

# Mechanical properties of solids: density functional theory calculations

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# Early history

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Hooke's law

1676 *ut tensio, sic vis* ("as the extension, so the force")

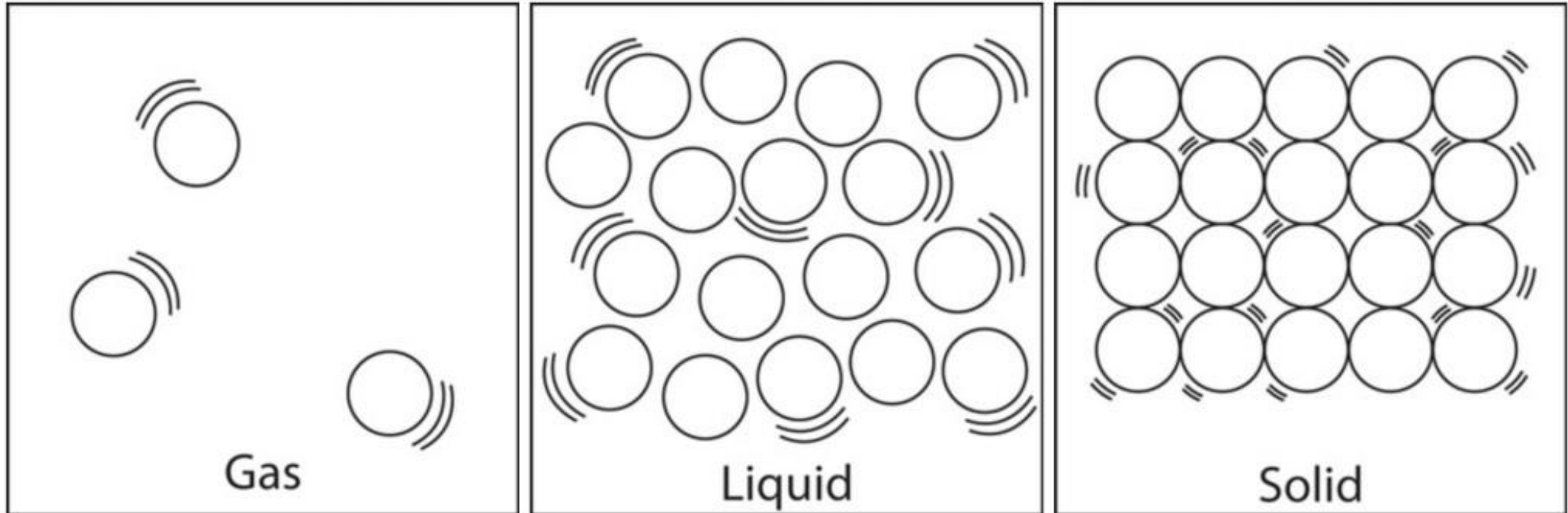
$$F_s = -kx$$

$$\mathbf{F} = \begin{bmatrix} F_1 \\ F_2 \\ F_3 \end{bmatrix} = \begin{bmatrix} \kappa_{11} & \kappa_{12} & \kappa_{13} \\ \kappa_{21} & \kappa_{22} & \kappa_{23} \\ \kappa_{31} & \kappa_{32} & \kappa_{33} \end{bmatrix} \begin{bmatrix} X_1 \\ X_2 \\ X_3 \end{bmatrix} = \boldsymbol{\kappa} \mathbf{X}$$

