

## **Single-crystal elasticity**

### **Assigned Reading:**

Nye JF (1957) *Physical Properties of Crystals*. Oxford University Press, Oxford, UK (Chapters 5 and 6).

Nye, J. F. "Elastic behavior of single crystals: Anisotropy", pp. 2415-2423, in *Encyclopedia of Materials: Science and Technology*, Elsevier Science, 2001 (<http://www.elsevier.com/mrwclus/15/show/Main.htm>) From MIT campus.

### **Resource reading (If you would like to brush up on stress, strain, and elasticity):**

Malvern LE (1969) *Introduction to the Mechanics of a Continuous Medium*. Prentice Hall, Englewood Cliffs, NJ. (A rigorous introduction to continuum mechanics.)

Oertel G (1996) *Stress and Deformation: A handbook on Tensors in Geology*. Oxford University Press, New York. (Many problems on which to practice.)

## Elasticity

### *Elastic and inelastic behavior*

For small strains at constant temperatures, the amount of strain is determined by the magnitude of the stress causing it.

#### *Perfectly Elastic:*

Purely elastic behavior implies thermodynamic reversibility. All the work put into deforming the body is recoverable. Deformation is not time-dependent.

The relation between stress and strain may be linear or non-linear.

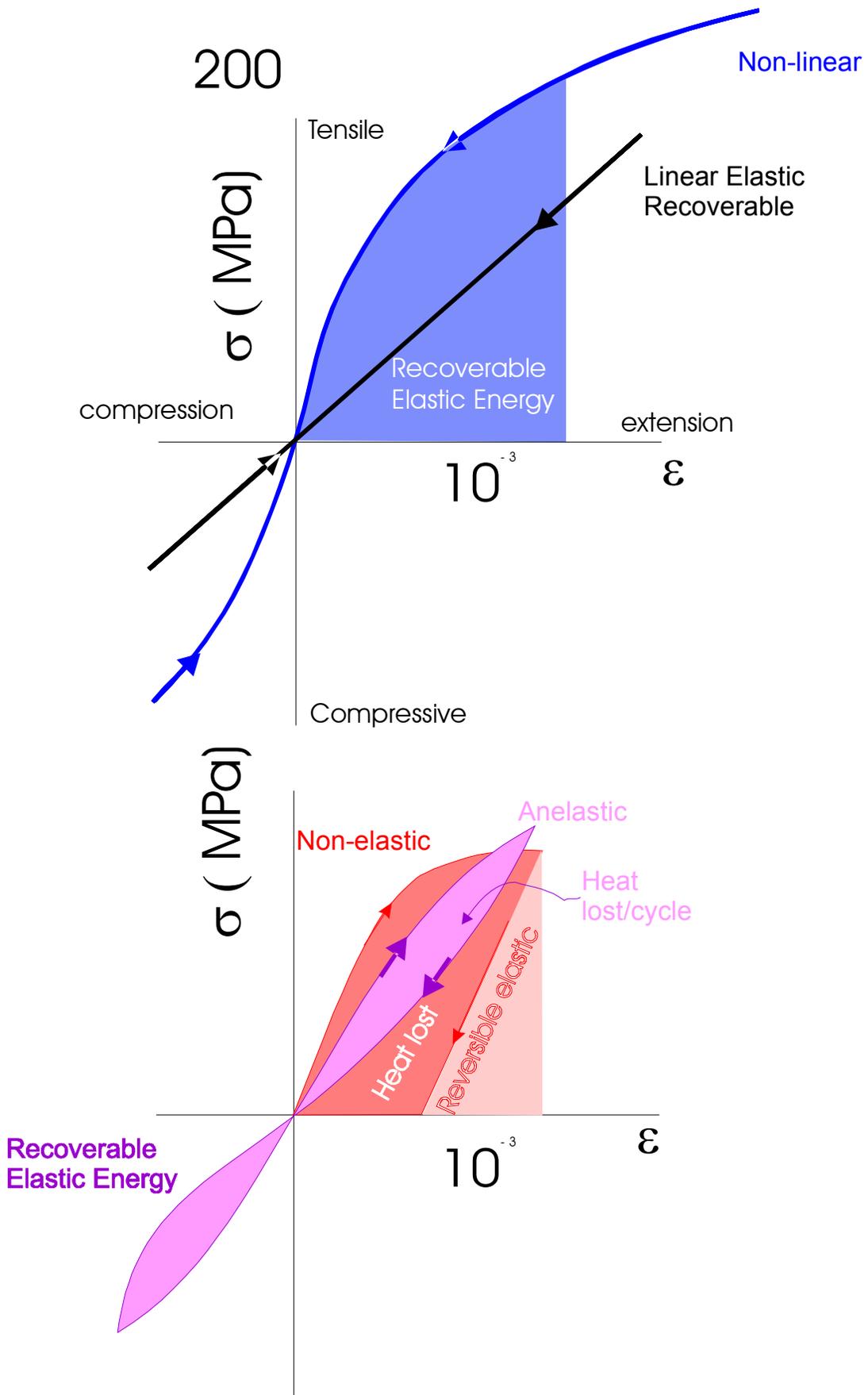
#### *Anelastic:*

Time-dependent behavior in which the material strain is recoverable

#### *Plastic and viscoplastic behavior:*

When a material is deformed to large strains, some of the strain is permanent and not recoverable; this permanent strain is plastic (if time independent) or viscoplastic (if time dependent).

Elastic		Recoverable	Time-independent	Linear
				Nonlinear
Inelastic	Anelastic	Part. Recov.	Time-dependent	Lin or Non-lin.
	Plastic	Not recover.	Time-indep.	"
	Visco-plas.	"	time-dep	"



## **Anisotropic (Single Crystal) Elasticity**

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### Coordinate Conventions for Elasticity Tensor

