CRYSTAL SYMMETRY, X-RAY DIFFRACTION, AND PHYSICAL PROPERTIES

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Lecture 58(A): Effect of Crystal Symmetry on Second Rank Property Tensor-I

In this lecture, I am going to discuss how a second-rank property tensor transforms under a symmetry operation. We have already learned a considerable amount about symmetry in crystals. If we have a crystal with a certain symmetry, the crystal remains unchanged under that symmetry operation. Now, if the crystal remains unchanged by the symmetry operation, then if I make a property measurement, for example electrical conductivity, with reference to some fixed axes, and then apply the symmetry operation to the crystal and again make the same measurement with respect to the same fixed axes, I will obtain the same property. Therefore, it follows that the property tensor must also remain unchanged.

What does this mean mathematically? If there is a transformation of the tensor given by

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

where T'_{ij} represents the transformed components under a coordinate transformation, then the individual components of the tensor remain unchanged. One can also write this in matrix form, where the transformed tensor T' is obtained by multiplying the direction cosine matrix A, the tensor T, and the transpose of the direction cosine matrix, that is,

$$T' = A\,T\,A^T.$$

Therefore, this implies that after the transformation, $T' = T$, meaning that the property tensor has the same components before and after the transformation.

Another important aspect of second-rank tensors is that almost all second-rank property tensors are symmetric. What does this mean? This means that the tensor components satisfy

$$T_{ij} = T_{ji}.$$

If we write out the components of the tensor as $T_{11}, T_{12}, T_{13}, T_{21}, T_{22}, T_{23}, T_{31}, T_{32}, T_{33}$,

$$\begin{pmatrix} T_{11} & T_{12} & T_{13} \\ T_{21} & T_{22} & T_{23} \\ T_{31} & T_{32} & T_{33} \end{pmatrix}.$$

then the conditions $T_{12} = T_{21}$, $T_{13} = T_{31}$, and $T_{23} = T_{32}$ indicate that the tensor is symmetric. In matrix form, this means that the matrix is symmetric. A prime example of such a tensor is the electrical conductivity tensor.

This symmetry property of almost all second-rank property tensors does not arise from crystal symmetry. Instead, it arises from the underlying physics, and a detailed discussion of this lies beyond the scope of this course. Therefore, we will assume that all second-rank property tensors that we deal with are symmetric.

Now, let us consider a particular symmetry operation, namely an inversion center. If there is an inversion center, how do the coordinate axes transform? Let us first examine this. Consider the Cartesian axes x_1, x_2, and x_3, with an inversion center located at the origin of the coordinate system. The inversion operation will invert the x_1 axis to x'_1, the x_2 axis to x'_2, and the x_3 axis to x'_3. Thus, we go from the coordinate system (x_1, x_2, x_3) to (x'_1, x'_2, x'_3).

We now determine the direction cosine matrix for this transformation. Recall that the components of the direction cosine matrix are $a_{11}, a_{12}, a_{13}, a_{21}, a_{22}, a_{23}, a_{31}, a_{32}, a_{33}$, where, for example, a_{11} is the cosine of the angle between x'_1 and x_1, a_{12} is the cosine of the angle between x'_1 and x_2, and so on. The angle between x'_1 and x_1 is 180° or π, so

$cos\pi = -1$, and hence $a_{11} = -1$. The angles between x'_1 and x_2, and between x'_1 and x_3, are both 90°, so $a_{12} = a_{13} = 0$.

Similarly, x'_2 makes an angle of 90° with x_1, so $a_{21} = 0$, and an angle of 180° with x_2, so $a_{22} = -1$, while $a_{23} = 0$. Finally, x'_3 makes angles of 90° with both x_1 and x_2, so $a_{31} = a_{32} = 0$, and an angle of 180° with x_3, giving $a_{33} = -1$. Thus, the direction cosine matrix for inversion is obtained.

We now transform the tensor using the matrix form,

$$T' = A\,T\,A^T.$$

From the properties of the direction cosine matrix, we note that the transpose of this matrix is the same as the matrix itself. Furthermore, this matrix is simply the identity matrix multiplied by -1, that is,

$$A = -I.$$

Therefore, the transformed tensor can be written as

$$T' = (-I)\,T\,(-I).$$

The product of the two factors of -1 gives $+1$, and hence

$$T' = I\,T\,I.$$

Multiplication by the identity matrix leaves the tensor unchanged, so we obtain

$$T' = T.$$

This shows that under inversion symmetry, the second-rank tensor remains unchanged. This leads to the important conclusion that all second-rank tensors possess inversion symmetry intrinsically. Whether or not the tensor is symmetric is irrelevant in this context; central inversion symmetry is always present.