$$\boldsymbol{\sigma} = -\mathbf{c}\boldsymbol{\varepsilon}$$

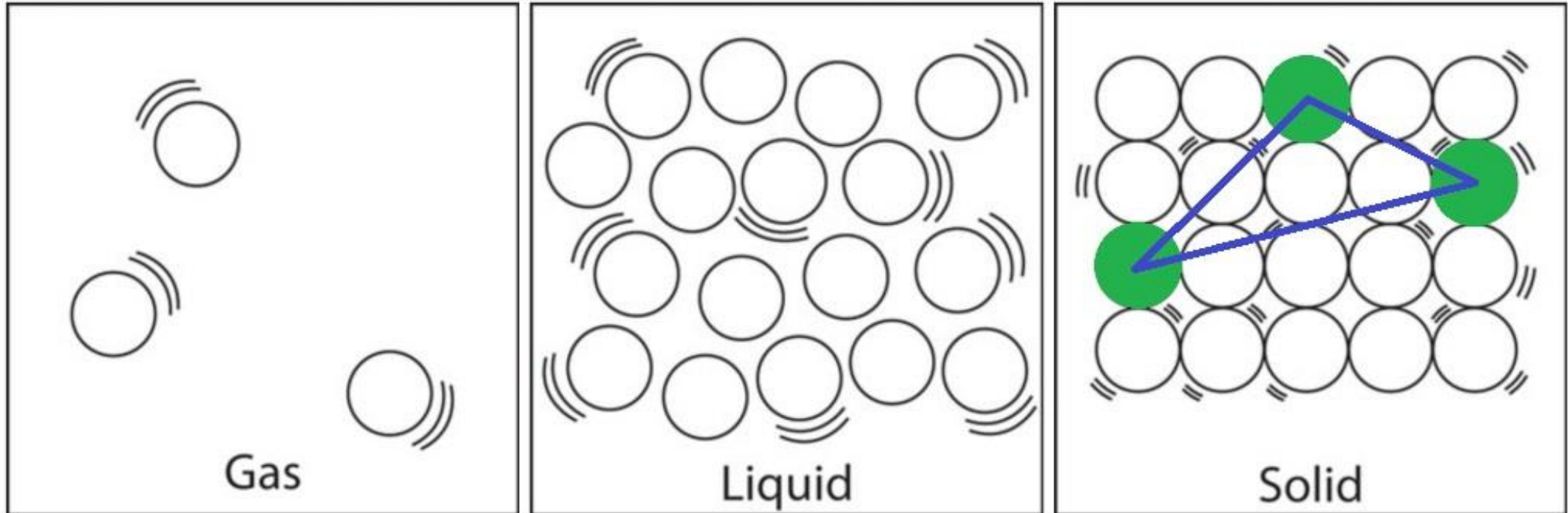
# Solids

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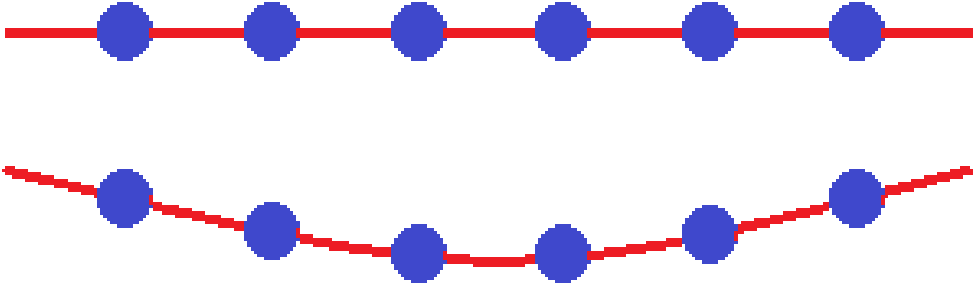
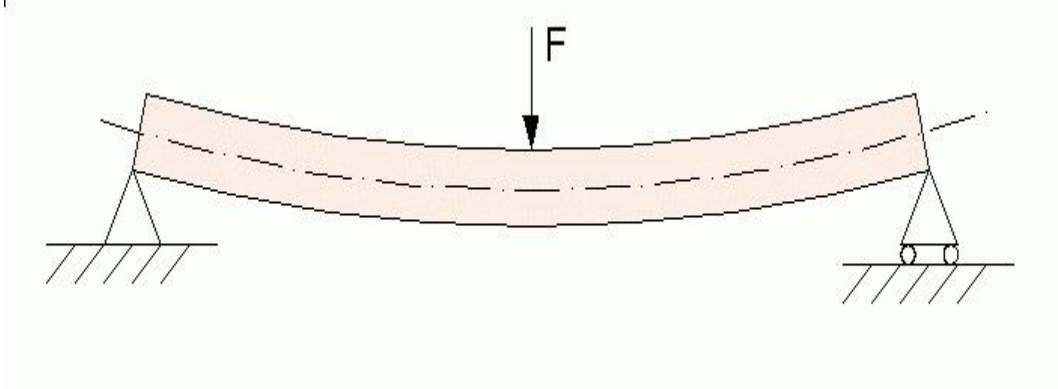
# Solids

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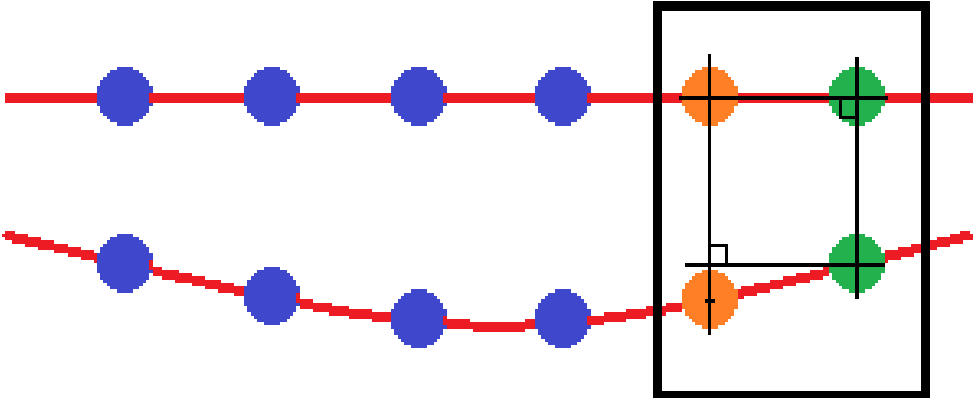
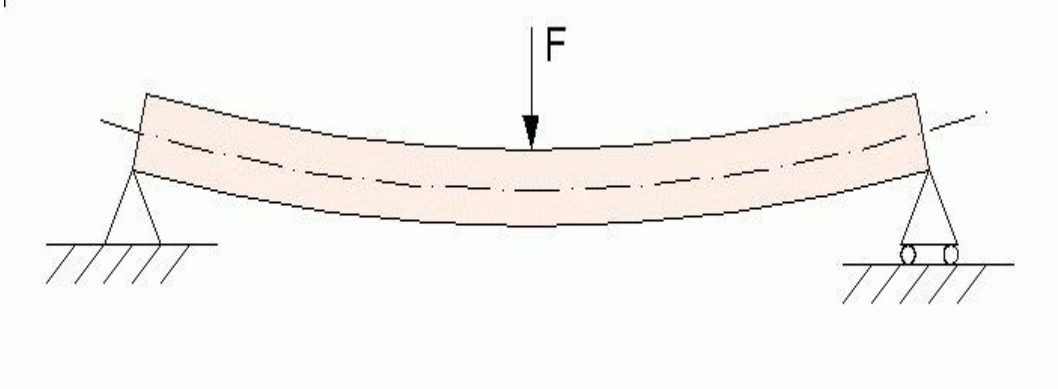


