Chapter #3:
Crystal Binding
Lecture 5: Elasticity in Crystals

1. Linear Elasticity and Hooke's Law

In three dimensions, stress and strain are generally tensors, and the linear relationship requires a set of elastic constants. We use tensors because strain and stress involve multiple directions and must be described consistently under a change of coordinate frame. In compact notation:

$$\sigma_i = \Sigma_j C_{ij} \varepsilon_j \quad (i, j = 1, \ldots, 6)$$

Here C_{ij} are the elastic stiffness coefficients. Their values depend on the material and its crystal symmetry. The inverse relationship uses the compliance coefficients S_{ij}:

$$\varepsilon_i = \Sigma_j S_{ij} \sigma_j, \quad \text{with } S = C^{-1}$$

The stiffness coefficients have units of pressure (Pa); the compliance coefficients have units of inverse pressure (Pa^{-1}).

2. Stress and Strain as Tensors

2.1 Stress

The stress tensor is a second-rank tensor with components σ_{ij}. Using the convention that the first index identifies the force direction and the second identifies the normal direction of the surface, σ_{xy} is the x-directed stress acting on a surface whose normal is along y.

We represent stress using a 3x3 matrix:

$$\boldsymbol{\sigma} = \begin{pmatrix} \sigma_{xx} & \sigma_{xy} & \sigma_{xz} \\ \sigma_{yx} & \sigma_{yy} & \sigma_{yz} \\ \sigma_{zx} & \sigma_{zy} & \sigma_{zz} \end{pmatrix}$$

In ordinary classical elasticity, when couple stresses are neglected, the stress tensor is symmetric:

$$\sigma_{ij} = \sigma_{ji}$$

It therefore has six independent components: three normal stresses (σ_{xx}, σ_{yy}, σ_{zz}) and three shear stresses (σ_{yz}, σ_{xz}, σ_{xy}).

2.2 Strain

Strain describes the relative deformation of a material. It measures changes in length, angle, or volume rather than the overall translation of the body. For small displacements, the strain tensor is defined by

$$\varepsilon_{ij} = \tfrac{1}{2} (\partial u_i/\partial x_j + \partial u_j/\partial x_i)$$

where u is the displacement vector. The strain tensor is symmetric, $\varepsilon_{ij} = \varepsilon_{ji}$, and has six independent components.

- Normal strains: ε_{xx}, ε_{yy}, ε_{zz} describe extension or compression along the coordinate axes.
- Shear strains: ε_{yz}, ε_{xz}, ε_{xy} describe angular distortion.

We represent strain using a 3x3 matrix:

$$\boldsymbol{\epsilon} = \begin{pmatrix} \epsilon_{xx} & \epsilon_{xy} & \epsilon_{xz} \\ \epsilon_{yx} & \epsilon_{yy} & \epsilon_{yz} \\ \epsilon_{zx} & \epsilon_{zy} & \epsilon_{zz} \end{pmatrix}.$$

For small deformation, the volume strain (fractional change in volume) is

$$\delta = \Delta V/V \approx \varepsilon_{xx} + \varepsilon_{yy} + \varepsilon_{zz}$$

A positive volume strain represents **expansion**; a negative volume strain represents **compression**.

3. Voigt Notation and Elastic Constants

In three-dimensional, crystal can experience several stress components simultaneously. In the general case, each strain component may depend on multiple stress components.

We therefore write

$$\sigma_{ij} = \sum_{k=1} \sum_{l=1} C_{ijkl} \varepsilon_{kl}$$

Here, C_{ijkl} is the fourth-rank elastic stiffness tensor. Each index *i,j,k,l* can take the values 1,2,3 corresponding to *x,y,z*.

Since there are three possible values for each of the four indices, the tensor initially has

$$3^4 = 81\ components$$

In fact, these 81 components are not independent.

In ordinary classical elasticity, the stress and strain tensors are symmetric:

$$\sigma_{ij} = \sigma_{ji} \qquad \text{and} \qquad \varepsilon_{kl} = \varepsilon_{lk}$$

These symmetries impose two corresponding symmetries on the stiffness tensor:

$$C_{ijkl} = C_{jikl} \qquad \text{and} \qquad C_{ijkl} = C_{ijlk}$$

Consequently, each stress pair and each strain pair has only six distinct combinations, rather than nine. We can therefore replace the four-index tensor by a $6x6$ matrix which has 36 components.

