CRYSTAL SYMMETRY, X-RAY DIFFRACTION, AND PHYSICAL PROPERTIES

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Lecture 60: Fourth Rank Elasticity Tensor

This is the final lecture of this course. In this lecture, a specific material property represented by the elasticity tensor is discussed. The elasticity tensor is a fourth-rank tensor. Its role is to relate the applied stress to the resulting strain, or equivalently, the applied strain to the stress that develops in the material.

For isotropic materials, this relationship is already familiar. For example, consider a bar made of an isotropic material subjected to a uniaxial tensile stress. An elastic strain develops, and the relationship between the elastic strain ϵ and the applied stress σ is given through Young's modulus E, such that

$$\epsilon = \frac{\sigma}{E}.$$

Here, E is Young's modulus, σ denotes the applied stress, and ϵ is the resulting strain, as described by Hooke's law. The stress σ is a second-rank tensor, details of which were discussed earlier in the course during the introduction to material properties. Similarly, strain is also a second-rank tensor, and the strain tensor was introduced in the previous lecture.

In the general case of an anisotropic crystal, the relationship between stress and strain must be expressed in tensor notation. The stress tensor component σ_{kl} and the strain tensor component ϵ_{ij} are related through a fourth-rank property tensor denoted as S_{ijkl}. Alternatively, one may write the stress σ_{ij} on the left-hand side and the strain ϵ_{kl} on the right-hand side, relating them through another fourth-rank tensor C_{ijkl}. Both S and C are elasticity tensors, with S referred to as the compliance tensor and C as the stiffness tensor. Either representation may be used; however, the stiffness tensor will be used here.

The terminology compliance and stiffness arises from historical usage in a language other than English. Since the elasticity tensor is of fourth rank, the total number of components is

$$3^4 = 81.$$

To illustrate this, consider the expansion of one stress component. For σ_{11}, the constitutive relation is

$$\sigma_{11} = C_{11kl}\epsilon_{kl},$$

where summation is carried out over $k = 1$ to 3 and $l = 1$ to 3. Expanding explicitly,

$$\sigma_{11} = C_{1111}\epsilon_{11} + C_{1112}\epsilon_{12} + C_{1113}\epsilon_{13} + C_{1121}\epsilon_{21}$$
$$+ C_{1122}\epsilon_{22} + C_{1123}\epsilon_{23} + C_{1131}\epsilon_{31} + C_{1132}\epsilon_{32} + C_{1133}\epsilon_{33}.$$

Thus, each stress component contains nine terms. Since there are nine stress components, this results in a total of $9 \times 9 = 81$ terms. However, not all components of the stiffness tensor are independent, and the same is true for the compliance tensor.

Both the stress tensor and the strain tensor are symmetric. The stress tensor components are

$$\sigma = \begin{pmatrix} \sigma_{11} & \sigma_{12} & \sigma_{13} \\ \sigma_{21} & \sigma_{22} & \sigma_{23} \\ \sigma_{31} & \sigma_{32} & \sigma_{33} \end{pmatrix}$$

and the strain tensor components are

$$\epsilon = \begin{pmatrix} \epsilon_{11} & \epsilon_{12} & \epsilon_{13} \\ \epsilon_{21} & \epsilon_{22} & \epsilon_{23} \\ \epsilon_{31} & \epsilon_{32} & \epsilon_{33} \end{pmatrix}$$

Due to symmetry, there are only six independent components in each tensor. The fourth-rank stiffness tensor C and the compliance tensor S are also symmetric, satisfying

$$C_{ijkl} = C_{ijlk}, \quad C_{ijkl} = C_{jikl}.$$

As a result, the number of independent components is reduced from 81 to 36.

Rewriting the constitutive relation,

$$\sigma_{ij} = C_{ijkl}\epsilon_{kl},$$

and expanding σ_{11} again, symmetry implies that terms such as $C_{1121}\epsilon_{21}$ are equal to $C_{1112}\epsilon_{12}$. Hence, these terms can be combined, introducing a factor of 2. Applying this reduction to all symmetric pairs leaves only six terms per equation. Since the stress tensor itself is symmetric, there are only six independent equations, resulting in 36 independent components.