The exact values of the elasticity tensor depend on the definition of the coordinate system.

The convention used is that the moduli are referred to an orthonormal coordinate systems,  $x_1, x_2, x_3$ , with unit vectors,  $\hat{\mathbf{e}}_1, \dots$ . These axes are related to the mineral lattice vectors by the following convention

Monoclinic	$\hat{\mathbf{e}}_2 \parallel \mathbf{b}$
Tetragonal, trigonal, hexagonal	$\hat{\mathbf{e}}_1 \parallel \mathbf{a}, \hat{\mathbf{e}}_3 \parallel \mathbf{c},$
Orthorhombic and cubic	$\hat{\mathbf{e}}_1 \parallel \mathbf{a}, \hat{\mathbf{e}}_2 \parallel \mathbf{b}, \hat{\mathbf{e}}_3 \parallel \mathbf{c},$

### Linear Elastic Equations

Given the restrictions of reversibility and linearity,

Hooke's law can be written for strain as a function of stress	
$\varepsilon_{ij} = c_{ijkl} \sigma_{kl} \quad (i, j, k, l = 1, \dots, 3)$	$\varepsilon_I = c_{IJ} \sigma_J \quad (I, J = 1, \dots, 6)$
$\sigma_{ij} = s_{ijkl} \varepsilon_{kl} \quad (i, j, k, l = 1, \dots, 3)$	$\varepsilon_I = c_{IJ} \sigma_J \quad (I, J = 1, \dots, 6)$

The matrix notation (right-hand set of equations) reduces the number of subscripts to two, but the equations do not strictly obey tensor transformation rules and require factors of 2 and 4 to be inserted in the relations between  $s_{ijkl}$  and  $s_{IJ}$ .

<b>s</b>	Compliance	Modulus	Stress <sup>-1</sup>
<b>c</b>	Stiffness	Constant	Stress

The reduction from 81 separate components to 36 occurs because the stress and strain tensors are symmetric.

Because the material behavior is thermodynamically reversible, a chemical potential energy, the Helmholtz free energy, can be defined to express the energy of the elastic solid. For this thermodynamic potential to exist, requires the stiffness and compliance tensors and matrices to be symmetric. This limits the number of independent components of the most general elasticity tensor to 21.

