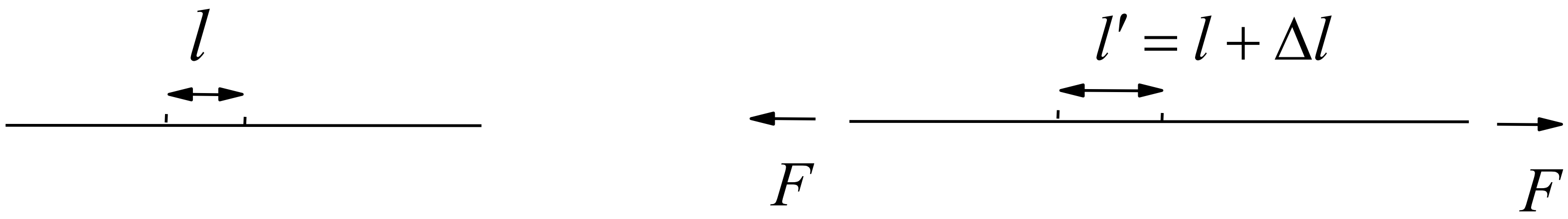
Lecture 5 (week 5: 17-18 March 2025)

Elastic response

- Hook's law for anisotropic materials
- Neumann principle application in 4th rank tensors
- Tensor and matrix forms for elasticity constants

Elastic response of solids

Deformation in 1 dimension



Hook’s law

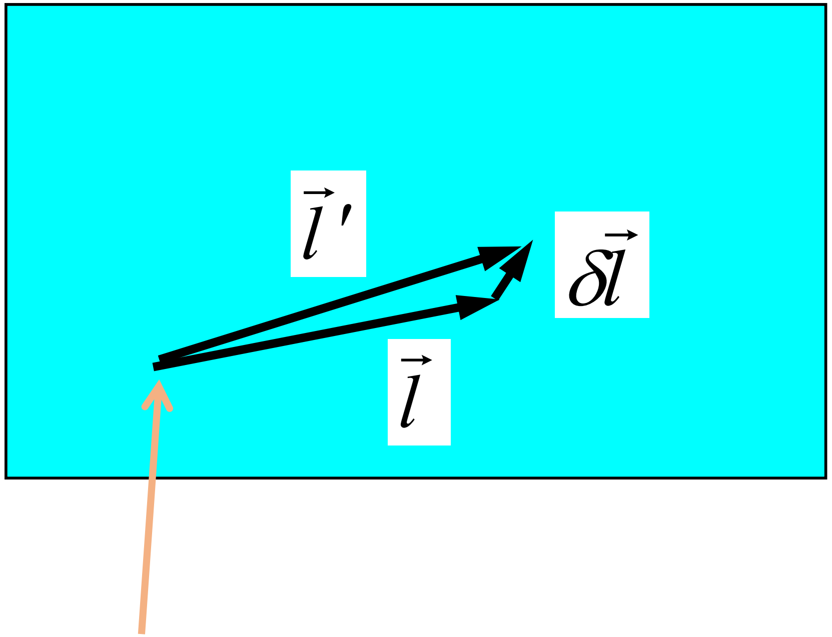
$$\frac{\Delta l}{l} = \varepsilon$$

$$\varepsilon << 1$$

$$\varepsilon = sF$$

Motion of material under the strain

Change of a vector under small strain



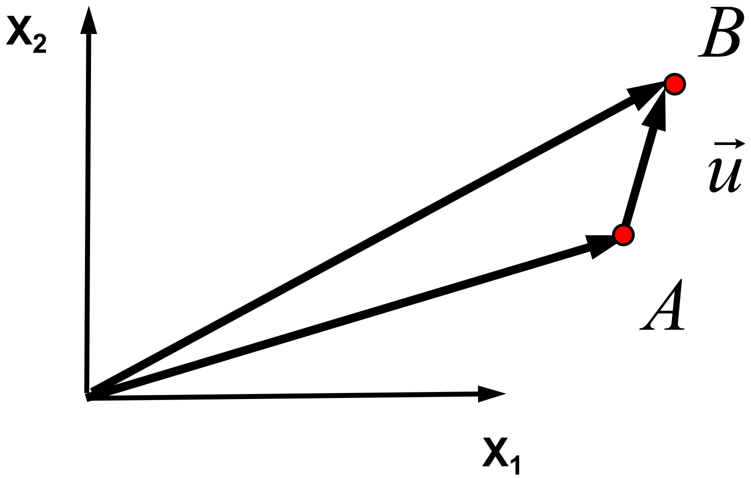
Immobile point

$$\vec{l} \xrightarrow{\varepsilon_{ij}} \vec{l}\,'$$

$$\delta l_i = \varepsilon_{ij} l_j \qquad |\varepsilon_{ij}| << 1$$

Strain is a second rank tensor

Motion of material under the strain



$\vec{u}$ **vector displacement**

$$\varepsilon_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)$$

$$\varepsilon_{ij} = \varepsilon_{ji}$$

A position of a point without strain

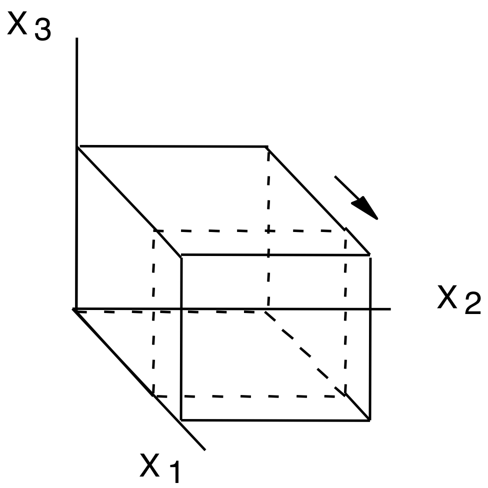
B position of the point under the strain ε_{ij}

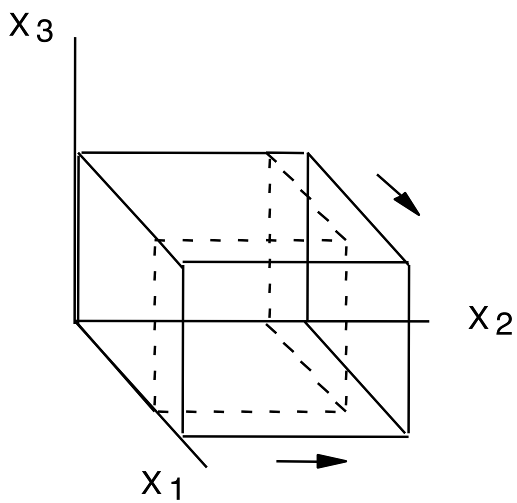
$$\frac{\Delta l}{l} = A(\vec{n}) = n_i \varepsilon_{ij} n_j$$

Strain tensor: symmetric 2nd rank tensor

Note: as shown in Lect. 4, similarly $K_{eff} = n_i K_{ij} n_j$

Example – tensile strain

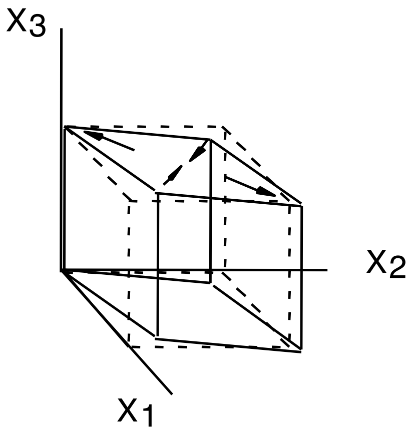




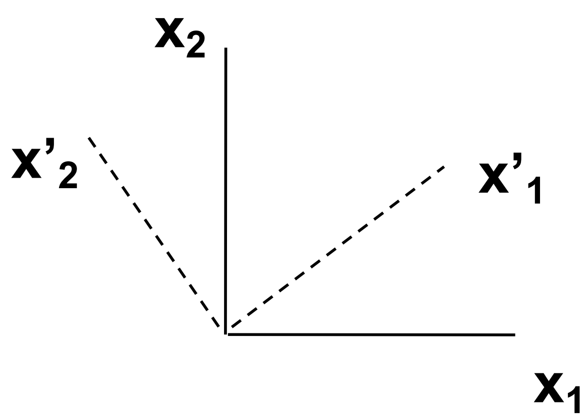
$$\varepsilon_{ij} = \begin{pmatrix} a & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

$$\varepsilon_{ij} = \begin{pmatrix} a & 0 & 0 \\ 0 & b & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