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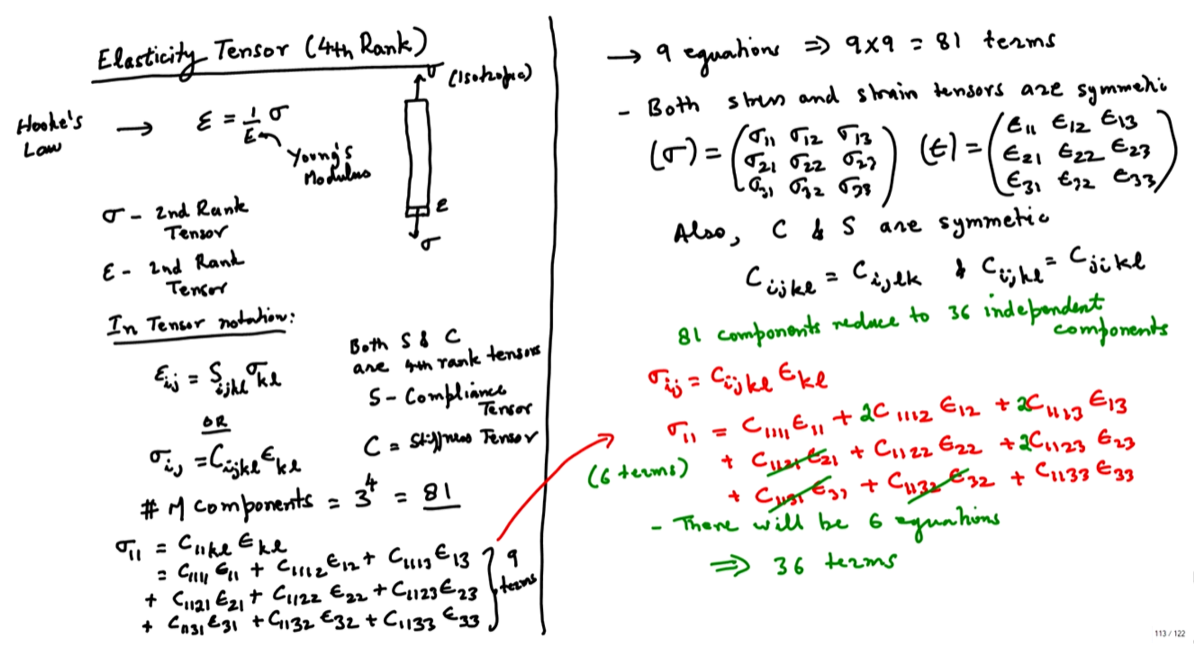

To represent the stiffness or compliance tensor more compactly, index reduction is employed, similar to the procedure used for the third-rank piezoelectric tensor. The fourth-rank tensor is reduced to a second-rank matrix, while the stress and strain tensors are reduced from second rank to first rank.

The strain tensor components

$$\epsilon = \begin{pmatrix} \epsilon_{11} & \epsilon_{12} & \epsilon_{13} \\ \epsilon_{21} & \epsilon_{22} & \epsilon_{23} \\ \epsilon_{31} & \epsilon_{32} & \epsilon_{33} \end{pmatrix}$$

are mapped to reduced indices as follows:

$$\epsilon_{11} \rightarrow \epsilon_1, \quad \epsilon_{22} \rightarrow \epsilon_2, \quad \epsilon_{33} \rightarrow \epsilon_3,$$

$$\epsilon_{23} \rightarrow \epsilon_4, \quad \epsilon_{13} \rightarrow \epsilon_5, \quad \epsilon_{12} \rightarrow \epsilon_6.$$

Due to symmetry,

$$\epsilon_{21} = \epsilon_{12} = \epsilon_6, \quad \epsilon_{31} = \epsilon_{13} = \epsilon_5, \quad \epsilon_{32} = \epsilon_{23} = \epsilon_4.$$