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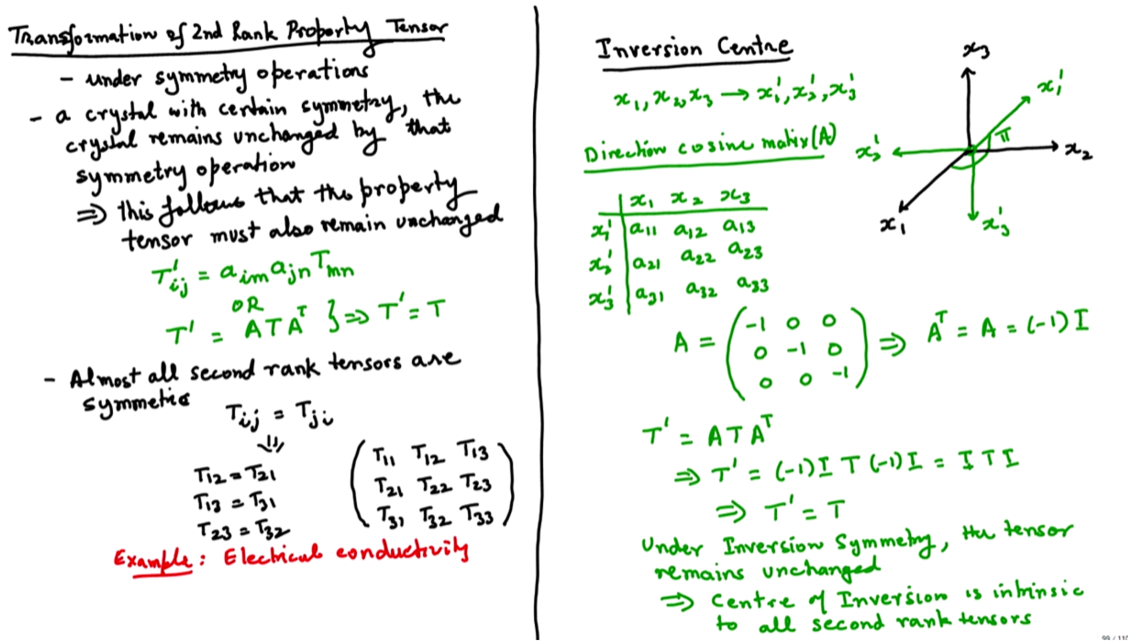

This result connects directly to Neumann's principle, which states that the symmetry of the physical properties of a crystal must include all the symmetries of the crystal, and may include additional symmetries. In this case, all second-rank tensors possess inversion symmetry, irrespective of whether the crystal itself has inversion symmetry.

Let us now consider another symmetry operation. Suppose we have a two-fold rotation axis along the x_3 axis. A two-fold axis corresponds to a rotation of 180°. Rotating about the x_3 axis by 180° takes x_1 to x'_1 and x_2 to x'_2, while the x_3 axis remains unchanged and coincides with x'_3.

We now determine the direction cosine matrix for this transformation. The angle between x'_1 and x_1 is 180°, so $a_{11} = -1$, while x'_1 is at 90° to both x_2 and x_3, giving $a_{12} = a_{13} = 0$. For x'_2, the angle with x_1 is 90°, so $a_{21} = 0$, the angle with x_2 is 180°, so $a_{22} = -1$, and $a_{23} = 0$. For x'_3, the axis coincides with x_3, so the angle is 0° and

$cos0 = 1$, giving $a_{33} = 1$, with $a_{31} = a_{32} = 0$. This gives the direction cosine matrix for a two-fold rotation about x_3.

The tensor transformation in tensor notation is given by

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

Let us expand one component of this tensor, namely T'_{11}. Here, $i = 1$ and $j = 1$ are the free indices, so we write

$$T'_{11} = \sum_{m=1}^{3}\sum_{n=1}^{3} a_{1m}a_{1n}T_{mn}.$$

Expanding this summation explicitly, we start with $m = 1$ and vary n from 1 to 3. For $m = 1$ and $n = 1$, we obtain the term $a_{11}a_{11}T_{11}$. For $m = 1$ and $n = 2$, we obtain $a_{11}a_{12}T_{12}$. For $m = 1$ and $n = 3$, we obtain $a_{11}a_{13}T_{13}$. Thus, for $m = 1$, we obtain three terms contributing to T'_{11}.