Example – shear strain



In 45^0-rotated frame (principal axes of the strain tensor)



$$\varepsilon_{ij} = \begin{pmatrix} 0 & b & 0 \\ b & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

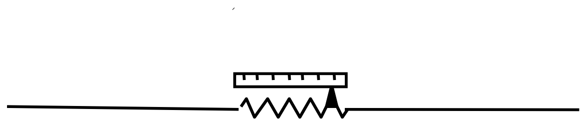
$$\varepsilon'_{ij} = \begin{pmatrix} b & 0 & 0 \\ 0 & -b & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

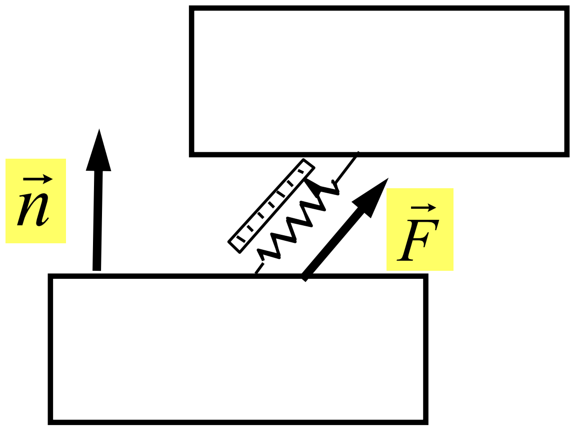
$$\delta l_i = \varepsilon_{ij} l_j$$

Stress tensor

1 dimension

3 dimensions





$$f_i = F_i / S$$

Force

$$F$$

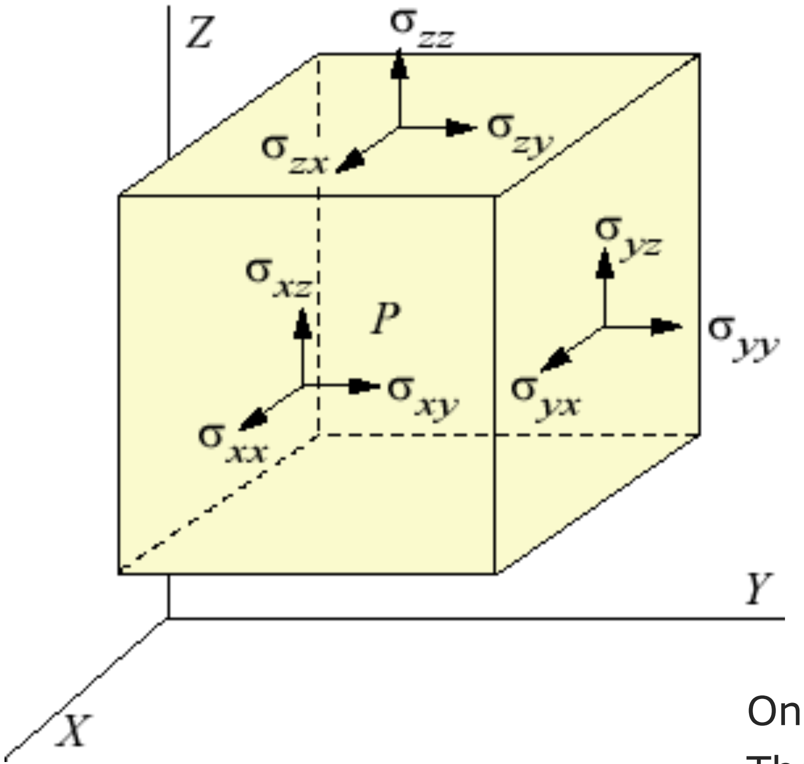
Stress tensor

$$f_i = \sigma_{ij} n_j$$

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

Symmetric
2nd rank tensor

Stress tensor



$$\begin{bmatrix} \sigma_{xx} & \sigma_{xy} & \sigma_{xz} \\ \sigma_{yx} & \sigma_{yy} & \sigma_{yz} \\ \sigma_{zx} & \sigma_{zy} & \sigma_{zz} \end{bmatrix}$$

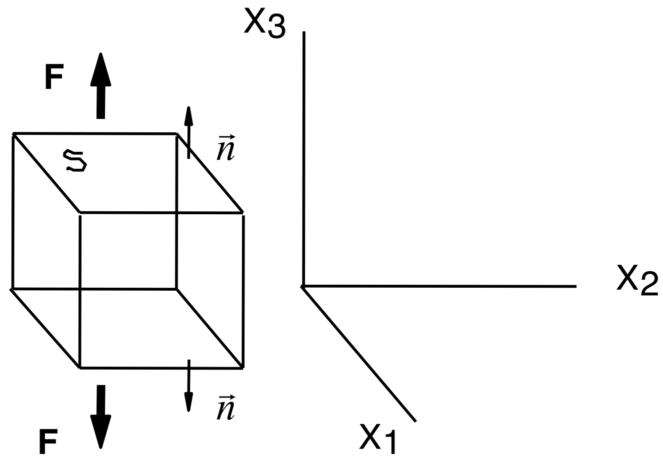
One suffix refers to the direction of the force

The other suffix – to the normal to the face on which the force acts

Symmetry: Shear stresses across the diagonal are identical (i.e. $\sigma_{xy} = \sigma_{yx}$, $\sigma_{yz} = \sigma_{zy}$, and $\sigma_{zx} = \sigma_{xz}$) as a result of static equilibrium (no net moment).