The stiffness tensor components C_{ijkl} are similarly reduced by mapping index pairs (ij) and (kl) to single indices (m, n), forming C_{mn}. For example,

$$C_{11} \leftrightarrow C_{1111}, \quad C_{12} \leftrightarrow C_{1122}, \quad C_{15} \leftrightarrow C_{1113}.$$

Using this notation, the stress–strain relation can be written in matrix form as

$$\begin{pmatrix} \sigma_1 \\ \sigma_2 \\ \sigma_3 \\ \sigma_4 \\ \sigma_5 \\ \sigma_6 \end{pmatrix} = \begin{pmatrix} C_{11} & C_{12} & C_{13} & C_{14} & C_{15} & C_{16} \\ C_{21} & C_{22} & C_{23} & C_{24} & C_{25} & C_{26} \\ C_{31} & C_{32} & C_{33} & C_{34} & C_{35} & C_{36} \\ C_{41} & C_{42} & C_{43} & C_{44} & C_{45} & C_{46} \\ C_{51} & C_{52} & C_{53} & C_{54} & C_{55} & C_{56} \\ C_{61} & C_{62} & C_{63} & C_{64} & C_{65} & C_{66} \end{pmatrix} \begin{pmatrix} \epsilon_1 \\ \epsilon_2 \\ \epsilon_3 \\ \epsilon_4 \\ \epsilon_5 \\ \epsilon_6 \end{pmatrix}.$$

This reduced representation is a matrix, not a tensor, and therefore tensor transformation rules cannot be directly applied to it.

The transformation of the stiffness tensor follows the general fourth-rank tensor transformation rule. If the coordinate axes x_1, x_2, x_3 transform to x_1', x_2', x_3', then

$$C_{ijkl}' = a_{ip} a_{jq} a_{kr} a_{ls} C_{pqrs},$$

where a_{ij} are the direction cosines.

Consider first an inversion center at the origin. Under inversion,

$$x_1^{'} = - x_1, \quad x_2^{'} = - x_2, \quad x_3^{'} = - x_3.$$

The direction cosine matrix is

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

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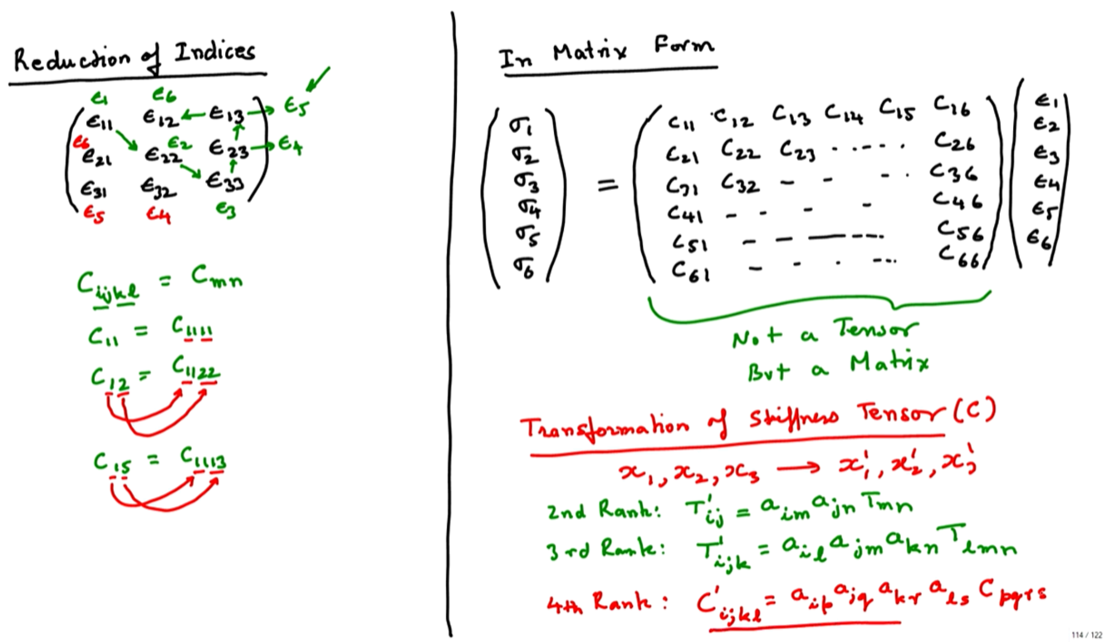