# Deformations

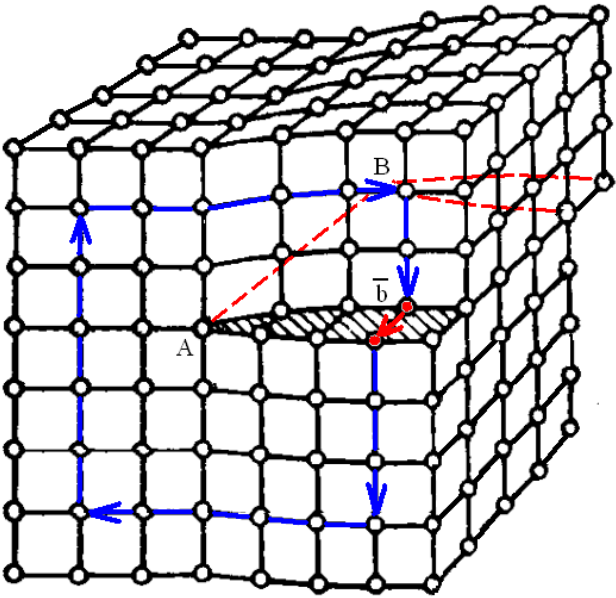
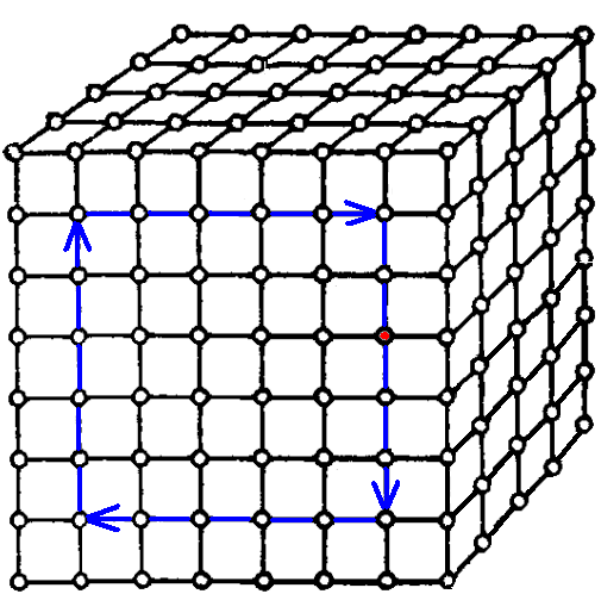
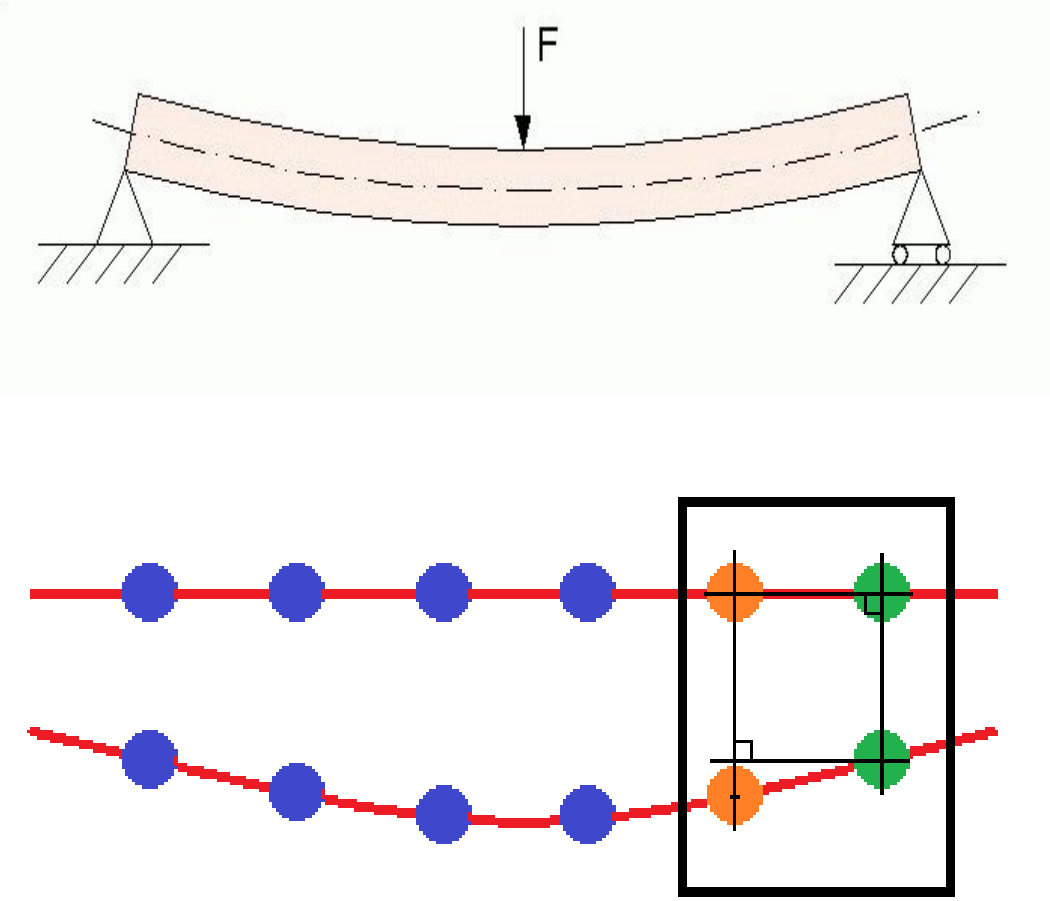
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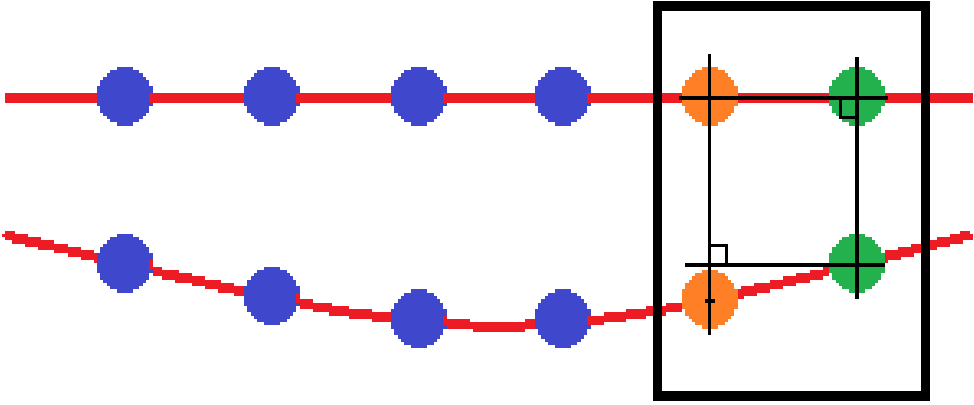
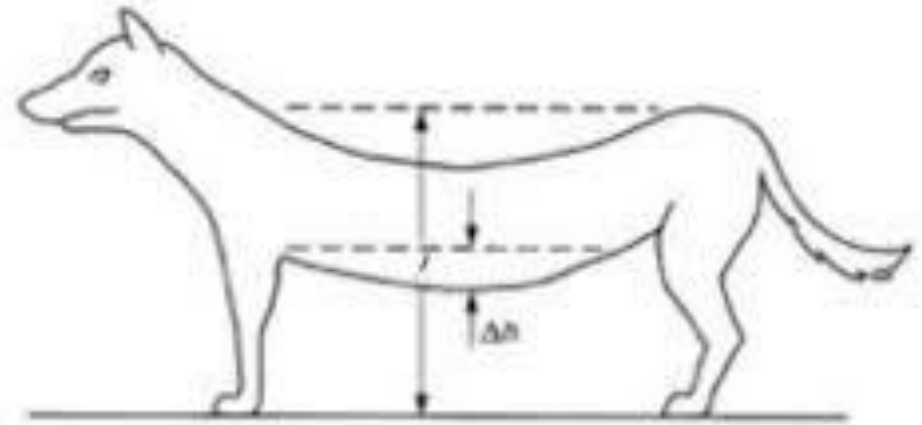
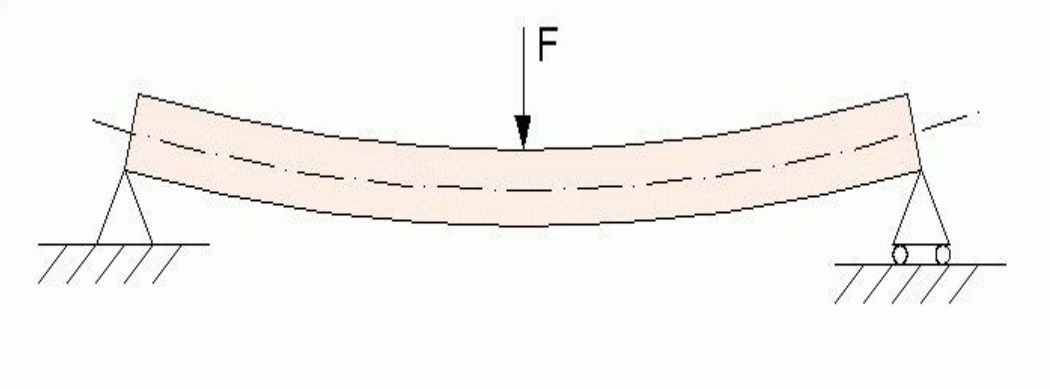
# Deformations