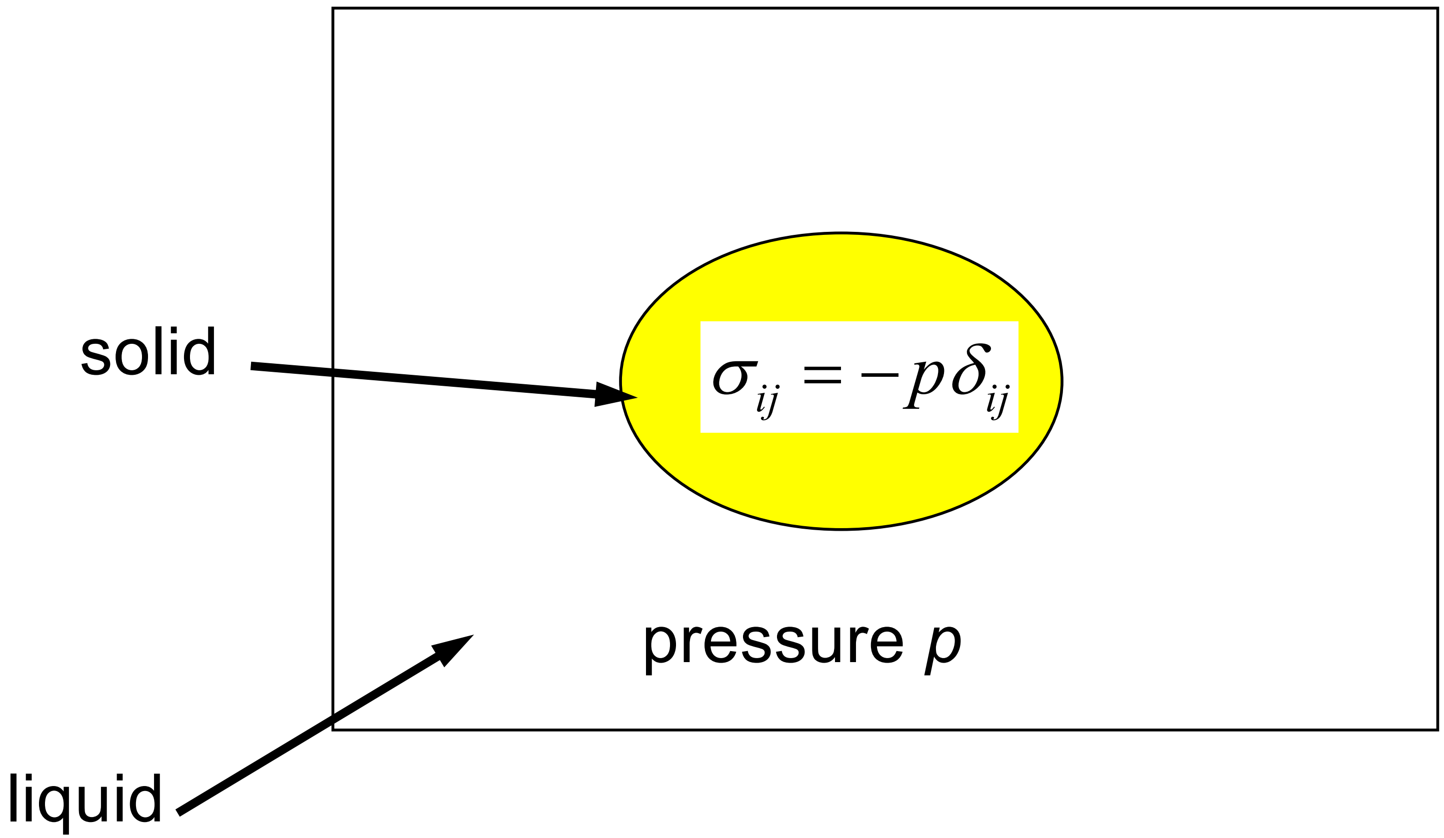
Stress tensor

Example- uniaxial stress



$$\sigma_{ij} = \begin{pmatrix} 0 & 0 & 0 \\ & 0 & 0 \\ & & F/S \end{pmatrix}$$

Example- hydrostatic pressure



Elastic response of solids

Stain tensor

$$\delta l_i = \varepsilon_{ij} l_j$$

Stress tensor

$$f_i = \sigma_{ij} n_j$$

Hook's law

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

Compliance tensor

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

Stiffness tensor
Young's modulus

Elastic response of solids

Strain tensor	$\varepsilon_{ij} = \varepsilon_{ji}$	**symmetric**
Stress tensor	$\sigma_{ij} = \sigma_{ji}$	**symmetric**
Compliance tensor	$s_{\underline{ij}kl} = s_{\underline{ji}kl}$ $s_{ij\underline{kl}} = s_{ij\underline{lk}}$ $s_{\underline{ij}\,\underline{kl}} = s_{\underline{kl}\,\underline{ij}}$	**symmetric × 3**
Stiffness tensor	$c_{\underline{ij}kl} = c_{\underline{ji}kl}$ $c_{ij\underline{kl}} = c_{ij\underline{lk}}$ $c_{\underline{ij}\,\underline{kl}} = c_{\underline{kl}\,\underline{ij}}$	**symmetric × 3** **(Thermodynamics)**

Matrix description (Voigt notations)

Stress tensor

$$\begin{pmatrix} \sigma_{11} & \sigma_{12} & \sigma_{13} \\ & \sigma_{22} & \sigma_{23} \\ & & \sigma_{33} \end{pmatrix} \Rightarrow \begin{pmatrix} \sigma_1 \\ \sigma_2 \\ \sigma_3 \\ \sigma_4 \\ \sigma_5 \\ \sigma_6 \end{pmatrix}$$

Strain tensor

$$\begin{pmatrix} \varepsilon_{11} & \varepsilon_{12} & \varepsilon_{13} \\ & \varepsilon_{22} & \varepsilon_{23} \\ & & \varepsilon_{33} \end{pmatrix} \Rightarrow \begin{pmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \varepsilon_3 \\ \varepsilon_4 = 2\varepsilon_{23} \\ \varepsilon_5 = 2\varepsilon_{13} \\ \varepsilon_6 = 2\varepsilon_{12} \end{pmatrix}$$

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

$$\sigma_n = c_{nm}\varepsilon_m$$

21 independent components

$$\boxed{\begin{array}{l} \vec{\varepsilon} = \underline{s}\vec{\sigma} \quad ou \quad \vec{\sigma} = \underline{c}\vec{\varepsilon} \\ c_{nm} = c_{mn}, \quad s_{nm} = s_{mn} \end{array}}$$

Matrix description

Stiffness tensor

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

$$\sigma_n = c_{nm}\varepsilon_m$$

$$c_{ijkl} = c_{nm}$$

$$m, n = 1.....6$$

Compliance tensor

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

$$\varepsilon_n = s_{nm}\sigma_m$$

$$s_{ijkl} = s_{nm}$$ $m, n = 1, 2, 3$

$$s_{ijkl} = s_{nm}/2$$ one suffix 1, 2, 3 and one suffix 4, 5, 6

$$s_{ijkl} = s_{nm}/4$$ both suffixes 4, 5, 6

Matrix description

$$\vec{\varepsilon} = \underline{s}\vec{\sigma} \quad ou \quad \vec{\sigma} = \underline{c}\vec{\varepsilon}$$

$$\begin{pmatrix} c_{11} & c_{12} & c_{13} & c_{14} & c_{15} & c_{16} \\ c_{21} & c_{22} & c_{23} & c_{24} & c_{25} & c_{26} \\ c_{31} & c_{32} & c_{33} & c_{34} & c_{35} & c_{36} \\ c_{41} & c_{42} & c_{43} & c_{44} & c_{45} & c_{46} \\ c_{51} & c_{52} & c_{53} & c_{54} & c_{55} & c_{56} \\ c_{61} & c_{62} & c_{63} & c_{64} & c_{65} & c_{66} \end{pmatrix} = \begin{pmatrix} c_{1111} & c_{1122} & c_{1133} & c_{1123} & c_{1113} & c_{1112} \\ c_{1122} & c_{2222} & c_{2233} & c_{2223} & c_{2213} & c_{2212} \\ c_{1133} & c_{2233} & c_{3333} & c_{3323} & c_{3313} & c_{3312} \\ c_{1123} & c_{2223} & c_{3323} & c_{2323} & c_{2313} & c_{2312} \\ c_{1113} & c_{2213} & c_{3313} & c_{2313} & c_{1313} & c_{1312} \\ c_{1112} & c_{2212} & c_{3312} & c_{2312} & c_{1312} & c_{1212} \end{pmatrix}$$

$$\begin{pmatrix} s_{11} & s_{12} & s_{13} & s_{14} & s_{15} & s_{16} \\ s_{21} & s_{22} & s_{23} & s_{24} & s_{25} & s_{26} \\ s_{31} & s_{32} & s_{33} & s_{34} & s_{35} & s_{36} \\ s_{41} & s_{42} & s_{43} & s_{44} & s_{45} & s_{46} \\ s_{51} & s_{52} & s_{53} & s_{54} & s_{55} & s_{56} \\ s_{61} & s_{62} & s_{63} & s_{64} & s_{65} & s_{66} \end{pmatrix} = \begin{pmatrix} s_{1111} & s_{1122} & s_{1133} & 2s_{1123} & 2s_{1113} & 2s_{1112} \\ s_{1122} & s_{2222} & s_{2233} & 2s_{2223} & 2s_{2213} & 2s_{2212} \\ s_{1133} & s_{2233} & s_{3333} & 2s_{3323} & 2s_{3313} & 2s_{3312} \\ 2s_{1123} & 2s_{2223} & 2s_{3323} & 4s_{2323} & 4s_{2313} & 4s_{2312} \\ 2s_{1113} & 2s_{2213} & 2s_{3313} & 4s_{2313} & 4s_{1313} & 4s_{1312} \\ 2s_{1112} & 2s_{2212} & 2s_{3312} & 4s_{2312} & 4s_{1312} & 4s_{1212} \end{pmatrix}$$

Matrix description

$$\vec{\varepsilon} = \underline{s}\vec{\sigma} \quad ou \quad \vec{\sigma} = \underline{c}\vec{\varepsilon}$$