Substituting into the transformation equation, only diagonal terms contribute, yielding

$$C_{ijkl}^{'} = (-1)^4 C_{ijkl} = C_{ijkl}.$$

Thus, the fourth-rank stiffness tensor is invariant under inversion. Consequently, the elasticity tensor is centrosymmetric irrespective of whether the crystal itself possesses a center of symmetry. This represents an intrinsic symmetry of fourth-rank tensors, consistent with Neumann's principle.

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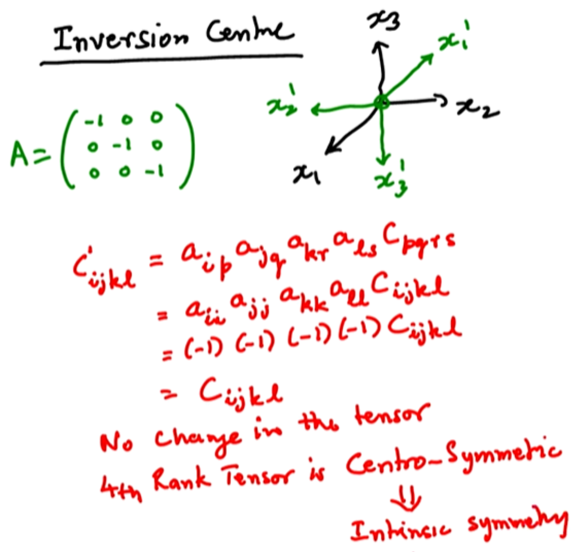

Next, consider a twofold rotation axis parallel to x_3, as in a monoclinic crystal. The coordinate transformation reverses x_1 and x_2 while leaving x_3 unchanged. The corresponding direction cosine matrix is

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

The implications of this symmetry on the stiffness tensor components can be determined using the same transformation rule.

This transformation implies that the axis x_1' points in the opposite direction to x_1, x_2' points in the opposite direction to x_2, and x_3' coincides with x_3. Therefore, the direction cosine matrix is simply

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

Now, let us determine some of the components of the stiffness tensor. We begin with the transformation

$$C'_{ijkl} = a_{ip}a_{jq}a_{kr}a_{ls}C_{pqrs}.$$

Let us calculate C'_{1111}. This becomes

$$C'_{1111} = a_{1p}a_{1q}a_{1r}a_{1s}C_{pqrs}.$$

The only non-zero contribution arises when all indices correspond to a_{11}. Thus, we have

$$C'_{1111} = a_{11}a_{11}a_{11}a_{11}C_{1111}.$$

Since each $a_{11} =- 1$, the product gives

$$C'_{1111} = C_{1111}.$$

In reduced notation, this corresponds to $C'_{11} = C_{11}$.

If we now write the reduced stiffness matrix, the C_{11} component is non-zero, which we indicate by a filled circle. This is the same convention used in the previous lecture for the piezoelectric tensor. If this notation is unclear, one may refer back to that lecture. A filled circle indicates a non-zero component and is more convenient than writing out individual tensor components.

This argument can be extended to show that when all indices are equal,

$$C'_{iiii} = C_{iiii}.$$

The only non-zero direction cosine components are a_{ii}, leading to

$$C'_{iiii} = a_{ii}a_{ii}a_{ii}a_{ii}C_{iiii} = C_{iiii}.$$

In reduced notation, this implies $C'_{ii} = C_{ii}$. Hence, there is no change in these components for $i = 1, 2, 3$.

Thus, the diagonal elements of the stiffness tensor referred to the original axes x_1, x_2, x_3 remain unchanged. In reduced notation, we may write $C_{44} = C_{2323}$, $C_{55} = C_{1313}$, and $C_{66} = C_{1212}$.

