CRYSTAL SYMMETRY, X-RAY DIFFRACTION, AND PHYSICAL PROPERTIES

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Lecture 58(B): Effect of Crystal Symmetry on Second Rank Property Tensor-II

Continuing from the previous lecture, where we discussed how a second-rank property tensor transforms for a crystal possessing a twofold rotation symmetry, such as a monoclinic crystal, we recall the result obtained earlier. By placing a twofold rotation axis along the x_3 direction, the transformed tensor was found to have the form

$$\begin{pmatrix} T_{11} & T_{12} & 0 \\ T_{12} & T_{22} & 0 \\ 0 & 0 & T_{33} \end{pmatrix}.$$

Now, suppose that in addition to the twofold rotation symmetry along x_3, we also introduce a twofold rotation symmetry along the x_1 direction. We wish to examine how this tensor further transforms. A rotation of 180° about the x_1 axis takes the x_2 axis to x'_2 and the x_3 axis to x'_3, while the x_1 axis itself remains unchanged, since the rotation is performed about this axis. Thus, x'_1 coincides with x_1.

We now write down the direction cosine matrix corresponding to this transformation. Since x'_1 coincides with x_1, the angle between them is 0°, and hence $a_{11} = cos0 = 1$. The axis x'_1 is perpendicular to both x_2 and x_3, so the corresponding direction cosines are zero. The axis x'_2 makes an angle of 180° with x_2, giving $a_{22} = cos\pi = -1$, and is perpendicular to the other axes. Similarly, x'_3 makes an angle of 180° with x_3, giving $a_{33} = -1$. Thus, the direction cosine matrix is

$$A = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}.$$

The tensor transformation is given by

$$T'_{ij} = a_{im} a_{jn} T_{mn}.$$

Since the twofold rotation about the x_3 axis has already reduced the tensor to the form given above, we focus on the off-diagonal component T_{12} and examine how it transforms under this additional symmetry. We have

$$T'_{12} = a_{1m} a_{2n} T_{mn}.$$

Inspecting the direction cosine matrix, the only nonzero contribution comes from $m = 1$ and $n = 2$, giving

$$T'_{12} = a_{11} a_{22} T_{12}.$$

Since $a_{11} = 1$ and $a_{22} = -1$, this yields

$$T'_{12} = -T_{12}.$$

For the tensor to remain unchanged under this symmetry operation, the only possible value is

$$T_{12} = 0.$$

It is straightforward to show that under this transformation $T'_{11} = T_{11}$, $T'_{22} = T_{22}$, and $T'_{33} = T_{33}$. Therefore, the final tensor under the combined action of twofold rotations about x_1 and x_3 is

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

The components T_{13} and T_{23} were not considered here because they were already forced to be zero by the twofold rotation about the x_3 axis. Hence, when two twofold rotation axes are present at 90° to each other, one along x_1 and one along x_3, the tensor has only three independent components: T_{11}, T_{22}, and T_{33}.

From crystallography, we recall that if two twofold rotation axes exist at right angles to each other, a third twofold rotation axis automatically appears at right angles to both of them. In this case, a third twofold axis lies along x_2. Therefore, the point group corresponding to three mutually perpendicular twofold axes is 222. This point group is associated with the orthorhombic crystal system. Consequently, for all orthorhombic crystals, a second-rank property tensor has only three independent components.