**Symmetry causes further restrictions:**

Crystal symmetry requires further reductions in the number of the stiffnesses and compliances

Triclinic	21
Monoclinic	13
Orthorhombic	9
Tetragonal	7,6
Trigonal	7,6
Hexagonal	5
Cubic	3
Isotropic	2

## Stiffness Moduli

### Cubic

	$C_{ii}$	$C_{44}$	$C_{12}$ (GPa)	Remark	$\rho$	$T_m$ (°C)
Gold (Au)	191	42	162	metal	19.3	1063
Halite NaCl	165	34	47	halide	2.2	801
Spinel (Mg Al <sub>2</sub> O <sub>4</sub> )	283	155	155	Al <sub>2</sub> O <sub>4</sub>	3.6	2135
Wustite (FeO)	246	45	149	Oxide	5.73	~1400
Periclase (MgO)	294	155	93	Oxide	3.6	2800
$\alpha$ -Iron (Fe)	230	117	135	metal	7.9	1408
Grossular Garnite <sup>3</sup>	322	105	91	Al. Silicate	3.6	(~1400)
Pyrite FeS <sub>2</sub>	361	105	34	Sulfide		5.0
Diamond	1079	578	124	covalent	3.5	(3652)

### Hexagonal

	$C_{11}$	$C_{33}$	$C_{44}$	$C_{12}$	$C_{13}$	Remark	$\rho$	$T_m$ (°C)
Graphite (C)	1060	36.5	0.3	180	15	Sp <sup>2</sup> bonding	2.26	(3652)
Ice-I (H <sub>2</sub> O)	13.5	15	3.0	65	6	hydrogen	0.9	0
$\beta$ -quartz (SiO <sub>2</sub> )	117	110	36	16	33	framework	-	1470-

### Trigonal

	$C_{11}$	$C_{33}$	$C_{44}$	$C_{12}$	$C_{13}$	$C_{14}$	Remark	$\rho$	$T_m$ (°C)
Calcite (CaCO <sub>3</sub> )	144	84	33.5	53.9	51	-20.5	carbonate		(1339°C)
Hematite (Fe <sub>2</sub> O <sub>3</sub> )	242	227	85.7	54.6	15.4	-125	oxide		~1550
Corundum (Al <sub>2</sub> O <sub>3</sub> )	497	501	147	162	116	-22	oxide		1840
$\alpha$ -quartz (SiO <sub>2</sub> )	86.5	107	58	7	12	-18	framework		(1470)

### Orthorhombic

	$C_{11}$	$C_{22}$	$C_{33}$	$C_{44}$	$C_{55}$	$C_{66}$	$C_{12}$	$C_{13}$	$C_{23}$	Remark	$\rho$
Perovskite (MgSiO <sub>3</sub> )	515	525	435	179	202	175	117	117	139	Clspckd	
Olivine (Mg <sub>2</sub> SiO <sub>4</sub> )	328	200	235	67	81	81	69	69	73	Isolated	3.20
Fayalite (Fe <sub>2</sub> SiO <sub>4</sub> )	266	168	232	32.3	47	57	94	92	92	Isolated	4.38
Enstatite (MgSiO <sub>3</sub> )	224	178	214	78	76	82	72	54	53	Chain	3.20
Ferrosilite (FeSiO <sub>3</sub> )	198	136	175	59	58	49	84	72	55	Chain	4.00
Wadsleyite <sup>4</sup>	360	383	273	112	118	98	75	110	105	Chain	3.47

#### Sources:

Simmons, M. G., and H. Wang, *Single crystal elastic constants and calculated aggregate properties*, MIT Press, 1975.

Bass, J. D., Elasticity of Minerals, Glasses, and Melts, pp.45-63, in *Mineral Physics and crystallography: a handbook of physical constants*, edited by T. J. Ahrens, AGU, Washington, DC., 1995.