# Deformations



# Deformations

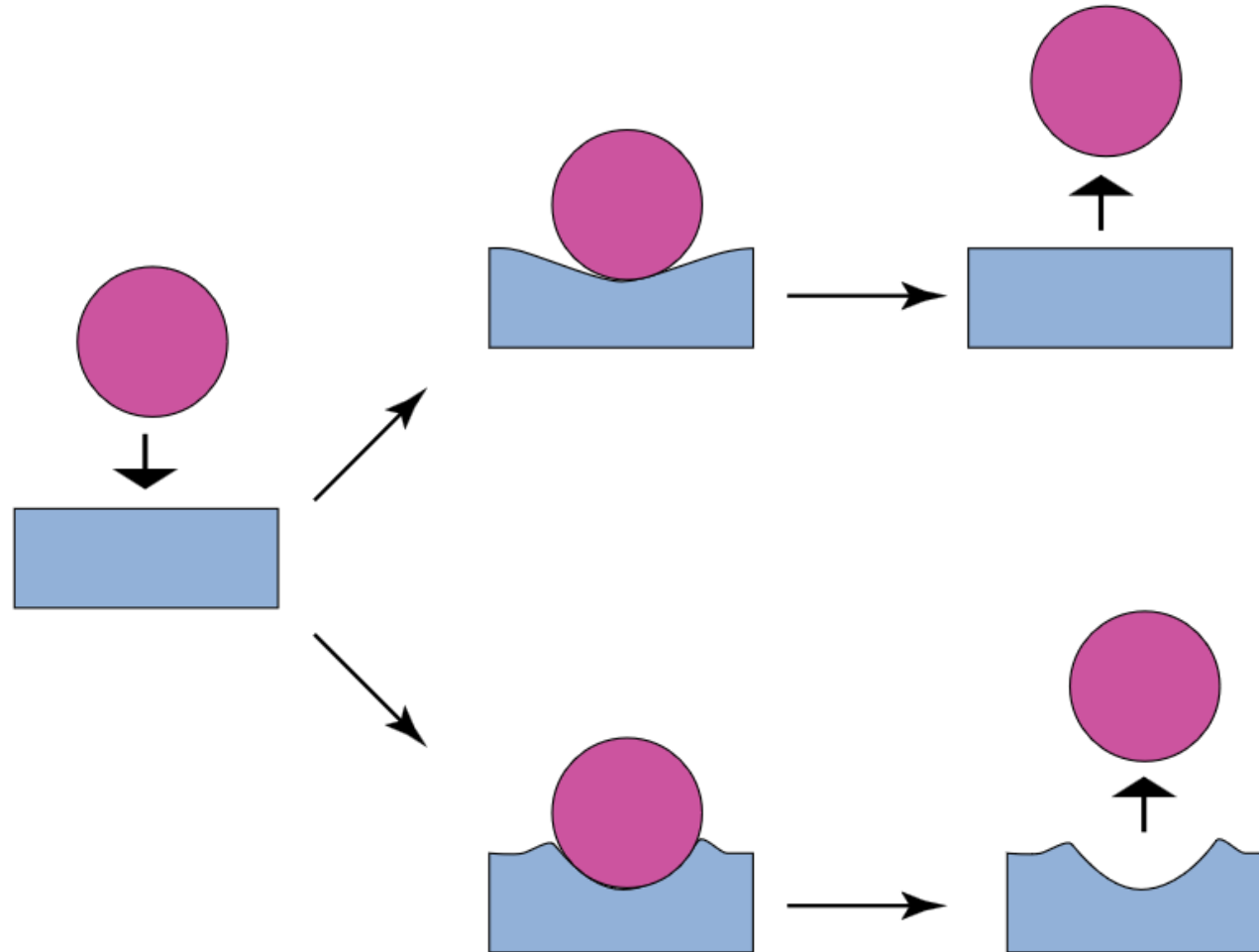


# Deformations

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Elastic deformations

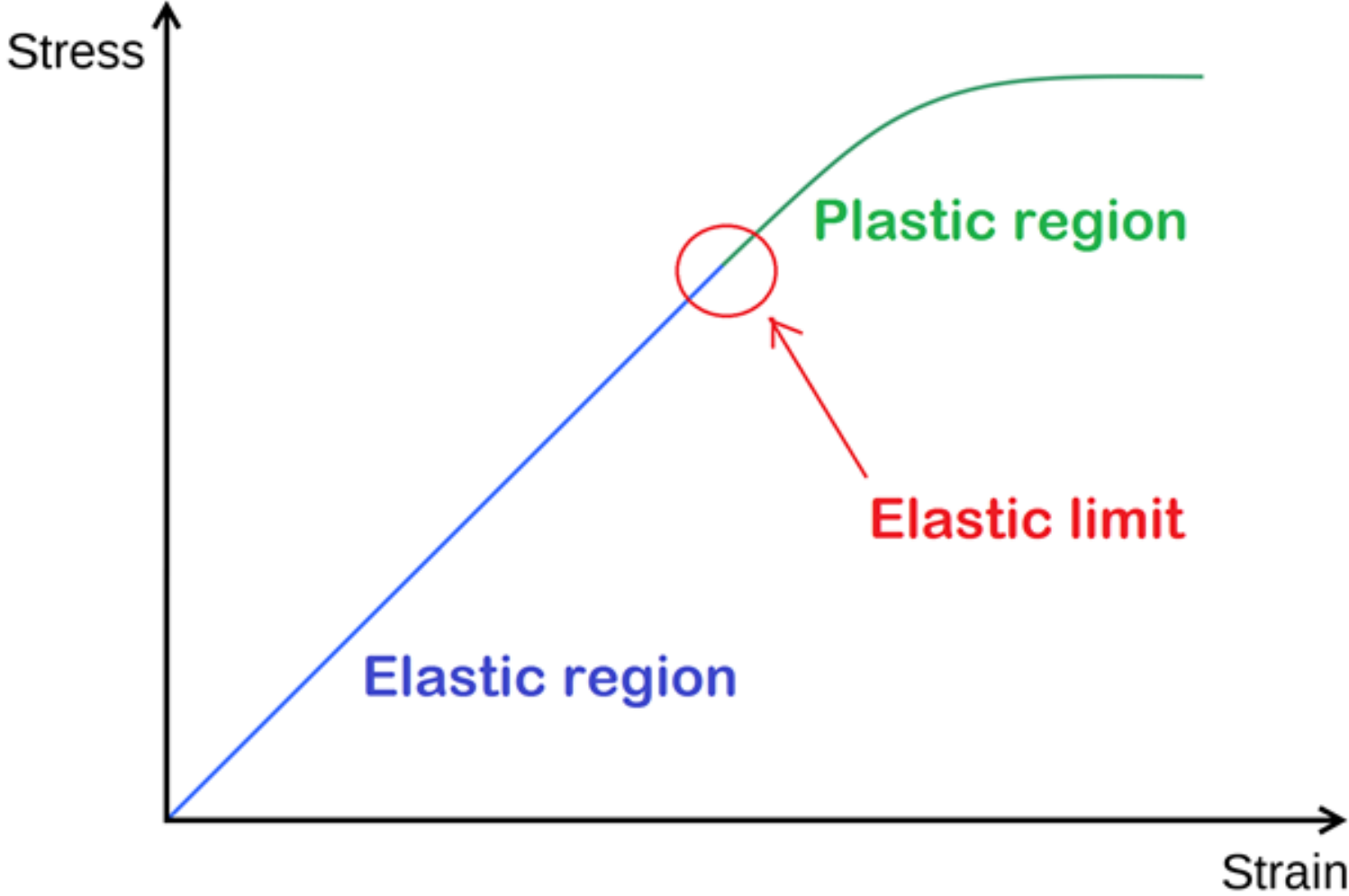
Plastic deformations



# Deformations

Elastic deformations

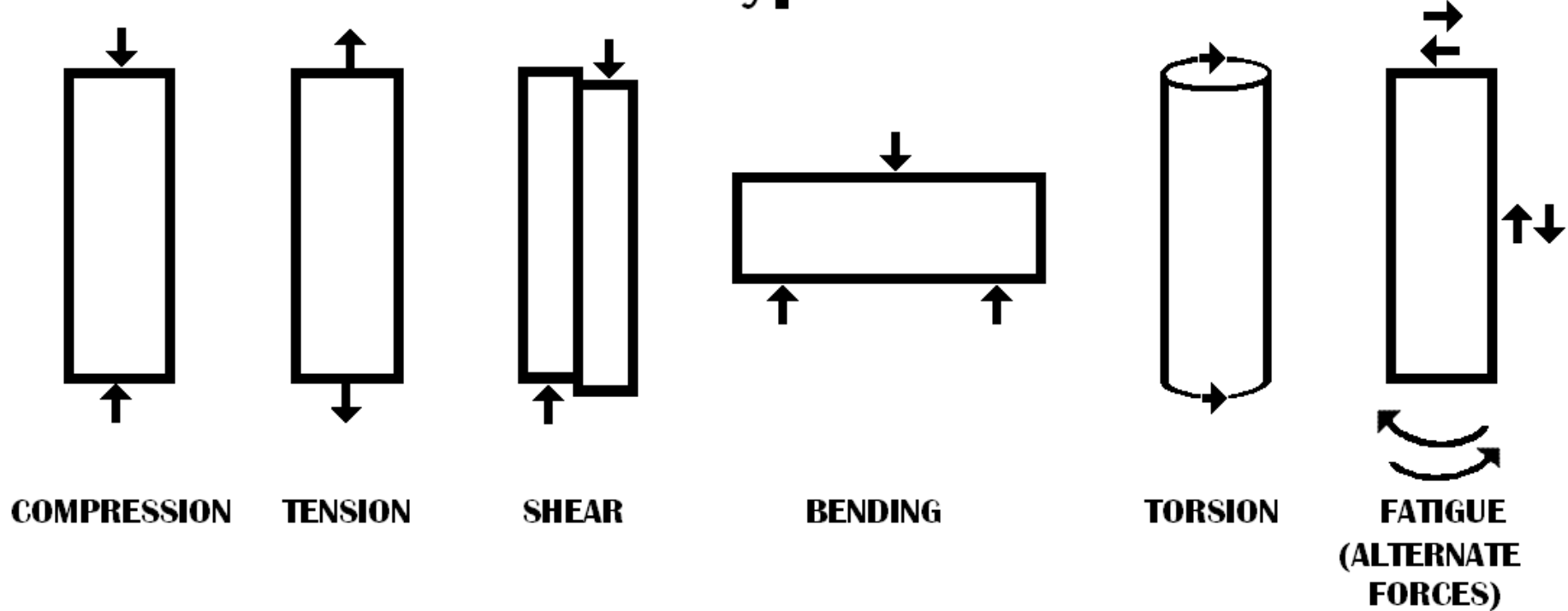
Plastic deformations



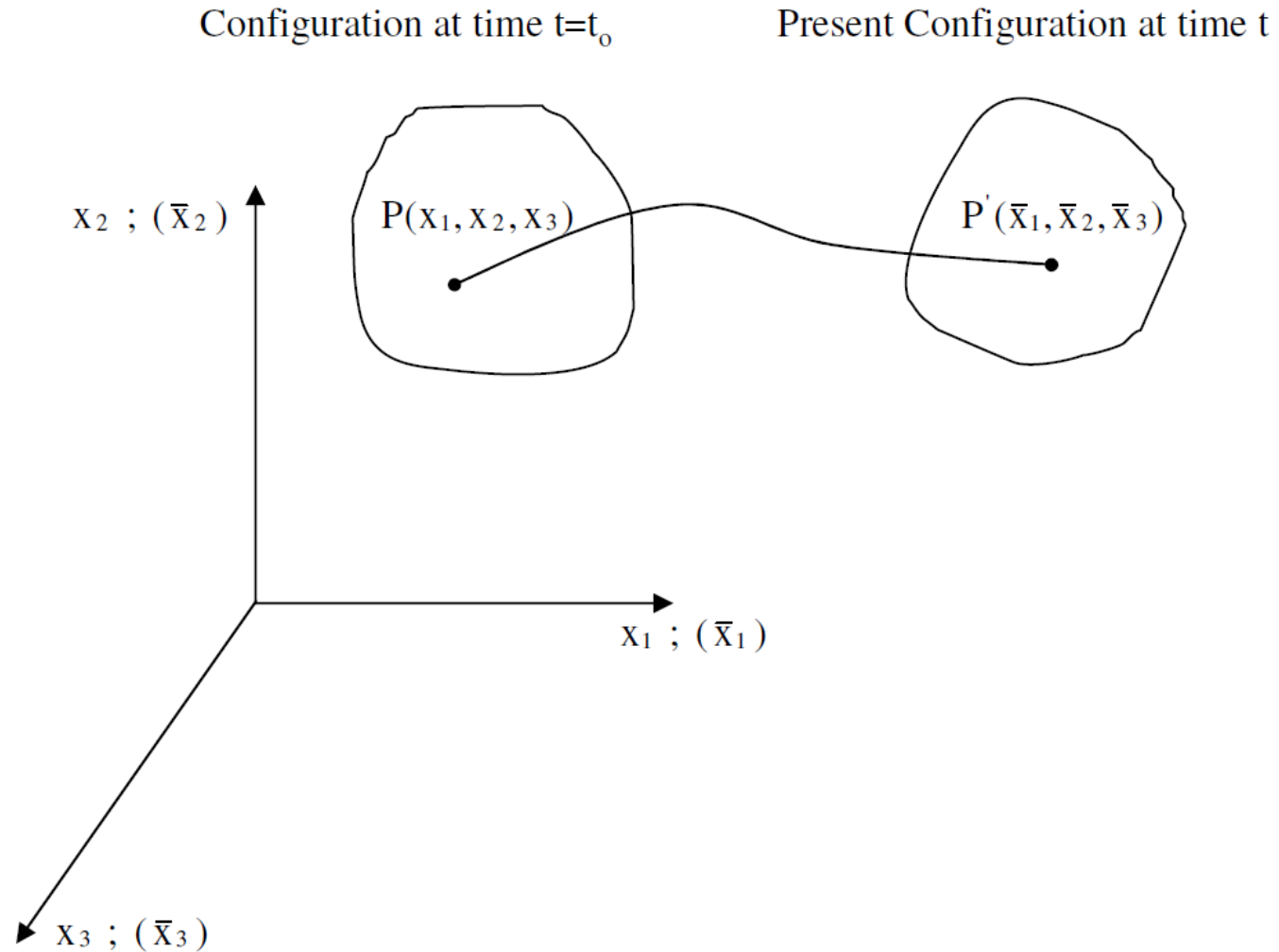
# Deformations

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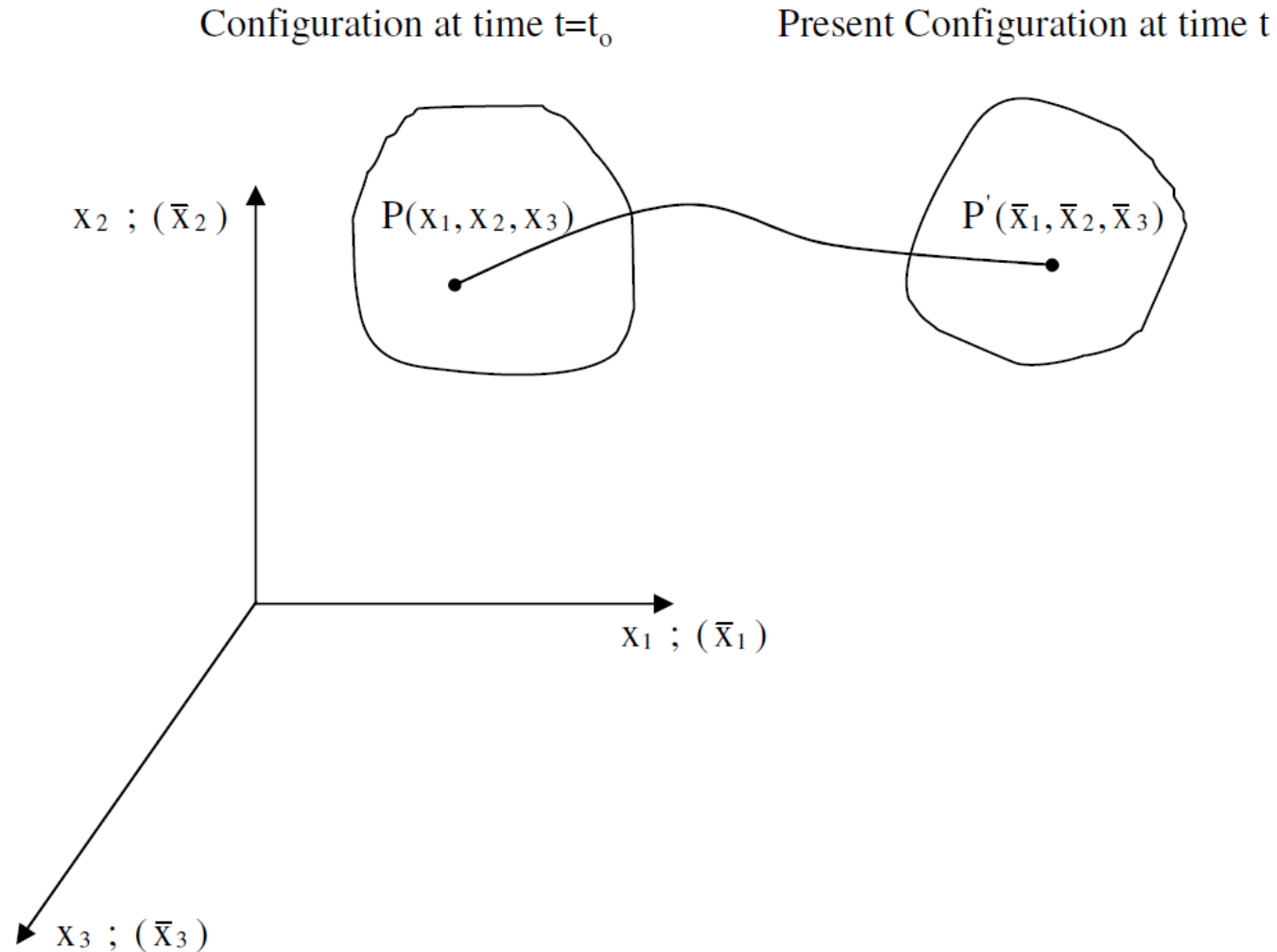
## Different types of stress



# Some math formulas



# Some math formulas



$$\bar{x}_1 = \bar{x}_1(x_1, x_2, x_3, t)$$

$$\bar{x}_2 = \bar{x}_2(x_1, x_2, x_3, t)$$