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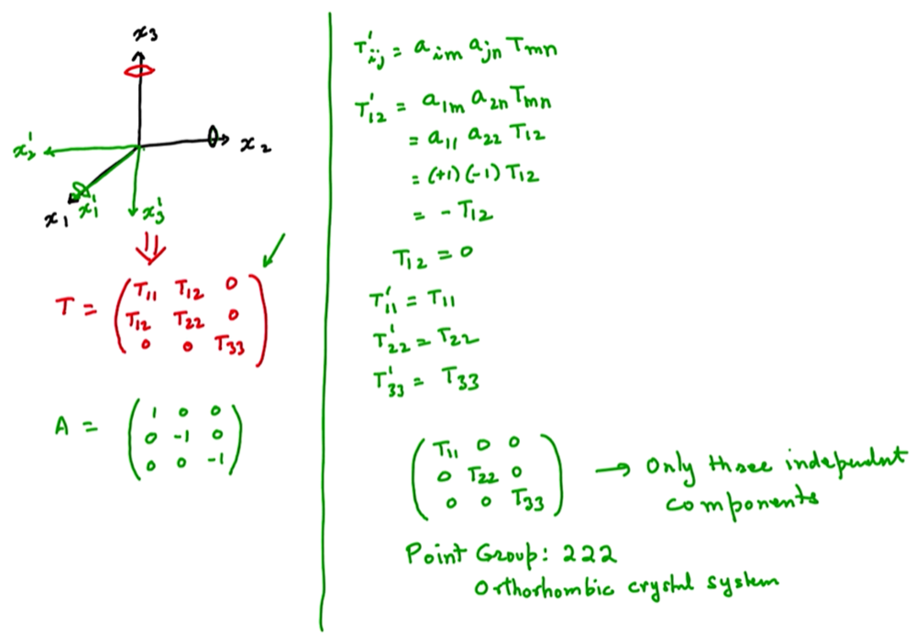

Next, let us consider another symmetry operation, namely that of a tetragonal crystal system. The axial point group associated with the tetragonal system is the point group 4. We place a fourfold rotation axis along the x_3 direction. A 90° rotation about x_3 takes the x_1 axis into the x_2 direction, so that x'_1 coincides with x_2, while x'_2 coincides with the negative of the x_1 direction. The x_3 axis remains unchanged.

From this, the direction cosine matrix can be written as

$$A = \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

The tensor transformation is again given by

$$T'_{ij} = a_{im}a_{jn}T_{mn}.$$

Consider first the component $T'_{11} = a_{1m}a_{1n}T_{mn}$. Inspection of the direction cosine matrix shows that the only nonzero term is $a_{12}a_{12}T_{22}$. Since $a_{12} = 1$, we obtain

$$T'_{11} = T_{22}.$$

Similarly,

$$T'_{22} = a_{2m}a_{2n}T_{mn} = a_{21}a_{21}T_{11} = T_{11},$$

and

$$T'_{33} = a_{33}a_{33}T_{33} = T_{33}.$$

For the tensor to remain unchanged under the fourfold rotation, we must therefore have

$$T_{11} = T_{22}.$$

Next, consider the off-diagonal components. For T'_{12},

$$T'_{12} = a_{1m}a_{2n}T_{mn} = a_{12}a_{21}T_{21} =- T_{21}.$$

Since the tensor is symmetric, $T_{21} = T_{12}$, and invariance under the symmetry operation requires