Next, we proceed with the case $m = 2$, followed by $m = 3$. In this way, for $m = 2$ we will obtain three additional terms, and for $m = 3$ another three terms, so that in total we will end up with nine terms.

Let us first consider the next three terms corresponding to $m = 2$. In this case, the first coefficient becomes a_{12}, and we begin with $n = 1$. Thus, the first term is $a_{12}a_{11}T_{21}$. When $n = 2$, we obtain $a_{12}a_{12}T_{22}$. When $n = 3$, we obtain $a_{12}a_{13}T_{23}$.

Now consider the last three terms corresponding to $m = 3$. These are $a_{13}a_{11}T_{31}$, $a_{13}a_{12}T_{32}$, and $a_{13}a_{13}T_{33}$.

At this stage, we have all nine terms. Although this appears quite cumbersome, we note that most of the elements of the direction cosine matrix are zero. Therefore, we examine the individual terms carefully. Starting with the first term, $a_{11}a_{11}T_{11}$, we see that a_{11} is nonzero and equal to -1. Since both factors are nonzero, this term survives. In the second term, although a_{11} is nonzero, a_{12} is zero, so the entire term vanishes. In the third term, a_{13} is zero, so that term also vanishes.

Now consider the second set of three terms. Each of these terms contains the factor a_{12}, and since $a_{12} = 0$, all three of these terms vanish. Similarly, in the final set of three terms, each contains the factor a_{13}, which is also zero, and hence these terms also vanish. Therefore, we are left with only one nonzero contribution, and we obtain

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

Since $a_{11} =- 1$, this gives

$$T'_{11} = (-1)(-1)T_{11} = T_{11}.$$

Thus, the T_{11} component remains unchanged under a twofold rotation.

Next, let us examine the second diagonal component, T'_{22}. This can be written as

$$T'_{22} = a_{2m}a_{2n}T_{mn}.$$

Although this expression formally contains nine terms, inspection of the second row of the direction cosine matrix shows that the only nonzero element is a_{22}. Therefore, the only surviving term is

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

Since $a_{22} =- 1$, we obtain

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

In a similar manner, one can show that

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

Now let us examine an off-diagonal component, T'_{12}. This is given by

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

Again, considering only the nonzero elements of the direction cosine matrix, the surviving term is

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

Since both a_{11} and a_{22} are equal to -1, we find

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

Thus far, the components T_{11}, T_{22}, T_{33}, and T_{12} all remain unchanged under this symmetry operation.

Now consider another off-diagonal component, T'_{13}. This component is given by

$$T'_{13} = a_{1m}a_{3n}T_{mn}.$$

Keeping only the nonzero terms, this becomes

$$T'_{13} = a_{11}a_{33}T_{13}.$$

Here, $a_{11} = -1$ and $a_{33} = +1$, so we obtain

$$T'_{13} = -T_{13}.$$

This result is significant. Under the symmetry operation, the transformed component is the negative of the original component. However, since this is a symmetry operation, the tensor must remain unchanged. The only way this condition can be satisfied is if

$$T_{13} = 0.$$

In a similar fashion, consider the component T'_{23}, which is given by

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

One finds that

$$T'_{23} = -T_{23},$$

which implies that

$$T_{23} = 0.$$

We have already stated that all second-rank property tensors under consideration are symmetric, which means that $T_{12} = T_{21}$, $T_{13} = T_{31}$, and $T_{23} = T_{32}$. Therefore, for a crystal with a single twofold rotation axis, the tensor takes the form

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

Such a tensor has five nonzero components, but only four of them are independent.

A crystal that possesses a single twofold rotation axis is a monoclinic crystal. Therefore, for monoclinic crystals, the second-rank property tensor has four independent components. The twofold rotation corresponds to point group 2. There are other point groups associated with monoclinic crystals, such as $2/m$, which includes an inversion center. Since inversion symmetry is intrinsic to second-rank property tensors, the tensors corresponding to point groups 2, $2/m$, and even m are identical.

As an assignment, consider the point group m, with a mirror plane in the x_1x_2 plane. In this case, x'_1 coincides with x_1, x'_2 coincides with x_2, and x'_3 is inverted relative to x_3.

Using this transformation, show that the resulting second-rank property tensor has the same form as above.