Stiffness tensor **Compliance tensor**

$$c_{mn} = \begin{pmatrix} c_{11} & c_{12} & c_{13} & c_{14} & c_{15} & c_{16} \\ & c_{22} & c_{23} & c_{24} & c_{25} & c_{26} \\ & & c_{33} & c_{34} & c_{35} & c_{36} \\ & & & c_{44} & c_{45} & c_{46} \\ & & & & c_{55} & c_{56} \\ & & & & & c_{66} \end{pmatrix} \qquad s_{mn} = \begin{pmatrix} s_{11} & s_{12} & s_{13} & s_{14} & s_{15} & s_{16} \\ & s_{22} & s_{23} & s_{24} & s_{25} & s_{26} \\ & & s_{33} & s_{34} & s_{35} & s_{36} \\ & & & s_{44} & s_{45} & s_{46} \\ & & & & s_{55} & s_{56} \\ & & & & & s_{66} \end{pmatrix}$$

(36 - 6)/2 + 6 = 21 independent components

Examples: $c_{44} = c_{2323}$ $\qquad s_{44} = 4s_{2323}$

Stiffness – compliance relations

- we can combine the expressions for matrix C and S:

$\sigma = C\varepsilon$ and $\varepsilon = S\sigma$ to give:

$\sigma = CS\sigma$, which shows:

$I = CS$, or, $C = S^{-1}$ where I is identity matrix

- Note that the definition of Young's modulus $\boldsymbol{E_{33} = 1/S_{33}}$ does not mean that $\boldsymbol{E = C_{33}}$ because $\boldsymbol{C_{33} \neq 1/S_{33}}$

Young's moduli: $\boldsymbol{1/S_{11}}$ $\boldsymbol{1/S_{22}}$ $\boldsymbol{1/S_{33}}$

Poisson's ratio:

$\nu_{13} = -S_{13}/S_{11}$

S_{13}: the force applied to the face (001) and acting in the direction [001] causes the face (100) to move in the direction [100].

There are 6 different Poisson' ratios ν_{12} , ν_{13} ν_{23} , ν_{21} , ν_{31} ,ν_{32}

Neumann equations

$$c_{i'j'k'l'} = a_{i'i}(t_1)a_{j'j}(t_1)a_{k'k}(t_1)a_{l'l}(t_1)c_{ijkl}$$

$$c_{i'j'k'l'} = a_{i'i}(t_2)a_{j'j}(t_2)a_{k'k}(t_2)a_{l'l}(t_2)c_{ijkl}$$

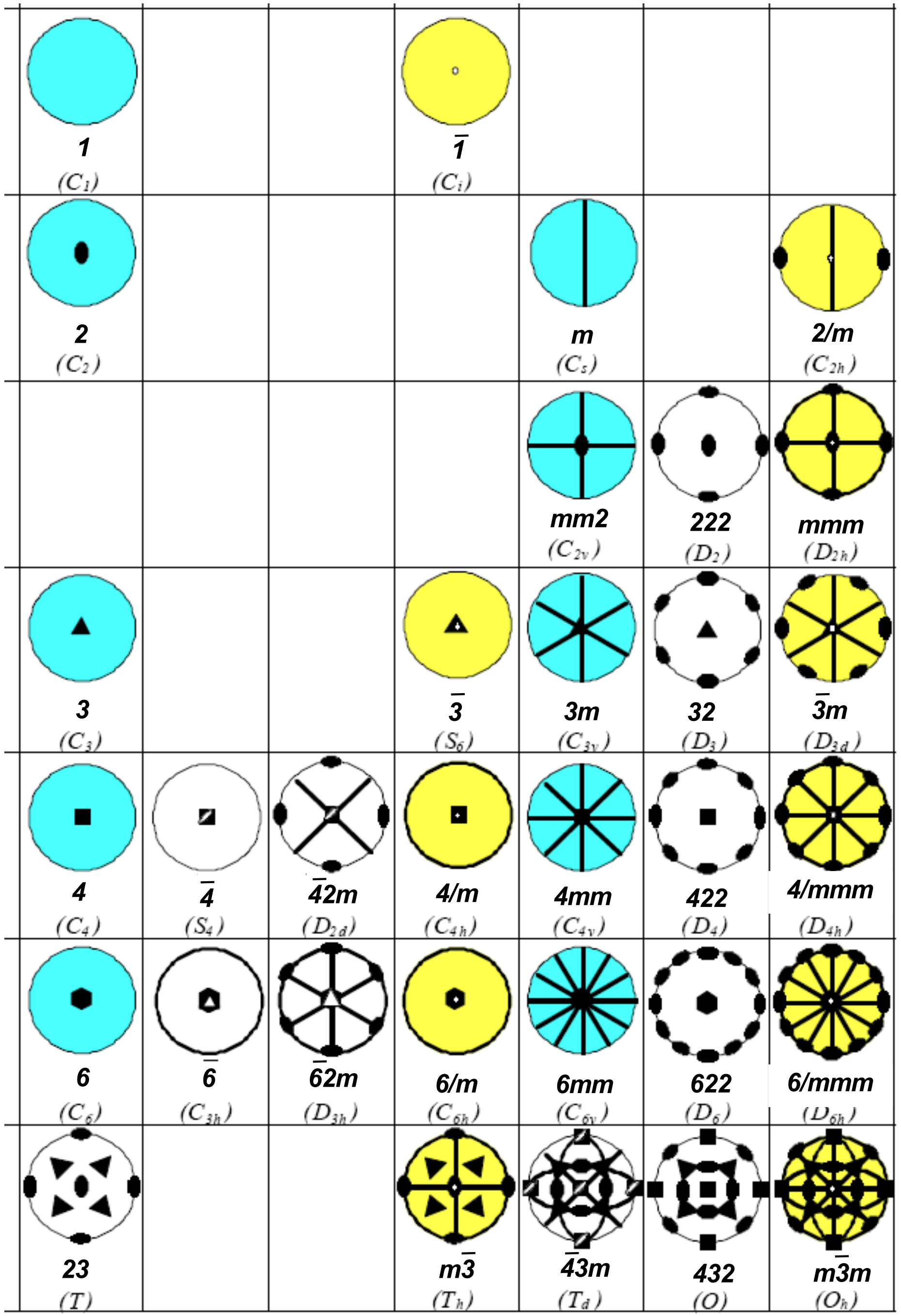
$$c_{i'j'k'l'} = a_{i'i}(t_3)a_{j'j}(t_3)a_{k'k}(t_3)a_{l'l}(t_3)c_{ijkl}$$