However, because stress and strain are symmetric tensors, their six independent components are often written as six-component vectors. This convention is called Voigt notation. One common ordering is

$$\varepsilon_1 = \varepsilon_{xx},\ \varepsilon_2 = \varepsilon_{yy},\ \varepsilon_3 = \varepsilon_{zz},\ \varepsilon_4 = \varepsilon_{yz},\ \varepsilon_5 = \varepsilon_{xz},\ \varepsilon_6 = \varepsilon_{xy}$$

$$\sigma_1 = \sigma_{xx},\ \sigma_2 = \sigma_{yy},\ \sigma_3 = \sigma_{zz},\ \sigma_4 = \sigma_{yz},\ \sigma_5 = \sigma_{xz},\ \sigma_6 = \sigma_{xy}$$

In Voigt notation, generalized Hooke's law is

$$\sigma_i = \Sigma_j\, C_{ij}\, \varepsilon_j$$

For a general elastic material, the stiffness matrix has 36 entries but, because of the symmetry of elastic energy, at most 21 independent elastic constants. Crystal symmetry reduces this number.

4. Elastic Strain Energy

For linear elastic behavior, the strain-energy density is quadratic in strain. It is analogous to the energy stored in a stretched or compressed spring.

$$u = \tfrac{1}{2}\, \Sigma_i\, \varepsilon_i\, \sigma_i \;\; = \tfrac{1}{2}\, \Sigma_{ij}\, \varepsilon_i\, C_{ij}\, \varepsilon_j \qquad (\text{Think about the familiar spring-energy equation})$$

Here u is elastic strain-energy density (J m^{-3}), which has the same units as pressure. The total elastic energy is U = uV for a uniformly strained volume V. In the absence of additional couplings, the stiffness matrix is symmetric, $C_{ij} = C_{ji}$.

In the following, we will focus on the elastic properties of cubic crystals, for which the x, y, and z axes are equivalent by symmetry.

5. Elasticity of Cubic Crystals

In a cubic crystal, the x, y, and z axes are symmetry-equivalent. Consequently, only three independent stiffness constants are required: C_{11}, C_{12}, and C_{44}.

For a cubic crystal, the matrix takes the form:

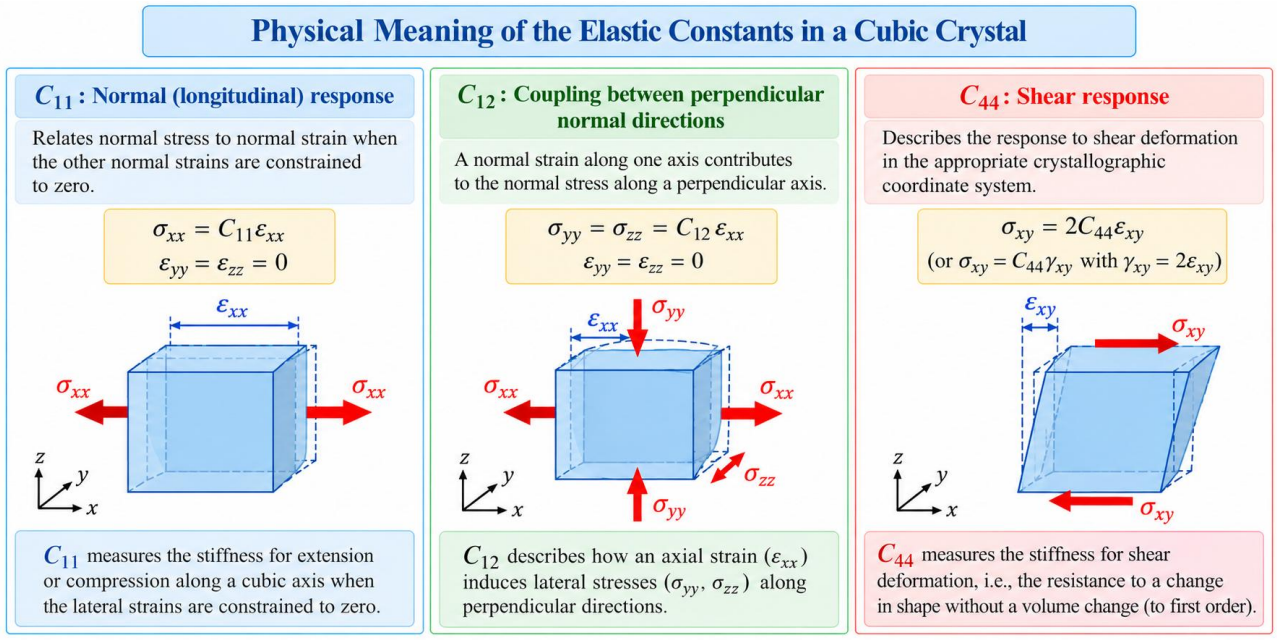
$$\mathbf{C} = \begin{pmatrix} C_{11} & C_{12} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{11} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{12} & C_{11} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & C_{44} \end{pmatrix}.$$