Next, we compute C'_{ijij} for $i \neq j$. This gives

$$C'_{ijij} = a_{ii}a_{jj}a_{ii}a_{jj}C_{ijij} = a_{ii}^2a_{jj}^2C_{ijij}.$$

Since the squares of the direction cosines are equal to unity, we obtain

$$C'_{ijij} = C_{ijij}.$$

These terms correspond to the diagonal elements C_{44}, C_{55}, and C_{66} in the reduced stiffness matrix. Hence, these components are also unchanged.

We now consider the off-diagonal terms. As an example, take

$$C'_{iijj},$$

which in reduced notation corresponds to C'_{ij} for $i \neq j$. This transforms as

$$C'_{iijj} = a_{ii}a_{ii}a_{jj}a_{jj}C_{iijj}.$$

Since each squared direction cosine equals unity, the result is

$$C'_{iijj} = C_{iijj}.$$

Thus, these off-diagonal components remain non-zero.

Consider next C'_{1112}, which in reduced notation corresponds to C'_{16}. This transforms to $-C_{1112}$, and hence this component vanishes. Similarly, for C'_{1113}, which corresponds to C'_{15} in reduced notation, we have

$$C'_{1113} = a_{11}a_{11}a_{11}a_{33}C_{1113}.$$

With three factors of -1 and one factor of $+1$, the result is

$$C'_{1113} =- C_{1113},$$

and therefore this term must be zero.

Filling in the remaining components, the non-zero terms are indicated by filled circles, while zeros are indicated by small dots. Since the stiffness matrix is symmetric, it suffices to write only the upper half. Counting the remaining independent components, we find a total of thirteen independent components in this case.

We now consider an orthorhombic example. Starting from the previously solved twofold rotation, we introduce an additional twofold axis along x_1. Under a 180° rotation about x_1, the x_2 axis transforms to x'_2, and x_3 transforms to x'_3. The direction cosine matrix for this transformation is

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

Evaluating one component, such as C'_{1112}, which corresponds to C'_{16} in reduced notation, we find

$$C'_{1112} =- C_{1112},$$

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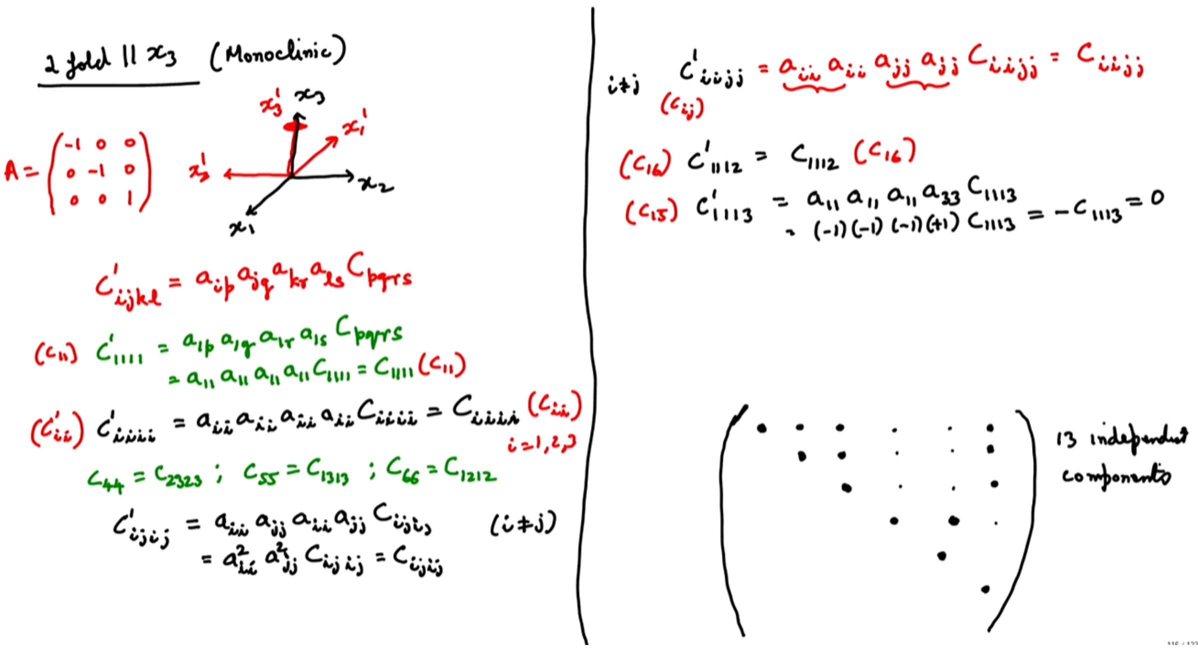