$$\bar{x}_3 = \bar{x}_3(x_1, x_2, x_3, t)$$

Let  $u_1, u_2, u_3$  be the displacements of point  $P(x_1, x_2, x_3)$

$$\bar{x}_1 = x_1 + u_1(x_1, x_2, x_3, t)$$

$$\bar{x}_2 = x_2 + u_2(x_1, x_2, x_3, t)$$

$$\bar{x}_3 = x_3 + u_3(x_1, x_2, x_3, t)$$

Inverse can be given as,

$$x_j = \bar{x}_j - \bar{u}_j(\bar{x}_i, t) \quad i, j = 1, 2, 3$$

# Some math formulas

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Jacobian matrix

$$[J(t)] = \frac{\partial\{\bar{x}\}}{\partial\{x\}} = \begin{bmatrix} \bar{x}_1, \bar{x}_2, \bar{x}_3 \\ x_1, x_2, x_3 \end{bmatrix} = \begin{bmatrix} \frac{\partial\bar{x}_1}{\partial x_1} & \frac{\partial\bar{x}_1}{\partial x_2} & \frac{\partial\bar{x}_1}{\partial x_3} \\ \frac{\partial\bar{x}_2}{\partial x_1} & \frac{\partial\bar{x}_2}{\partial x_2} & \frac{\partial\bar{x}_2}{\partial x_3} \\ \frac{\partial\bar{x}_3}{\partial x_1} & \frac{\partial\bar{x}_3}{\partial x_2} & \frac{\partial\bar{x}_3}{\partial x_3} \end{bmatrix}$$

Let  $W$  be the strain energy density function for elastic material

$$W = W([J])$$

# Some math formulas

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Expand  $W([\varepsilon])$  in Taylor series about  $[\varepsilon^0]$

$$W = W|_{[\varepsilon^0]} + \left. \frac{\partial W}{\partial \{\varepsilon\}} \right|_{[\varepsilon^0]} (\{\varepsilon\} - \{\varepsilon^0\}) + \frac{1}{2!} \left. \frac{\partial^2 W}{\partial \{\varepsilon\}^2} \right|_{[\varepsilon^0]} (\{\varepsilon\} - \{\varepsilon^0\})^2 + \frac{1}{3!} \left. \frac{\partial^3 W}{\partial \{\varepsilon\}^3} \right|_{[\varepsilon^0]} (\{\varepsilon\} - \{\varepsilon^0\})^3 + \dots$$

More precisely, using index notation, we can write the above equation as,

$$W = C_0 + C_{ij}(\varepsilon_{ij} - \varepsilon_{ij}^0) + \frac{1}{2!} C_{ijkl}(\varepsilon_{ij} - \varepsilon_{ij}^0)(\varepsilon_{kl} - \varepsilon_{kl}^0) + \frac{1}{3!} C_{ijklmn}(\varepsilon_{ij} - \varepsilon_{ij}^0)(\varepsilon_{kl} - \varepsilon_{kl}^0)(\varepsilon_{mn} - \varepsilon_{mn}^0) + \dots$$