$$\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots$$

$$c_{i'j'k'l'} = a_{i'i}(t_n)a_{j'j}(t_n)a_{k'k}(t_n)a_{l'l}(t_n)c_{ijkl}$$

$t_1, t_2, t_3 \dots\dots t_n$ **- symmetry elements of the material**

Number of independent components



21 independent components

13

9

6-7

6-7

5

3

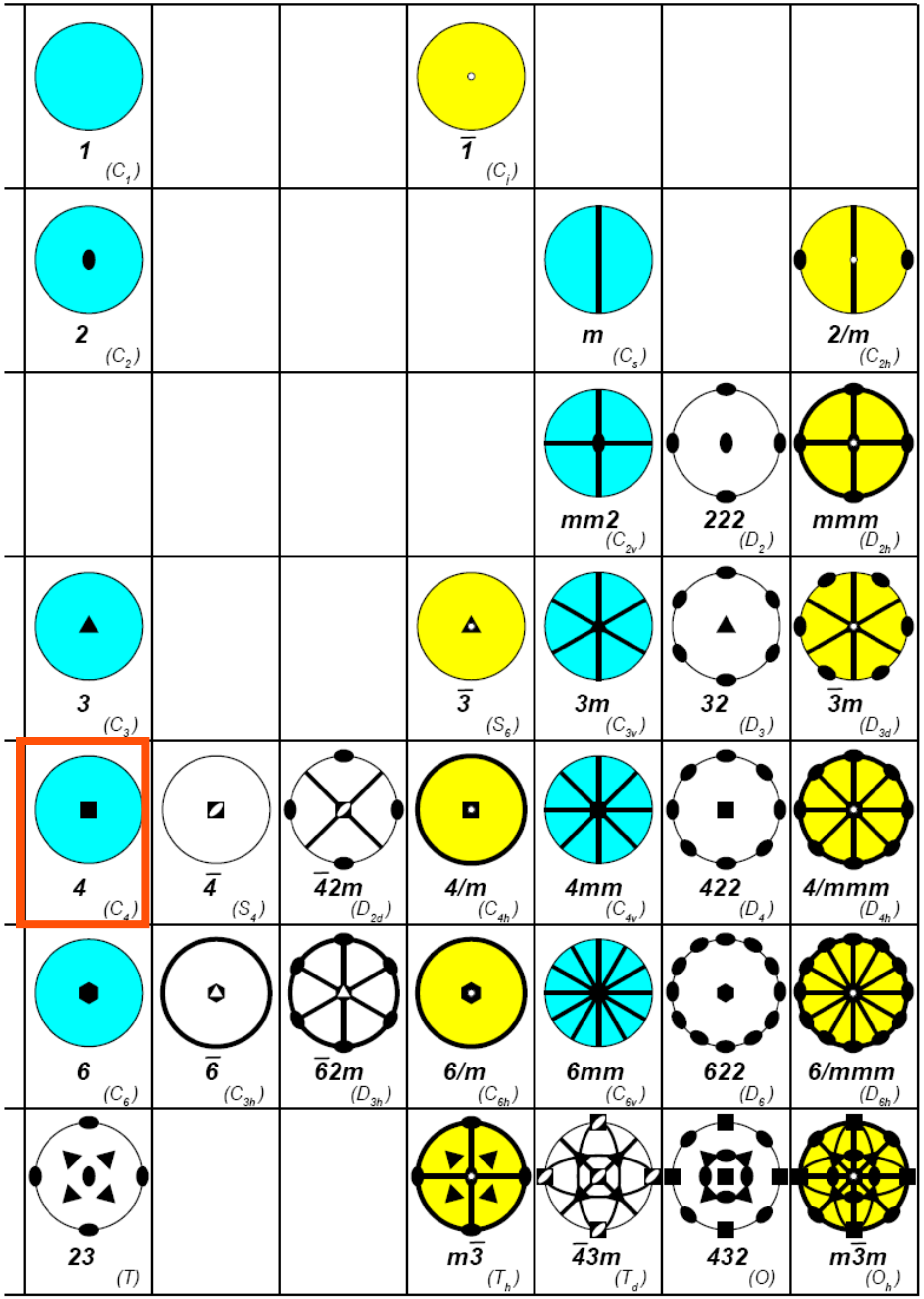
$\infty\infty$ $\quad$ $\infty\infty m$

2

∞ $\quad$ ∞m $\quad$ $\infty 2$

∞ / m $\quad$ ∞ / mm

Applications of Neumann equation



Example: group 4

Symmetry elements:

$90^0, 180^0$, and 270^0 rotations about OX_3 axis

Problem

$$c_{51} = ?$$

Applications of Neumann equation

Example: class 4

$$c_{51} = c_{1311}$$

$$\begin{pmatrix} \underset{1}{\sigma_{11}} & \overset{6}{\sigma_{12}} & \sigma_{13} \; 5 \\ & \underset{2}{\sigma_{22}} & \sigma_{23} \; 4 \\ & & \underset{3}{\sigma_{33}} \end{pmatrix}$$

180^0 rotation

$$p'_3 = p_3$$
$$p'_2 = -p_2$$
$$p'_1 = -p_1$$

$$p'_1\, p'_3 p'_1\, p'_1 = (-p_1)p_3(-p_1)(-p_1) = -p_1 p_3 p_1 p_1 \Rightarrow c'_{1311} = -c_{1311}$$

Neumann equation

$$c_{1311} = c'_{1311} \Longrightarrow c_{1311} = -c_{1311} \Longrightarrow c_{51} = c_{1311} = 0$$

$$c_{1311} = c_{1322} = c_{1333} = c_{1213} = c_{2311} = c_{2322} = c_{2333} = c_{2312} = 0$$

Applications of Neumann equation

Example: class 4

90° rotation:

$$c_{1111} = c_{2222}, \quad c_{2222} = c_{1111}, \quad c_{3333} = c_{3333},$$

$$c_{1212} = c_{2121}, \quad c_{1313} = c_{2323}, \quad c_{2323} = c_{1313},\ .$$

$$c_{1122} = c_{2211}, \quad c_{1133} = c_{2233}, \quad c_{2233} = c_{1133},$$

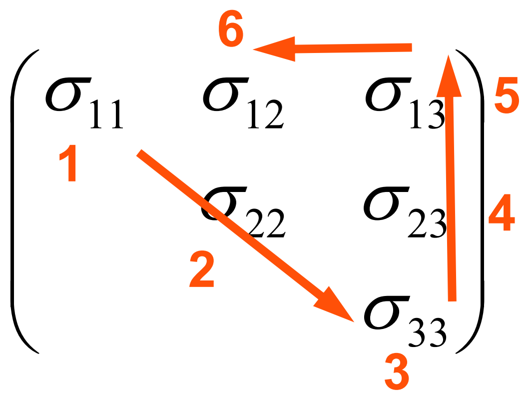
$$c_{1211} = -c_{2122}, \quad c_{1222} = -c_{2111}.$$

$$c_{1233} = -c_{2133}, \quad c_{2313} = -c_{1323}.$$

$$\boldsymbol{p'_1 = p_2}$$

$$\boldsymbol{p'_2 = -p_1}\ .$$

$$\boldsymbol{p'_3 = p_3}$$



$$\boxed{\begin{aligned} & c_{11} = c_{22},\ c_{33},\ c_{44} = c_{55},\ c_{66}, \\ & c_{12},\ c_{13} = c_{23},\ c_{61} = -c_{62} \end{aligned}}$$

11 different components, however only 7 are independent

Link:
material symmetry - property symmetry

39 groups of macroscopic symmetry

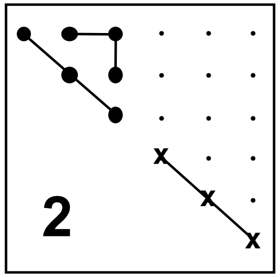
↓

10 structures of *c*-tensor and *s*-tensor in conventional axes

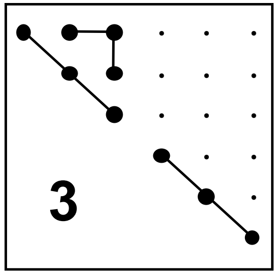
↓

8 types of symmetry of elastic response (elastic anisotropy)