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

$$C_{12} = C_{13} = C_{23}$$

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

Elastic constant	Physical interpretation
C_{11}	Relates normal stress to normal strain when the other normal strains are constrained to zero.
C_{12}	Describes coupling between normal strains along perpendicular crystal axes.
C_{44}	Describes the response to shear deformation in the appropriate crystallographic coordinate system.

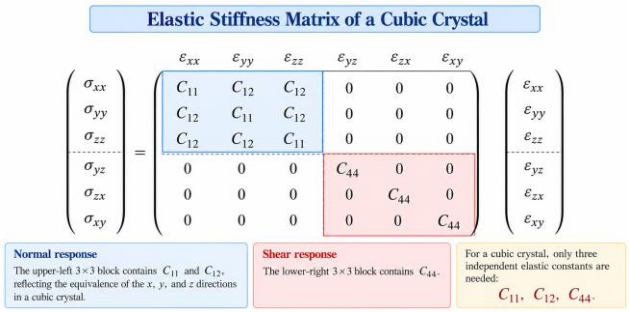


In tensor notation, the normal-stress relations are

$$\sigma_{xx} = C_{11}\,\varepsilon_{xx} + C_{12}(\varepsilon_{yy} + \varepsilon_{zz})$$

$$\sigma_{yy} = C_{11}\,\varepsilon_{yy} + C_{12}(\varepsilon_{xx} + \varepsilon_{zz})$$

$$\sigma_{zz} = C_{11}\,\varepsilon_{zz} + C_{12}(\varepsilon_{xx} + \varepsilon_{yy})$$



6. Bulk Modulus of a Cubic Crystal

A pure volume change corresponds, for small isotropic dilation, to equal normal strains along all three axes:

$$\varepsilon_{xx} = \varepsilon_{\gamma\gamma} = \varepsilon_{zz} = \delta/3, \qquad \delta = \Delta V/V$$

The bulk modulus B measures resistance to uniform compression. It is defined by

$$B = -V\,(dP/dV)$$

For a cubic crystal, the relationship between the bulk modulus and the stiffness constants is

$$B = (C_{11} + 2C_{12})/3$$

A large bulk modulus means that a relatively large pressure change is required to produce a given fractional change in volume. The compressibility is $\kappa = 1/B$.

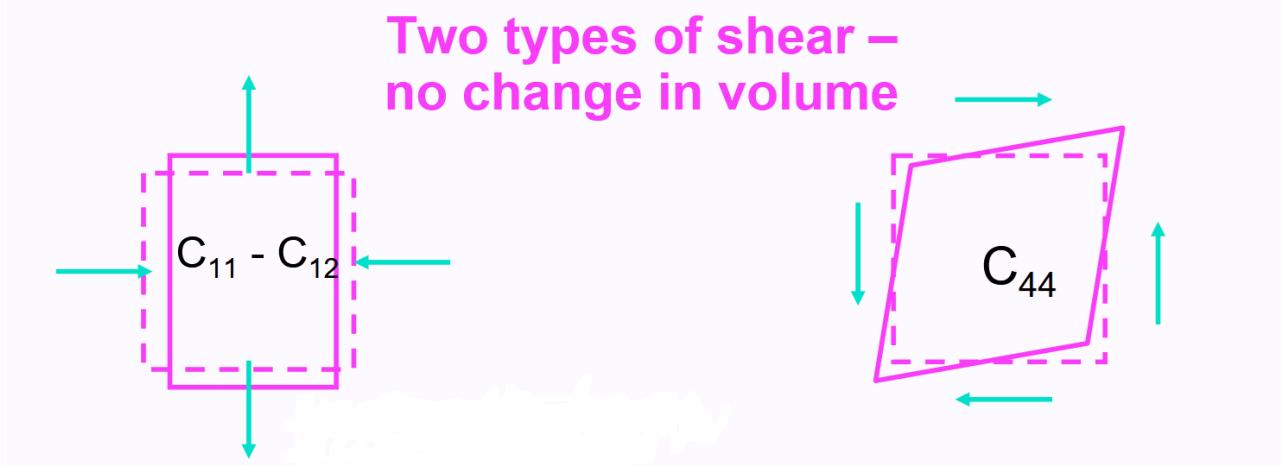
Homework:

From the elastic strain-energy density (given in 4), prove that the bulk modulus B for a cubic crystal is given by:

$$B = (C_{11} + 2C_{12})/3$$

You also need to read the following to see more examples about the properties of elastic stiffness.

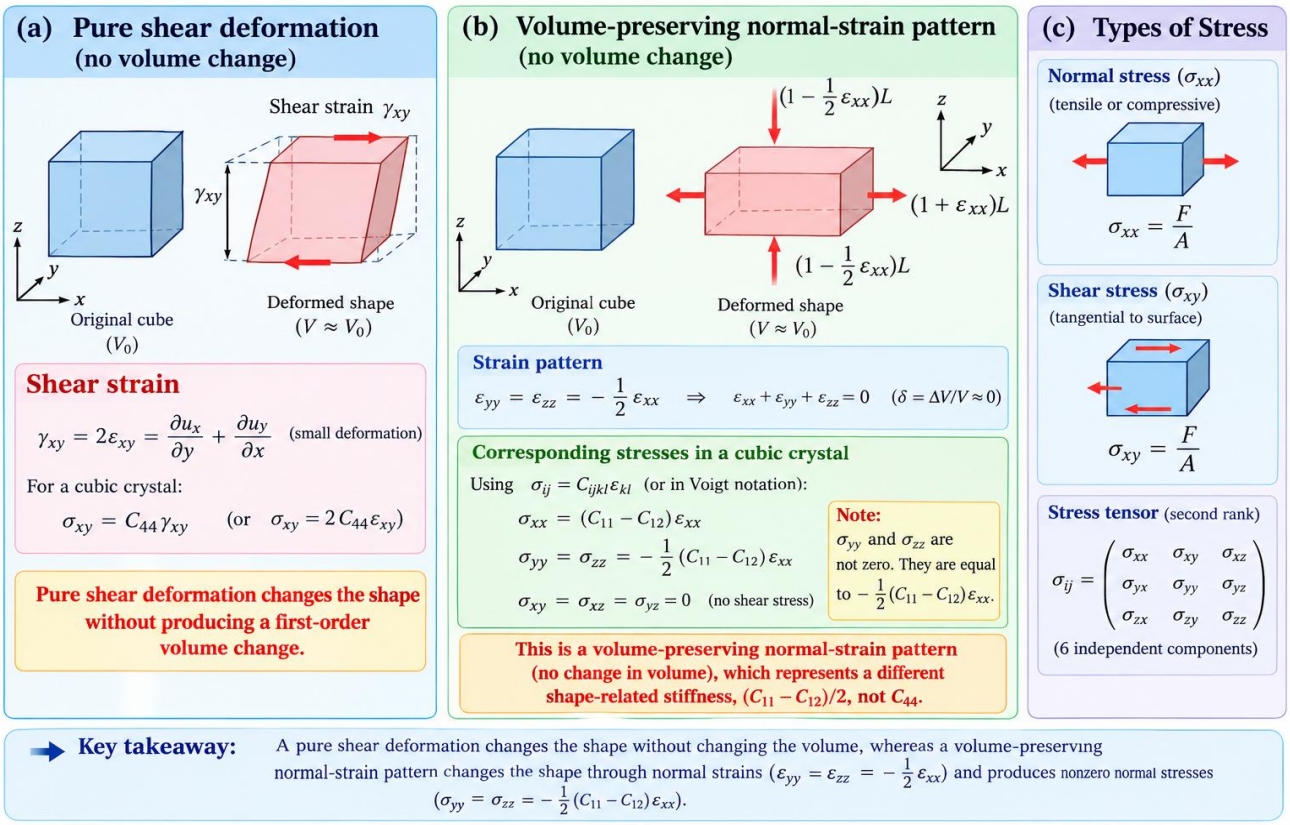
7. Shear Deformation and Volume-Preserving Strain in Cubic Crystals



- A pure shear deformation changes the shape without producing a first-order volume change. Cubic crystals can respond differently to distinct shear patterns, reflecting the fact that the shear stiffness C_{44} need not equal $(C_{11} - C_{12})/2$.
- For a volume-preserving normal-strain pattern, one example is

$$\varepsilon_{yy} = \varepsilon_{zz} = -\tfrac{1}{2}\,\varepsilon_{xx}$$

This gives $\varepsilon_{xx} + \varepsilon_{yy} + \varepsilon_{zz} = 0$, so the volume strain is zero to first order. The two characteristic shear-related stiffnesses in a cubic crystal are C_{44} and $(C_{11} - C_{12})/2$.