$$T_{12} = 0.$$

Similarly,

$$T'_{13} = a_{1m}a_{3n}T_{mn} = a_{12}a_{33}T_{23} = T_{23},$$

and

$$T'_{23} = a_{2m}a_{3n}T_{mn} = a_{21}a_{33}T_{13} =- T_{13}.$$

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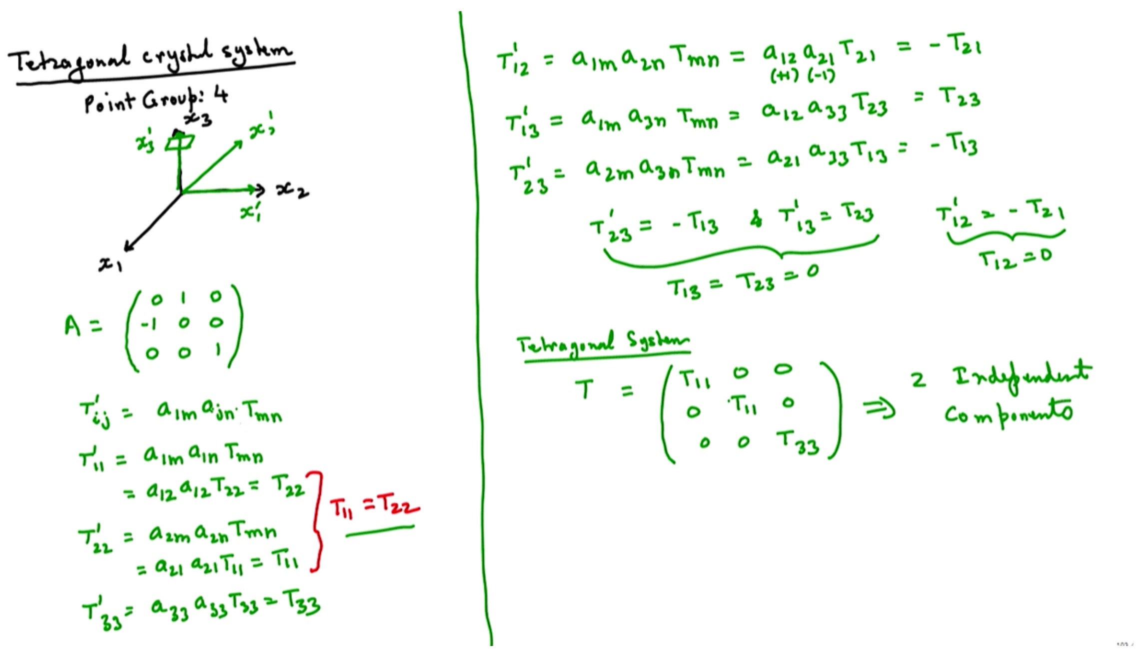

For the tensor to remain unchanged, these relations imply

$$T_{13} = T_{23} = 0.$$

Thus, for a tetragonal crystal system, the second-rank property tensor reduces to

$$\begin{pmatrix} T_{11} & 0 & 0 \\ 0 & T_{11} & 0 \\ 0 & 0 & T_{33} \end{pmatrix},$$

which contains only two independent components.

Now, consider combining a twofold rotation with a threefold rotation in a cubic crystal. Let the coordinate axes be x_1, x_2, and x_3, with a twofold rotation axis along x_3. As discussed previously, this symmetry reduces the tensor to

$$\begin{pmatrix} T_{11} & T_{12} & 0 \\ T_{12} & T_{22} & 0 \\ 0 & 0 & T_{33} \end{pmatrix}.$$

Next, introduce a threefold rotation axis along the body diagonal, that is, along the $[111]$ direction. In a cube, a 120° rotation about a body diagonal maps x_1 to x'_2, x_2 to x'_3, and x_3 to x'_1. Since each new axis coincides with one of the original axes, the direction cosine matrix is

$$A = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}.$$

Using matrix notation, the transformed tensor is given by

$$T' = ATA^{T}.$$

Substituting the tensor obtained after the twofold rotation and carrying out the matrix multiplication, one finds that invariance under the threefold rotation requires all off-diagonal components to vanish and the diagonal components to be equal, that is,

$$T_{11} = T_{22} = T_{33}.$$

Thus, the tensor reduces to

$$\begin{pmatrix} T_{11} & 0 & 0 \\ 0 & T_{11} & 0 \\ 0 & 0 & T_{11} \end{pmatrix},$$

with only one independent component.

This result implies that for this combination of symmetries the second-rank property tensor is isotropic. The corresponding point group is 23, which is one of the axial point groups of the cubic crystal system. Therefore, cubic crystals are isotropic with respect to second-rank property tensors. A familiar example of such a property is electrical conductivity.

There are other point groups associated with the cubic crystal system. For example, one may consider a fourfold rotation combined with a threefold rotation, giving the point group 432. Since the fourfold rotation contains a twofold rotation as a subgroup, this case also leads to an isotropic tensor. Alternatively, one may consider two different threefold rotations along different body diagonals of the cube; this again leads to the same conclusion. These cases are left as exercises for further study.

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