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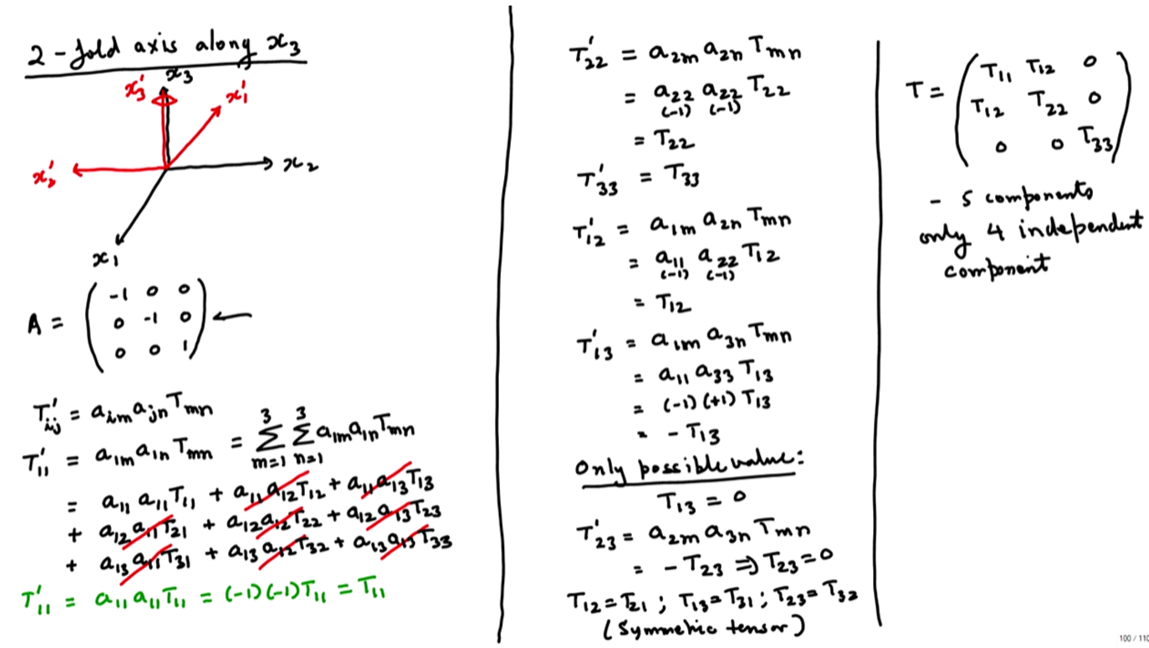

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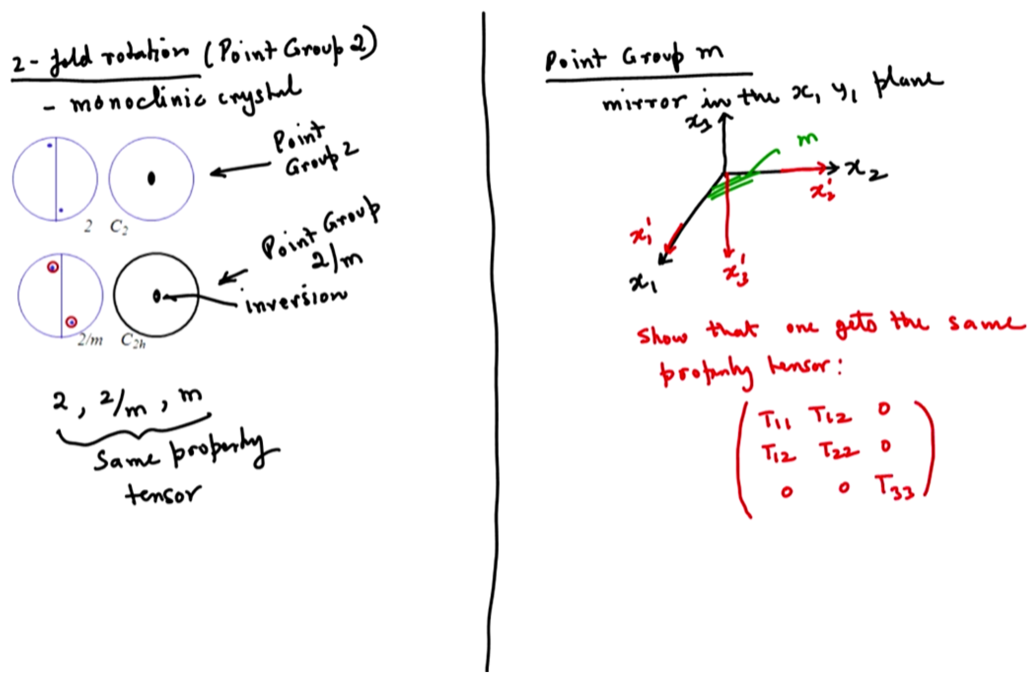

In the next lecture, we will consider additional symmetry operations, examine other point groups, and study how second-rank tensors change under those symmetries.