<sup>3</sup> (Mg,Fe,Mn)<sub>3</sub>Al<sub>2</sub>Si<sub>3</sub>O<sub>12</sub>

<sup>4</sup>  $\beta$ -(Mg<sub>2</sub>SiO<sub>4</sub>)

**Tetragonal**

	$C_{11}$	$C_{33}$	$C_{44}$	$C_{66}$	$C_{12}$	$C_{13}$	Remark	$\rho$	$T_m$ (°C)
Zircon (ZrSi <sub>2</sub> O <sub>7</sub> )	424	489	131	48	70	149		4.7	(1540 decp)
Stishovite (SiO <sub>2</sub> )	453	776	252	302	211	203	Framework	4.20	high pressure
$\alpha$ -Cristobalite (SiO <sub>2</sub> )	59.4	42.4	67	26	4	-4.4	Framework	2.335	1713

**Monoclinic**

	$C_{11}$	$C_{22}$	$C_{33}$	$C_{44}$	$C_{55}$	$C_{66}$	$C_{12}$	$C_{13}$	$C_{23}$	$C_{15}$	$C_{25}$	$C_{35}$	$C_{46}$	Remark	$\rho$	$T_m$ (°C)
Albite (NaAlSi <sub>3</sub> O <sub>8</sub> )	74	131	128	17	30	32	36	39	31	-6.6	-13	-20	-25	Framework	2.62	1100°C
Anorthite (CaAl <sub>2</sub> Si <sub>2</sub> O <sub>8</sub> )	124	205	156	24	40	42	66	50	42	-19	-7	-18	-1	Framework	2.76	1550°C
Microcline (KSi <sub>3</sub> AlO <sub>8</sub> )	67	169	118	14	24	36	45	27	20	-2	-	-15	-2	Framework	2.56	1150°C
Labradorite <sup>5</sup>	99	158	150	22	35	37	63	49	27	-25	-11	-12	-5	Framework	2.70	1280°C
Diopside (CaMgSi <sub>2</sub> O <sub>6</sub> )	204	175	238	68	59	71	84	88	48	-19	-20	-34	-11	Chain	3.31	1390°C
Hedenbergite (CaFeSi <sub>2</sub> O <sub>6</sub> )	222	176	249	55	63	60	69	79	86	12	13	26	-10	Chain	3.65	
Hornblende <sup>6</sup>	116	160	192	57	32	37	45	61	66	4.3	-2.5	10	-6.2	Chain	3.12	
Coesite (SiO <sub>2</sub> )	161	230	232	68	73	59	82	103	36	-36	2.6	-39	9.9	Framework	2.911	(1713)

<sup>5</sup> Albite 30-50%, Anorthite 70-50%<sup>6</sup> (Ca,Na)<sub>2-3</sub>(Mg,Fe,Al)<sub>5</sub>(Al,Si)<sub>8</sub>O<sub>2</sub>(OH)<sub>2</sub>

## Elastic stiffness or compliance in an arbitrary direction

### Vector Transformation

Express the components of a vector in a new coordinate system that has been rotated. The components of the vector in the new system are

$$E'_i = a_{ij} E_j$$

where  $E_i$  are the components of the vector in the old system,  $a_{ij}$  are the direction cosines between the old and new coordinate systems, and  $E'_j$  are the components in the new system.

### Tensor Transformation:

Tensors of the second rank transform in much the same way as vectors:

$$E'_{ij} = a_{ik} a_{jl} E_{kl}$$

Tensors of the fourth rank (like stiffness or compliance) transform as

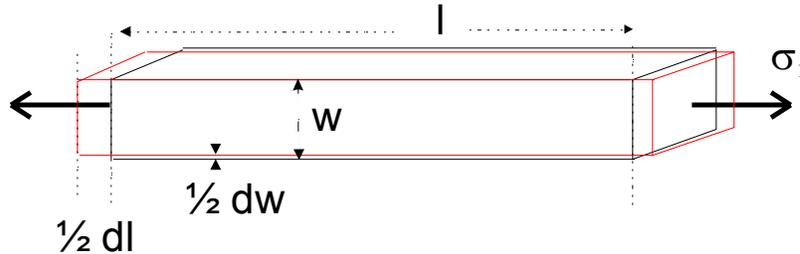
$$S'_{ijkl} = a_{im} a_{jn} a_{ko} a_{lp} S_{mnop}$$

Thus, the Young's modulus ( $c_{1111}$ ) could be calculated in any arbitrary direction.

