_3 - r_2) \sim \frac{1}{2}(e_{133} - e_{123} - e_{132} + e_{122}) \Rightarrow e'_{133} = -d$

One can see that the last method is much easier than the first one.

2.

The point group of highest symmetry in orthorhombic system is *mmm*, which contains seven symmetry operations (eight if one counts the trivial operation of identity):

- inversion
- two-fold axes: [100], [010], [001]
- mirror planes: (100), (010), (001)

Formally, we should verify that the tensor remains invariant under all these transformations. However, it is enough to check only three of them:

a) one mirror plane, e.g. (001)

b) one 2-fold axis parallel to this plane (e.g. [100])

c) inversion

a) Mirror plane (001) transforms vector coordinates as

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

We obtain: $T_{11}' = T_{11} = 1$, $T_{22}' = T_{22} = 2$, $T_{33}' = T_{33} = 3$, $T_{12}' = T_{12} = 0$, $T_{13}' = -T_{13} = 0$ and $T_{23}' = -T_{23} = 0$ – the tensor doesn't change.

b) Two-fold axis [100] transforms vector coordinates as

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

We obtain: $T_{11}' = T_{11} = 1$, $T_{22}' = T_{22} = 2$, $T_{33}' = T_{33} = 3$, $T_{12}' = -T_{12} = 0$, $T_{13}' = -T_{13} = 0$ and $T_{23}' = T_{23} = 0$ – the tensor doesn't change.

c) All even-rank tensors are invariant under inversion transformations.

Thus, the tensor is invariant with respect to all operations of point groups belonging to the orthorhombic system.

3.

The central atom is displaced in the (001) plane in arbitrary direction. As a result, all the symmetry elements of the group $m\bar{3}m$ are lost, except for the mirror plane (001). The system has monoclinic *m* symmetry.

In this reference frame for the system with *m* symmetry, where the mirror plane is directed as (001), the dielectric permittivity tensor has the following form:

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

Thus, in the material characterized in the cubic crystallographic reference frame the transition changes the structure of the tensor as follows:

$$\begin{pmatrix} K & & \\ & K & \\ & & K \end{pmatrix} \rightarrow \begin{pmatrix} K_{11} & K_{12} & \\ K_{12} & K_{22} & \\ & & K_{33} \end{pmatrix}$$

4.

The only element of symmetry we have is $(\bar{1}10)$ mirror plane. According to Neumann principle, the tensor should remain unchanged upon applying this symmetry operation:

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

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

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

To satisfy Neumann principle, the following requirements must be met:

$$K_{11} = K_{22} \qquad\qquad K_{13} = K_{23}$$

Thus, for cubic crystallographic reference frame, the transition changes the structure of the dielectric tensor as follows:

$$\begin{pmatrix} K & & \\ & K & \\ & & K \end{pmatrix} \rightarrow \begin{pmatrix} K_{11} & K_{12} & K_{13} \\ K_{12} & K_{11} & K_{13} \\ K_{13} & K_{13} & K_{33} \end{pmatrix}.$$

5.

Formally, we should show that tensor remains unchanged under all symmetry operations which exist in all groups of cubic system. The group $m\bar{3}m$ contains all these operations. Fortunately, it is enough to check only three of them, for example: 3-fold axis, 4-fold axis and inversion. This can be verified with the table of point symmetry groups: all combinations of a 3-fold axis, 4-fold axis, and inversion compose all the elements of $m\bar{3}m$ group.

Now we will check the tensor transformations for 3-fold axis, 4-fold axis, and inversion.

Inversion:

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

We automatically get $g_{ijkl}' = g_{ijkl}$, as for any even rank tenrsor.

3-fold axis [111]:

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

Using the same method we find, $g_{1111}' = g_{2222} = 1$

$g_{2222}' = g_{3333} = 1,\ g_{3333}' = g_{1111} = 1$. From (2) it is clear that if two indexes are different before the transformation, they will also be different after the transformation. Thus all components of g_{ijkl} with different indices remain 0 and satisfy this symmetry operation as well.

4-fold axis [001]:

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

Thus $g_{1111}' = g_{2222} = 1,\ g_{2222}' = g_{1111} = 1,\ g_{3333}' = g_{3333} = 1$. If two indexes are different before the transformation, they will also be different after the transformation. Thus all components of g_{ijkl} with different indices remain 0 and satisfy this symmetry operation as well.

6. The dielectric permittivity tensor must remain unchanged upon a rotation of $\frac{2\pi}{3}$ around 3-fold axis (we will put Ox_3 in this direction). The vector components will be transformed as:

$$p_1' = -\frac{1}{2}p_1 + \frac{\sqrt{3}}{2}p_2$$
$$p_2' = -\frac{\sqrt{3}}{2}p_1 - \frac{1}{2}p_2$$
$$p_3' = p_3$$

The tensor components will be transformed as:

$$K_{11}' = \frac{1}{4}K_{11} - \frac{\sqrt{3}}{2}K_{12} + \frac{3}{4}K_{22},\quad K_{22}' = \frac{3}{4}K_{11} + \frac{\sqrt{3}}{2}K_{12} + \frac{1}{4}K_{22},\quad K_{33}' = K_{33},$$
$$K_{12}' = \frac{\sqrt{3}}{4}K_{11} - \frac{1}{2}K_{12} - \frac{\sqrt{3}}{4}K_{22},\quad K_{13}' = -\frac{1}{2}K_{13} + \frac{\sqrt{3}}{2}K_{23},\quad K_{23}' = -\frac{\sqrt{3}}{2}K_{13} - \frac{1}{2}K_{23}$$

With Neumann principle from these equations we can get:

$$\left.\begin{aligned} K_{11} = K_{11}' = \frac{1}{4}K_{11} - \frac{\sqrt{3}}{2}K_{12} + \frac{3}{4}K_{22} \ &\Rightarrow\ K_{12} = \frac{\sqrt{3}}{2}(K_{22} - K_{11}) \\ K_{12} = K_{12}' = \frac{\sqrt{3}}{4}K_{11} - \frac{1}{2}K_{12} - \frac{\sqrt{3}}{4}K_{22} \ &\Rightarrow K_{12} = \frac{\sqrt{3}}{2}(K_{11} - K_{22}) \end{aligned}\right\} \Rightarrow K_{12} = 0,\ K_{11} = K_{22}$$

$$\left.\begin{aligned} K_{13} = K_{13}' = -\frac{1}{2}K_{13} + \frac{\sqrt{3}}{2}K_{23} \ &\Rightarrow K_{13} = \frac{1}{\sqrt{3}}\ K_{23} \\ K_{23} = K_{23}' = -\frac{\sqrt{3}}{2}K_{13} - \frac{1}{2}K_{23} \ &\Rightarrow\ K_{23} = -\frac{1}{\sqrt{3}}\ K_{13} \end{aligned}\right\} \Rightarrow K_{13} = K_{23} = 0$$

The tensor will finally have the form:

$$K = \begin{pmatrix} K_1 & 0 & 0 \\ & K_1 & 0 \\ & & K_3 \end{pmatrix}.$$

Therefore, this tensor has same form as for tetragonal systems e.g. ***4*** or ***4/mmm*** .
It describes dielectric response, which is isotropic in the plane perpendicular to the rotation axis.

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