and hence this component vanishes. Similar arguments show that other off-diagonal components also vanish, leaving only the diagonal terms and three additional components. Thus, the stiffness matrix for the orthorhombic point group 222 has nine independent components.

Finally, we consider the cubic case, specifically the point group 23. We have already considered the twofold rotation about x_3. We now add a threefold rotation axis along the body diagonal of the cube. Under this symmetry operation, x_1' coincides with x_2, x_2' coincides with x_3, and x_3' coincides with x_1.

The direction cosine matrix for this transformation is

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

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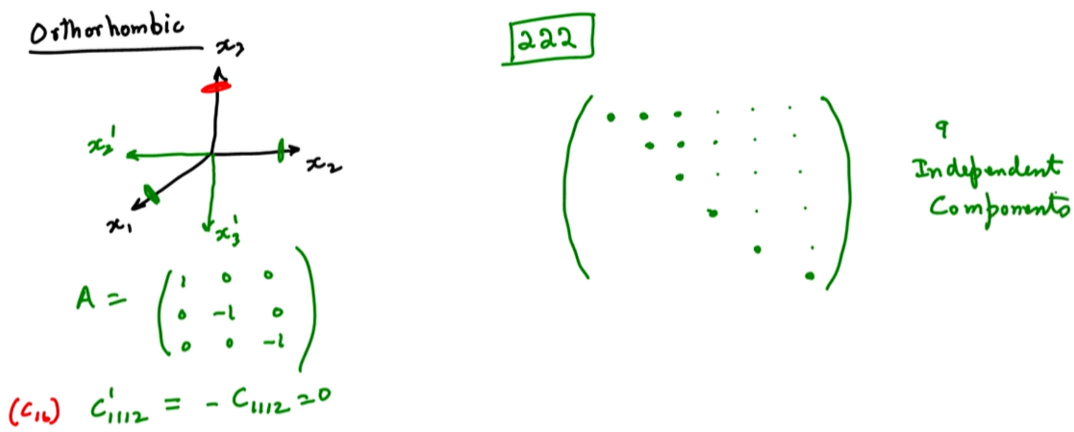

Let us evaluate C'_{1111}, which in reduced notation corresponds to C'_{11}. We obtain

$$C'_{1111} = a_{1p}a_{1q}a_{1r}a_{1s}C_{pqrs}.$$

The only non-zero contribution arises when all indices correspond to $p = q = r = s = 2$, giving

$$C'_{1111} = C_{2222}.$$

Similarly, evaluating C'_{2222} yields

$$C'_{2222} = C_{3333}.$$

Thus, invariance of the tensor under rotation implies

$$C_{1111} = C_{2222} = C_{3333},$$

or, in reduced notation,

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

Hence, the first three diagonal elements of the stiffness matrix are equal.

Carrying out a similar calculation for the remaining diagonal terms shows that

$$C_{44} = C_{55} = C_{66}.$$

Thus, the six diagonal elements form two triplets of equal values.

We next consider the off-diagonal terms C_{12}, C_{13}, and C_{23}. It can be shown that these three components are also equal. All remaining components vanish. Therefore, for the cubic case, only three independent elastic constants remain.

Thus, even in the cubic system, the stiffness tensor, and hence the elastic property, remains anisotropic.

With this, the lecture, as well as the course, is concluded. Thank you.

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