## Relations among moduli, stiffnesses and compliances

In isotropic elastic materials, the most commonly used elastic (moduli, constants, stiffnesses, compliances) are Young's Modulus, the Bulk modulus, the Volumetric compressibility, Poisson's ratio, and the Lamé parameters.

### Young's Modulus



The relation between the load on a bar and the fractional stretch of a bar along its long axis is known as Young's modulus.

$$\sigma_l = E \varepsilon_l \quad \varepsilon_l = \frac{1}{E} \sigma_l$$

where the subscript  $l$  is used to indicate the direction in which the measurement is made, but in an isotropic material the direction is immaterial.

In an anisotropic material, the equivalent measurement depends on the direction (relative to some fixed axes in the material) in which the measurement is made).

When the measurement is made along the 1 axis in a single crystal, the equivalent modulus (stiffness, compliance) is

$$\sigma_{11} = c_{1111} \varepsilon_{11} \text{ equivalently } \sigma_1 = c_{11} \varepsilon_1 \text{ or } \varepsilon_{11} = s_{1111} \sigma_{11}$$

When the Young's modulus measurement is made in the 1 direction,

$$E = 1/s_{1111}$$

When the measurement is made in another direction D

$$1/E = a_{Di} a_{Dj} a_{Dk} a_{Dl} s_{ijkl}$$

where  $a_{Di}$  is the direction cosine between D and the axis i.

### Some typical values of compressibility and Poisson's ratio

Rock/Material	Compressibility ( $10^{-5} \text{ MPa}^{-1}$ )	Poisson's Ratio
Obsidian	2.9-3.	0.12-0.16
Granite	1.9-2.0	0.23-0.27
Diorite	1.4-1.7	0.26-0.29
Gabbro	1.1-1.3	0.27-0.31
Diabase	1.2-1.4	0.27-0.30
Dunite	0.8-0.9	0.26-0.28
Slate	1.9-2.3	0.15-0.20
Limestone	1.3-1.4	0.27-0.30
Dolomite	1.0-1.1	0.30
Quartzite	2.4-2.6	0.12-0.15
Mica Schist	2.1-2.3	0.15-0.20
Feldspathic Gneiss	1.8-2.2	0.15-0.20
Amphibolite	1.1-1.3	0.28-0.30
Oligoclase	1.5-1.6	0.29
Anorthosite	1.2-1.4	0.31
Rocksalt	4.3	0.25
Anhydrite	1.8	0.30
Ice	12	0.36
Steel	0.6	0.28-0.29
Aluminum	1.3	0.34-0.36

### Poisson's Ratio

$$\nu \equiv \frac{-\varepsilon_{\perp l}}{\varepsilon_l}$$

for an isotropic material  $\sigma_l = E\varepsilon_l$

$$s_{22111} = \frac{\varepsilon_{22}}{\sigma_{11}} = \frac{\varepsilon_{22}}{E\varepsilon_{11}} = \boxed{\frac{\nu}{E} = s_{21}}$$

For rocks, Poisson's ratio is commonly 0.25. In some materials, it may be very small or even negative.

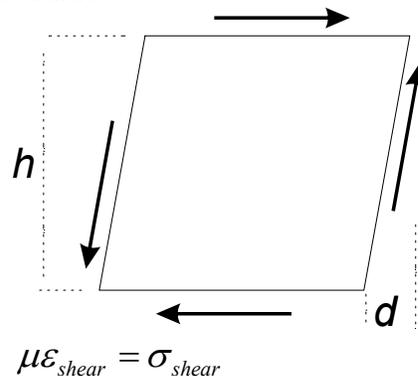
*Can you think of a common use for a material with a low or negative Poisson's ratio?*

For an incompressible material, Poisson's ratio is 0.5.