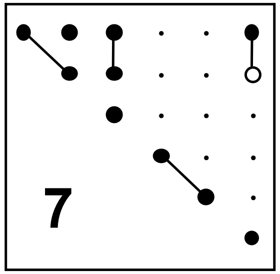
c and *s* tensors for all symmetries



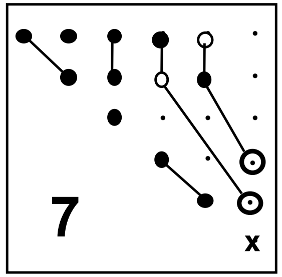
$\infty\infty, \infty\infty m$



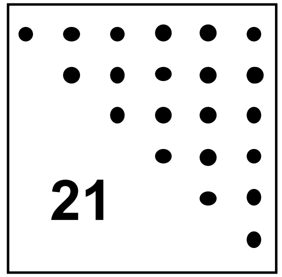
Cubic



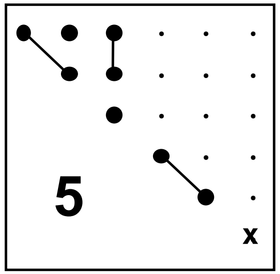
$4, \bar{4}, 4/m$



$3, \bar{3}$



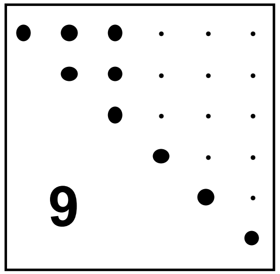
Triclinic



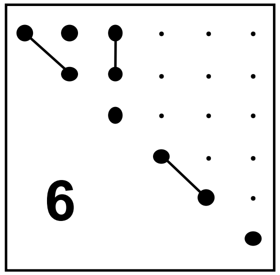
Hexagonal

$\infty, \infty m, \infty/2,$

$\infty/m, \infty/mmm$

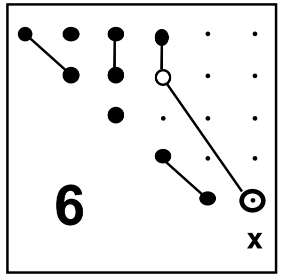


Orthorhombic

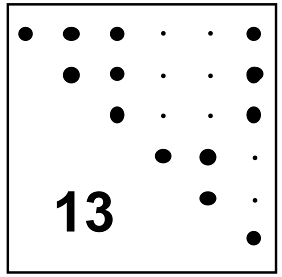


$4mm, \bar{4}2m,$

$422, 4/mmm$



$3m, \bar{3}m, 32$



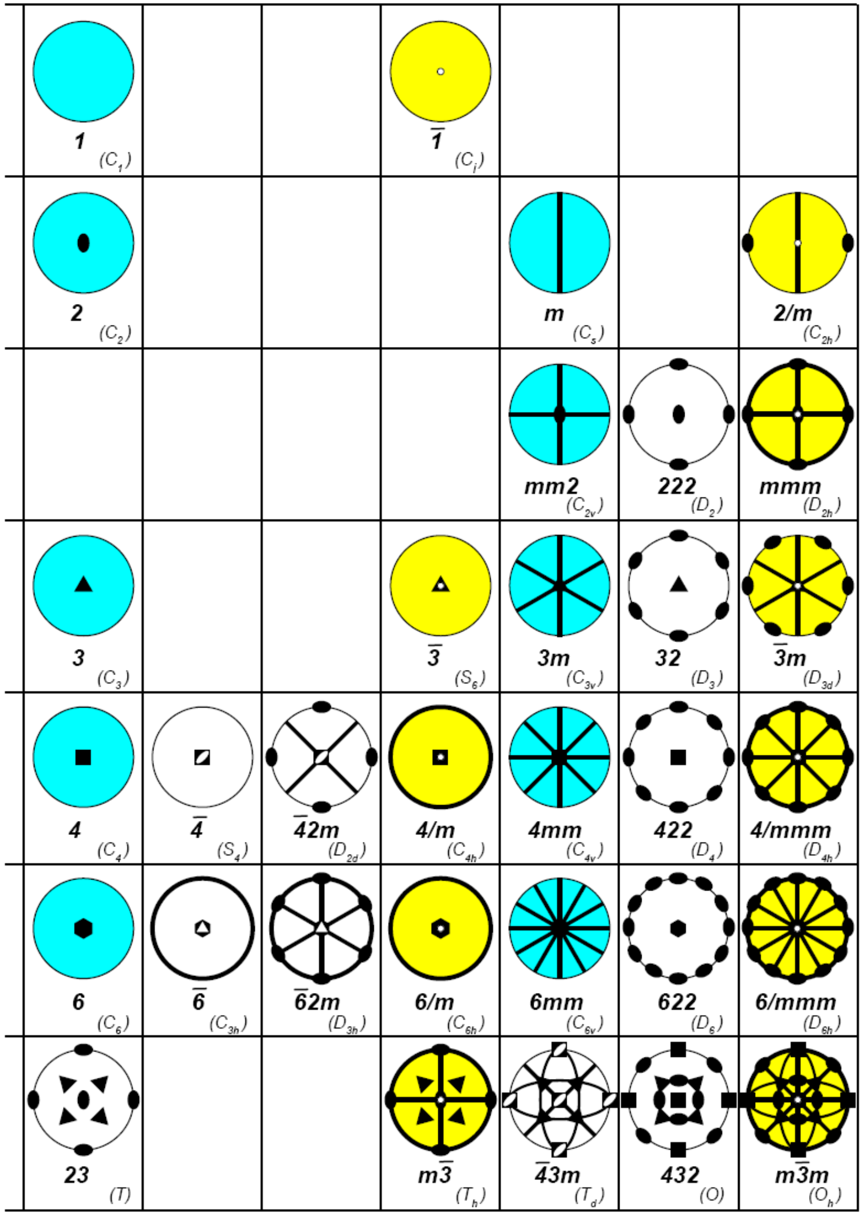
Monoclinic

● non-zero component, ⊙ a component equal to twice the heavy dot component to which it is joined,

●—● components numerically equal, ●—○ components numerically equal, but different in sign

for s x $2(s_{11} - s_{12})$, for c x $(c_{11} - c_{12})/2$

Effect of axis choice and symmetry of response



Isotropic medium

21	$\Rightarrow$	**18**	$\bar{1}$
13	$\Rightarrow$	**12**	$2/m$
		9	mmm
6-7	$\Rightarrow$	**6**	$\bar{3}m$
6-7	$\Rightarrow$	**6**	$4/mmm$
∞ ∞m ∞/m $\infty 2$ ∞/mm		**5**	∞/mm
		3	$m\bar{3}m$
$\infty\infty$ $\infty\infty m$		**2**	$\infty\infty m$

Sensitivity of tensors to material symmetry

4th rank *c*-tensor
is more sensitive to the material symmetry
than 2nd rank *K*-tensor

	K_{ij}	c_{ijkl}
$m\bar{3}m$	1	3
$\infty\infty m$	1	2

Number of independent components

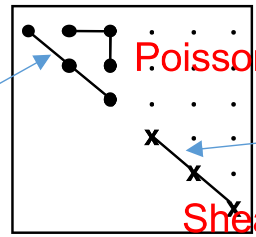
Elastic response: isotropic vs cubic materials

Isotropic material

Dielectric response

$$K_{ij} = K\delta_{ij}$$

Elastic response



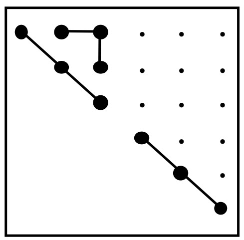
$$c_{44} = (c_{11} - c_{12})/2$$

Material of cubic symmetry

Dielectric response

$$K_{ij} = K\delta_{ij}$$

Elastic response



$$\begin{bmatrix} C_{11} & C_{12} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{11} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{12} & C_{11} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & C_{44} \end{bmatrix}$$

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Anisotropy in elasticity and thermodynamic properties of zirconium tetraboride under high pressure

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The recently predicted ZrB_4 with an *Amm*2 orthorhombic structure has great scientific and technical significance owing to its novel B–Zr–B "sandwich" layer bonding and evaluated high hardness. To better understand the performance of *Amm*2-ZrB_4, its elastic and thermodynamic properties under pressure and temperature are studied here by taking advantage of first principles calculations in combination with