8. Uniaxial Strain versus Uniaxial Stress

These two conditions must be distinguished.

8.1 Uniaxial strain (lateral strains constrained)

If ε_{xx} is nonzero but $\varepsilon_{yy} = \varepsilon_{zz} = 0$, then

$$\sigma_{xx} = C_{11}\,\varepsilon_{xx}$$

This is a constrained deformation: lateral strains are prevented, and nonzero lateral stresses may be required to maintain the constraint. The energy density for this strain state is $u = \tfrac{1}{2} C_{11}\,\varepsilon_{xx}^2$.

8.2 Uniaxial stress (lateral surfaces free)

For a specimen under uniaxial stress along x with free lateral surfaces, $\sigma_{yy} = \sigma_{zz} = 0$. The material generally develops lateral strains $\varepsilon_{\gamma\gamma}$ and εzz. In this case, Young's modulus is the ratio of axial stress to axial strain:

$$Y = \sigma_{xx}/\varepsilon_{xx}$$

Therefore, C_{11} is not generally equal to Young's modulus. This distinction is important when interpreting experiments and elastic constants.

9. Young's Modulus and Poisson's Ratio

Consider a crystal stretched or compressed along the x direction. If the lateral surfaces are free of stress, the crystal can change dimensions in the y and z directions as well.

$$\sigma_{yy} = \sigma_{zz} = 0$$

By symmetry, $\varepsilon_{yy} = \varepsilon_{zz}$. Applying these conditions to the cubic stress–strain equations leads to the expressions for Y and ν.

Young's modulus is

$$Y = \sigma_{xx}/\varepsilon_{xx}$$

Poisson's ratio describes the lateral strain relative to the axial strain. For loading along x,

$$\nu = -\varepsilon_{yy}/\varepsilon_{xx} = -\varepsilon_{zz}/\varepsilon_{xx}$$

The minus sign is used because a typical material contracts laterally when stretched longitudinally. For a cubic crystal under uniaxial stress with $\sigma_{yy} = \sigma_{zz} = 0$, the constants give

$$Y = (C_{11} - C_{12})(C_{11} + 2C_{12})/(C_{11} + C_{12})$$

$$\nu = C_{12}/(C_{11} + C_{12})$$

These expressions apply to a cubic crystal loaded along a cubic [100] direction under the stated uniaxial-stress conditions.

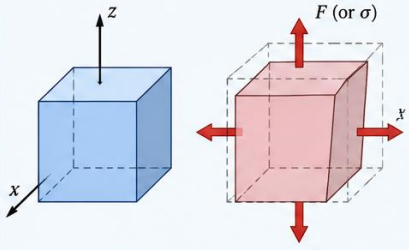
I recommend that you to watch these videos to better understand:

https://www.youtube.com/watch?v=NtTVEzZS3Bg

https://www.youtube.com/watch?v=UQ4GnWACesY

https://www.youtube.com/watch?v=5yZNKGxe0H8

(a) Deformation of a Crystal

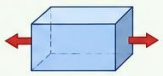


Original crystal (volume V_0)

Deformed crystal (volume $V = V_0 + \Delta V$)

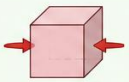
(b) Types of Strain

Normal strain (extension)



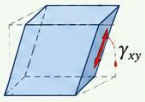
$$\varepsilon_{xx} = \frac{\Delta L}{L} \quad (\varepsilon_{xx} > 0)$$

Normal strain (compression)



$$\varepsilon_{xx} = \frac{\Delta L}{L} \quad (\varepsilon_{xx} < 0)$$

Shear strain



$$\gamma_{xy} = 2\varepsilon_{xy}$$

(γ_{xy} : engineering shear strain)

Volume strain (dilation)

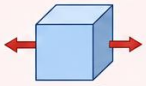
$$\delta = \frac{\Delta V}{V} \approx \varepsilon_{xx} + \varepsilon_{yy} + \varepsilon_{zz}$$