*Why?*

*Is it possible for  $\nu$  to be even larger than that?*

### Rigidity Modulus



When the body and the crystal axes are aligned,

$$\boxed{s_{44} = \frac{1}{\mu}}$$

### Lamé Constants

For an isotropic material, the stress strain relations are often written:

$$\sigma_1 = (\lambda + 2\mu)\varepsilon_1 + \lambda\varepsilon_2 + \lambda\varepsilon_3$$

$$\sigma_2 = \lambda\varepsilon_1 + (\lambda + 2\mu)\varepsilon_2 + \lambda\varepsilon_3$$

$$\sigma_3 = \lambda\varepsilon_1 + \lambda\varepsilon_2 + (\lambda + 2\mu)\varepsilon_3$$

From the equations above it is clear that if the crystal axis 1 is aligned with the exterior axis 1 then

$$\boxed{2\mu + \lambda = c_{1111} \text{ and } c_{1122} = \lambda}$$

**Compressibility**

Consider imposition of pressure  $\sigma_{ij} = -p\delta_{ij}$

Then the equation for the strain is

$$\varepsilon_{ij} = -ps_{ijkl}\delta_{kl}$$

define  $\Delta \equiv \varepsilon_{ii} = -ps_{iikk}$

and 
$$\boxed{\beta_T = -\frac{\Delta}{p} = s_{iikk}}$$

*Write the equation for the isothermal compressibility for a cubic crystal.*

$$\beta_{T \text{ cubic}} = 3(s_{11} + 2s_{12})$$

*Does the compressibility depend on the direction of measurement?*

*The bulk modulus is the inverse of the compressibility.*

### Relations among Various Moduli and Elastic Constants

Name	Symbol	Definition	S/C	Units	Relations
Inv. Young's Modulus	1/E	<u>Normal Strain</u> Normal Stress	S <sub>1111</sub>	Stress <sup>-1</sup>	$\frac{\lambda + \mu}{\mu(3\lambda + 2\mu)}$
Poisson's Ratio	$\nu, \sigma$	<u>Normal Strain</u> ⊥ Norm. Strain	S <sub>2211</sub> /S <sub>1111</sub>	---	$\frac{\lambda}{2(\lambda + \mu)}$
Shear Modulus	$\mu, G$	<u>Shear Stress</u> Shear Strain	C <sub>1212</sub>	Stress	$\frac{E}{2(1 + \nu)}$
Lame Const.	$\lambda$	Response of Stress to Volum.Change	C <sub>1111</sub>	Stress	$\lambda = \frac{E\nu}{(1 + \nu)(1 - \nu)}$
Compressibility	B	Dilation/Pressure		Stress <sup>-1</sup>	$\frac{E}{3(1 - 2\nu)} = \lambda + 2\frac{\mu}{3}$

### Equivalent formulations for isotropic elastic materials in principal stress representation:

$$\varepsilon_{11} = \frac{1}{E}\sigma_{11} - \frac{\nu}{E}\sigma_{22} - \frac{\nu}{E}\sigma_{33}$$

$$\varepsilon_{22} = \frac{1}{E}\sigma_{11} - \frac{\nu}{E}\sigma_{22} - \frac{\nu}{E}\sigma_{33}$$

$$\varepsilon_{33} = -\frac{\nu}{E}\sigma_{11} - \frac{\nu}{E}\sigma_{22} + \frac{1}{E}\sigma_{33}$$

$$\sigma_1 = (\lambda + 2\mu)\varepsilon_1 + \lambda\varepsilon_2 + \lambda\varepsilon_3$$

$$\sigma_2 = \lambda\varepsilon_1 + (\lambda + 2\mu)\varepsilon_2 + \lambda\varepsilon_3$$

$$\sigma_3 = \lambda\varepsilon_1 + \lambda\varepsilon_2 + (\lambda + 2\mu)\varepsilon_3$$

### In general:

$$\varepsilon_{ij} = \frac{1 + \nu}{E}\sigma_{ij} - \frac{\nu}{E}\delta_{ij}\sigma_{kk}$$

$$\sigma_{ij} = \lambda\delta_{ij}\varepsilon_{kk} + 2\mu\varepsilon_{ij}$$