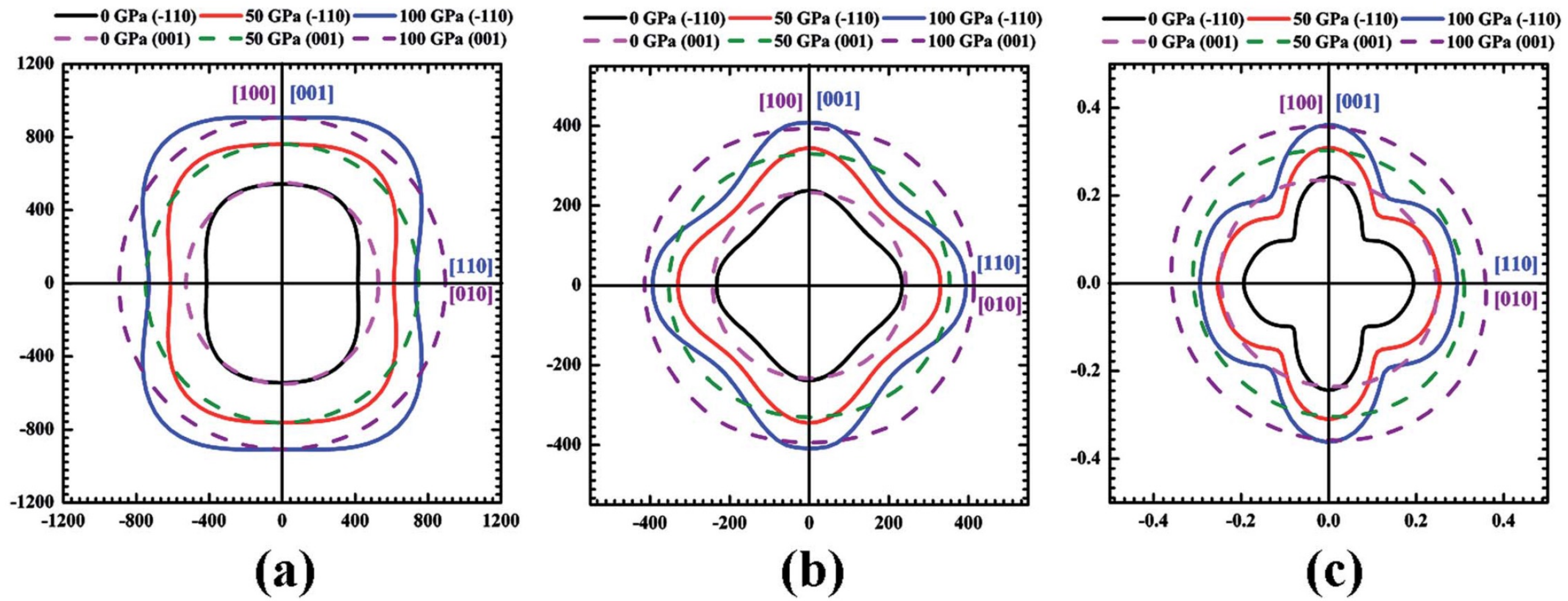


Fig. 3 The projections of Young's modulus *E* (a), shear modulus *G* (b) and Poisson's ratio υ (c) in (−110) plane and (001) plane at pressures 0 GPa, 50 GPa and 100 GPa respectively, the units are in GPa for *E* and *G*.

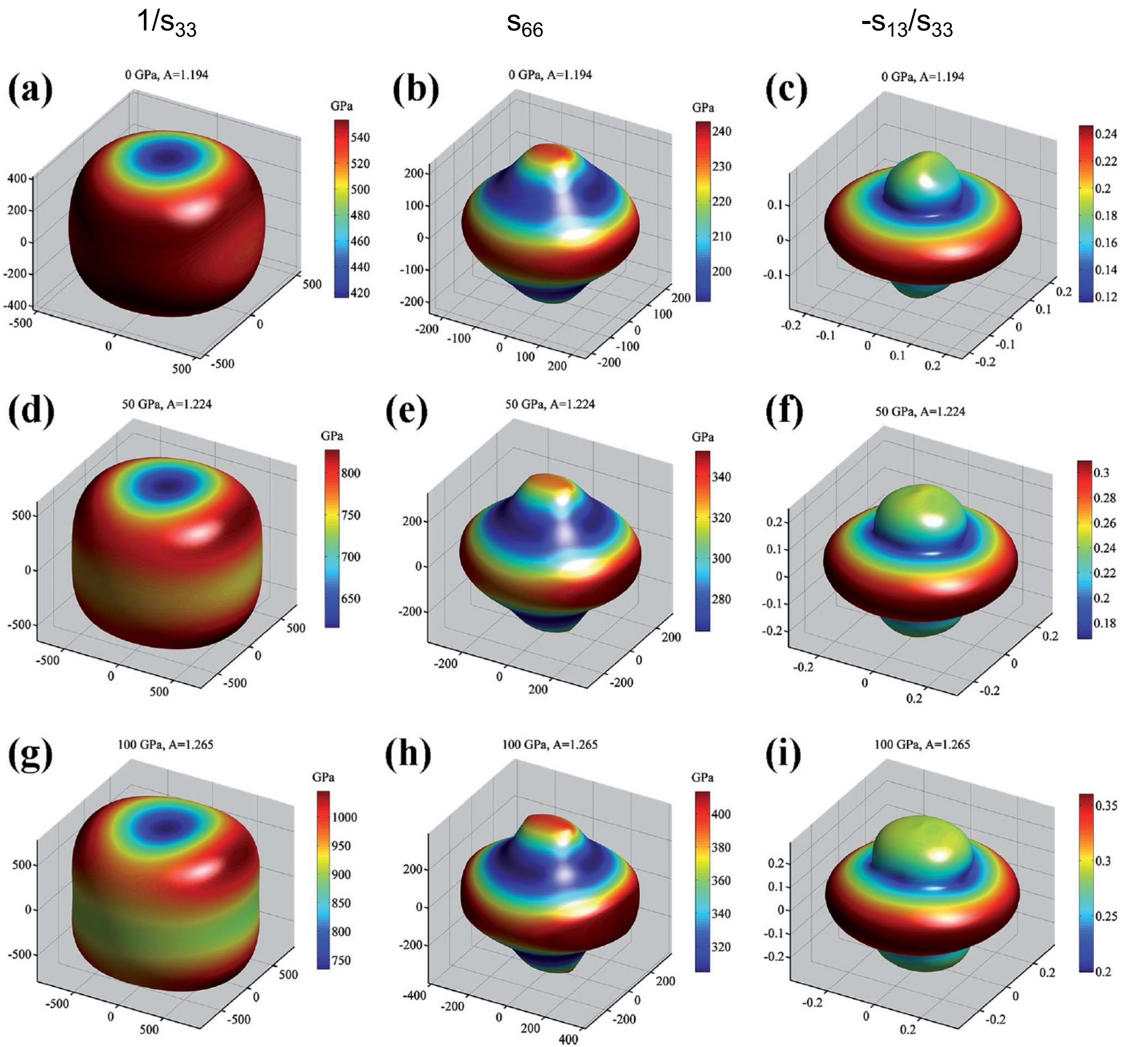
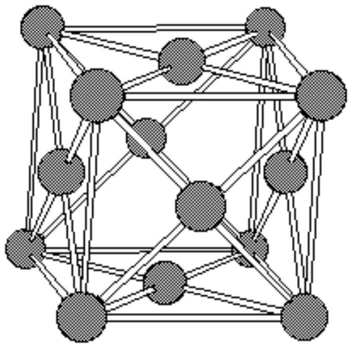
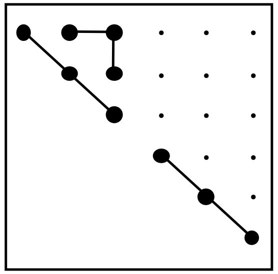


Fig. 2 Direction dependence of Young's modulus E (a), (d), (g), shear modulus G (b), (e), (h) and Poisson's ratio υ (c), (f), (i) under different pressures for ZrB_4, the units are in GPa for E and G.