$\delta > 0$: expansion

$\delta < 0$: compression

(c) Types of Stress

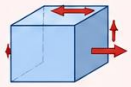
Normal stress (σ_{xx})



$$\sigma_{xx} = \frac{F}{A}$$

(tensile or compressive)

Shear stress (σ_{xy})



$$\sigma_{xy} = \frac{F}{A}$$

(tangential to surface)

Stress tensor (second-rank tensor)

$$\sigma_{ij} = \begin{pmatrix} \sigma_{xx} & \sigma_{xy} & \sigma_{xz} \\ \sigma_{yx} & \sigma_{yy} & \sigma_{yz} \\ \sigma_{zx} & \sigma_{zy} & \sigma_{zz} \end{pmatrix} \qquad \sigma_{ij} = \sigma_{ji}$$

(6 independent components)

(d) Generalized Hooke's Law

Tensor notation (general form)

$$\sigma_{ij} = C_{ijkl}\varepsilon_{kl}$$

σ_{ij} : stress tensor

ε_{kl} : strain tensor

C_{ijkl} : fourth-rank elastic stiffness tensor

Voigt notation (6 × 6 matrix form)

$$\sigma_i = \sum_j C_{ij}\varepsilon_j \qquad (i, j = 1, \ldots, 6)$$

$$\begin{pmatrix} \sigma_1 \\ \sigma_2 \\ \sigma_3 \\ \sigma_4 \\ \sigma_5 \\ \sigma_6 \end{pmatrix} = \begin{pmatrix} C_{11} & C_{12} & C_{13} & C_{14} & C_{15} & C_{16} \\ C_{21} & C_{22} & C_{23} & C_{24} & C_{25} & C_{26} \\ C_{31} & C_{32} & C_{33} & C_{34} & C_{35} & C_{36} \\ C_{41} & C_{42} & C_{43} & C_{44} & C_{45} & C_{46} \\ C_{51} & C_{52} & C_{53} & C_{54} & C_{55} & C_{56} \\ C_{61} & C_{62} & C_{63} & C_{64} & C_{65} & C_{66} \end{pmatrix} \begin{pmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \varepsilon_3 \\ \varepsilon_4 \\ \varepsilon_5 \\ \varepsilon_6 \end{pmatrix}$$

$\varepsilon_1 = \varepsilon_{xx}$, $\varepsilon_2 = \varepsilon_{yy}$, $\varepsilon_3 = \varepsilon_{zz}$, $\varepsilon_4 = \gamma_{yz}$, $\varepsilon_5 = \gamma_{xz}$, $\varepsilon_6 = \gamma_{xy}$

(e) Elastic Strain Energy

For linear elastic behavior, the strain-energy density is

$$u = \frac{1}{2}\sum_i \varepsilon_i\sigma_i = \frac{1}{2}\sum_{ij} \varepsilon_i C_{ij}\varepsilon_j$$

u : energy per unit volume (J m^{-3}) – same unit as pressure (Pa)

Total elastic energy for a uniformly strained volume V:

$$U = u\,V$$

(f) Cubic Crystal: Elastic Constants and Examples

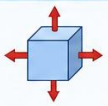
Cubic stiffness matrix (Voigt notation)

$$C_{ij} = \begin{pmatrix} C_{11} & C_{12} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{11} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{12} & C_{11} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & C_{44} \end{pmatrix}$$

Three independent elastic constants

- C_{11} : normal stiffness
- C_{12} : coupling between normal strains
- C_{44} : shear stiffness

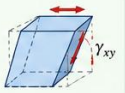
Bulk modulus (hydrostatic compression)



$$\varepsilon_{xx} = \varepsilon_{yy} = \varepsilon_{zz} = \frac{\delta}{3}$$

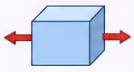
$$B = \frac{1}{3}(C_{11} + 2C_{12})$$

Shear deformation



$$\sigma_{xy} = C_{44}\gamma_{xy}$$

Uniaxial stress (Young's modulus)



$$\sigma_{xx} \neq 0, \quad \sigma_{yy} = \sigma_{zz} = 0$$

$$Y = \frac{(C_{11} - C_{12})(C_{11} + 2C_{12})}{C_{11} + C_{12}}$$

$$\nu = \frac{C_{12}}{C_{11} + C_{12}}$$