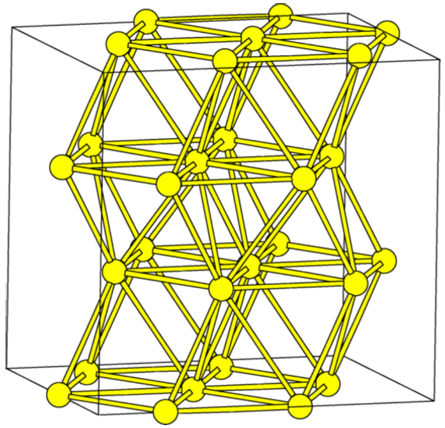
Elastic response: examples of materials

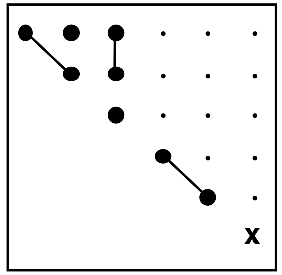
Cu $m\bar{3}m$





Zn $6/mmm$





$$s_{66} = 2(s_{11} - s_{12})$$

$$s_{11} = 1.49 \quad s_{12} = -0.63 \quad s_{44} = 1.33$$

$$s_{11} = 0.84 \quad s_{12} = 0.11 \quad s_{44} = 2.64$$

$$s_{33} = 2.87 \quad s_{13} = -0.78$$

Units → $10^{-11} m^2/N$

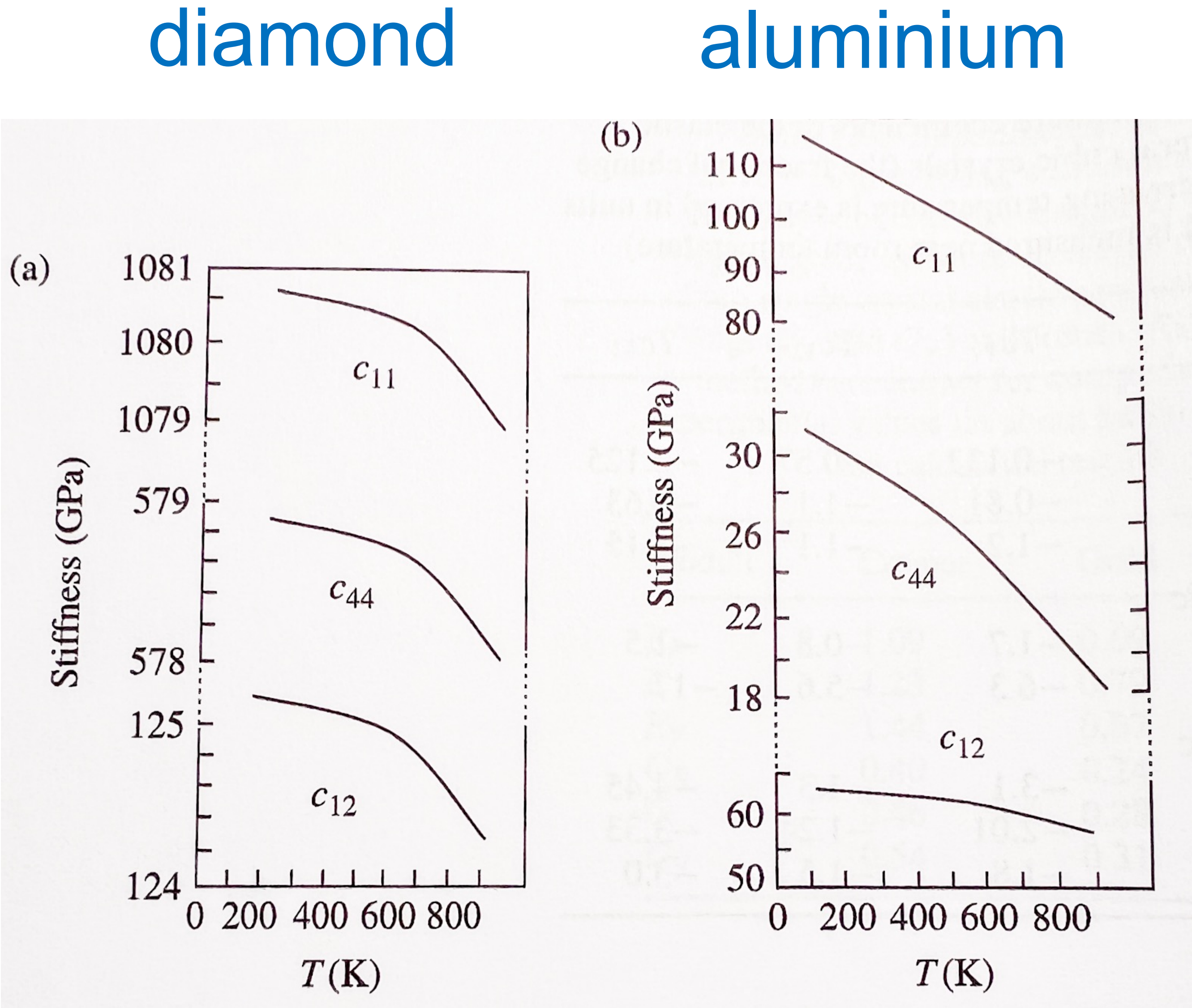
Stiffness coefficients for cubic materials

Material class	Material	C_{11} (10^{10} N/m^2)	C_{12} (10^{10} N/m^2)	C_{44} (10^{10} N/m^2)	Anisotropy ratio $(C_{11} - C_{12})/2C_{44}$
Metals	Ag	12.4	9.3	4.6	0.34
	Al	10.8	6.1	2.9	0.81
	Au	18.6	15.7	4.2	0.35
	Cu	16.8	12.1	7.5	0.31
	α-Fe	23.7	14.1	11.6	0.41
	Mo	46.0	17.6	11.0	1.29
	Na	0.73	0.63	0.42	0.12
	Ni	24.7	14.7	12.5	0.40
	Pb	5.0	4.2	1.5	0.27
	W	50.1	19.8	15.1	1.00
Covalent solids	Si	16.6	6.4	8.0	0.64
	Diamond	107.6	12.5	57.6	0.83
	TiC	51.2	11.0	17.7	1.14
Ionic solids	LiF	11.2	4.6	6.3	0.52
	MgO	29.1	9.0	15.5	0.65
	NaCl	4.9	1.3	1.3	1.38

Table 2.2
Stiffness coefficients for selected cubic materials

Stiffness generally decreases with the temperature increase

- the effect increases with the bond length



Compressibility of solids under hydrostatic pressure

K= -1/V (dV/dp),

K- coimpressibility, V – volume, p-hydrostatic pressure

- The change in volume per unit volume is equal to ε_{ii}

$\varepsilon_{ii} = \varepsilon_{11} + \varepsilon_{22} + \varepsilon_{33}$

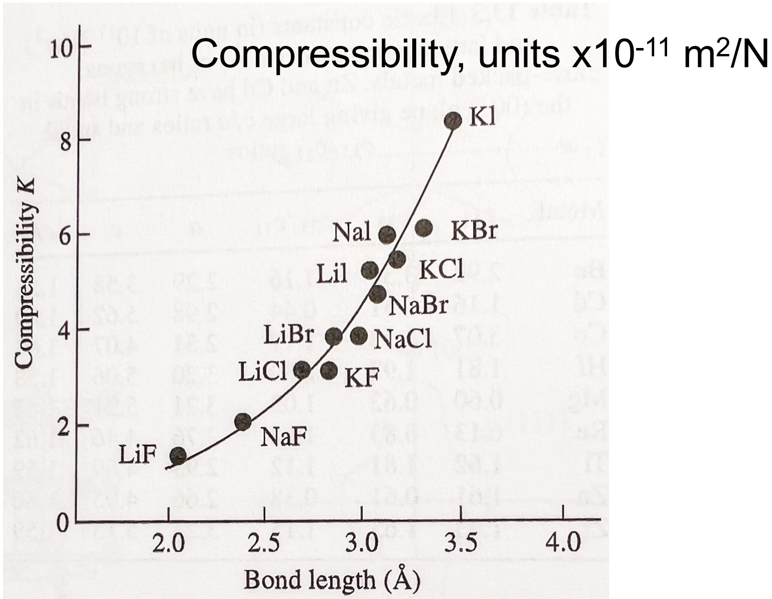
ε_{ii} can be expressed through elastic compliance moduli:

$\varepsilon_{ii} = s_{iikl}\sigma_{kl} = -\, s_{iikl}\, p\, \delta_{kl}$

Compressibility is $K = s_{iikk}$

Compressibility increases

with the bond length



Essential

1. The elastic response can be successfully treated with the Neumann principle.

2. The symmetry of the elastic response is often higher than that of the material.

3. The elastic response is controlled by a 4^{th} rank tensor. It is more sensitive to the material symmetry than the dielectric response controlled by a 2^{nd} rank tensor.