# Some math formulas

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$$W = \frac{E}{V} = \frac{1}{2} C_{ijkl} \varepsilon_{ij} \varepsilon_{kl}$$

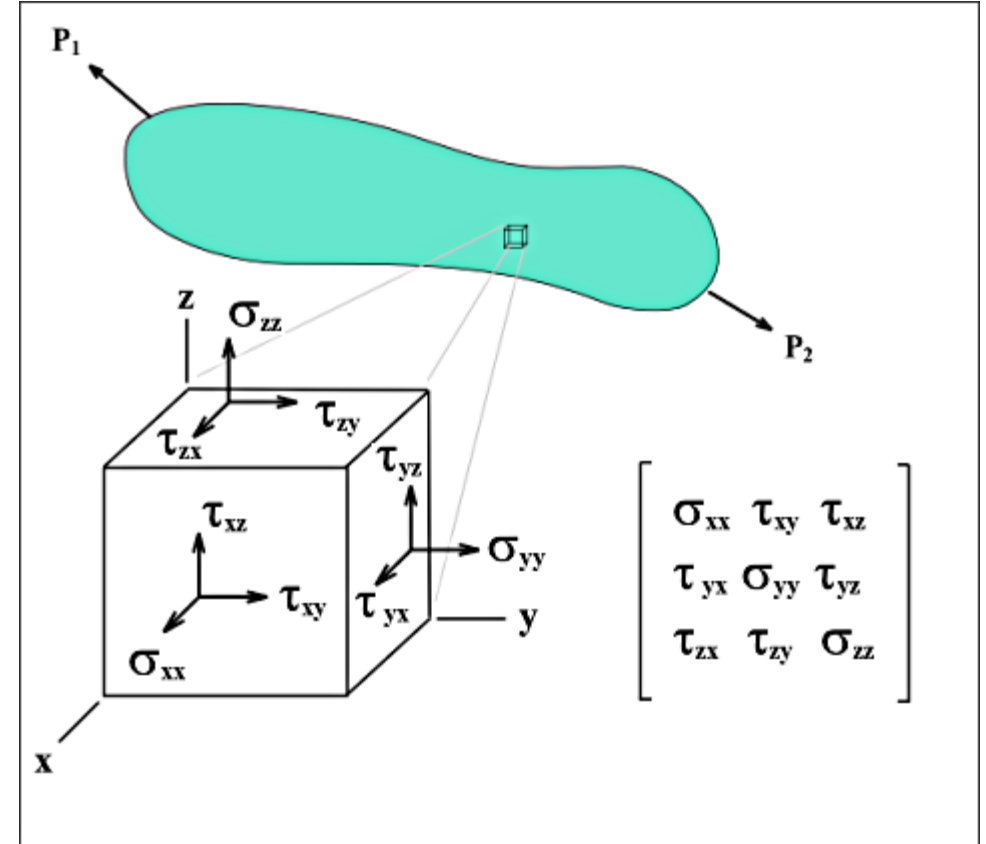
$$\varepsilon_{ij} = \frac{1}{2} \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} + \sum_l \frac{\partial u_l}{\partial x_i} \frac{\partial u_l}{\partial x_j} \right)$$

# Some math formulas

$$W = \frac{E}{V} = \frac{1}{2} C_{ijkl} \varepsilon_{ij} \varepsilon_{kl}$$

$$\sigma = -c\varepsilon$$

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



Cauchy stress tensor

# Some math formulas

We can write  $C_{ijkl}$  or  $[C]$  as follows:

$$[C] = \begin{bmatrix} C_{11} & C_{12} & C_{13} & C_{14} & C_{15} & C_{16} \\ & C_{22} & C_{23} & C_{24} & C_{25} & C_{26} \\ & & C_{33} & C_{34} & C_{35} & C_{36} \\ \text{symm.} & & & C_{44} & C_{45} & C_{46} \\ & & & & C_{55} & C_{56} \\ & & & & & C_{66} \end{bmatrix}$$

Thus we can write the following,

$$\{\sigma\} = [C]\{\varepsilon\}$$

$$\begin{aligned} 11 \rightarrow 1 \quad , \quad 22 \rightarrow 2 \quad , \quad 33 \rightarrow 3, \\ 23 \rightarrow 4 \quad , \quad 13 \rightarrow 5 \quad , \quad 12 \rightarrow 6 \end{aligned}$$

**Voigt notation**

# Birch-Murnaghan equation

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*THE COMPRESSIBILITY OF MEDIA UNDER EXTREME  
PRESSURES*

BY F. D. MURNAGHAN

DEPARTMENT OF MATHEMATICS, THE JOHNS HOPKINS UNIVERSITY

Communicated July 11, 1944

PHYSICAL REVIEW

VOLUME 71, NUMBER 11

JUNE 1, 1947

## **Finite Elastic Strain of Cubic Crystals\***

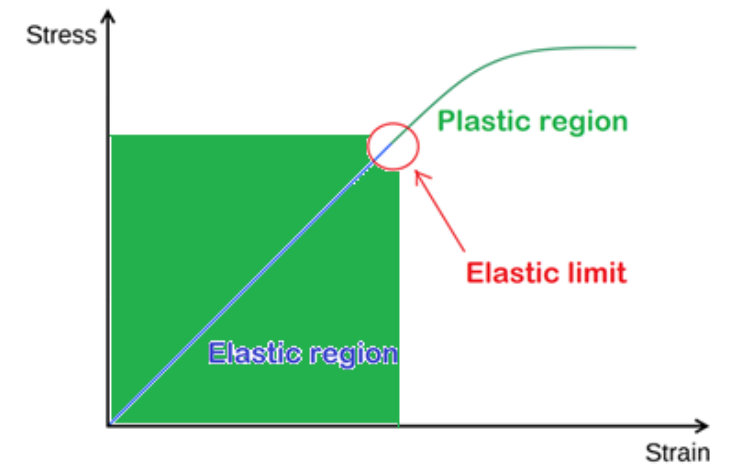
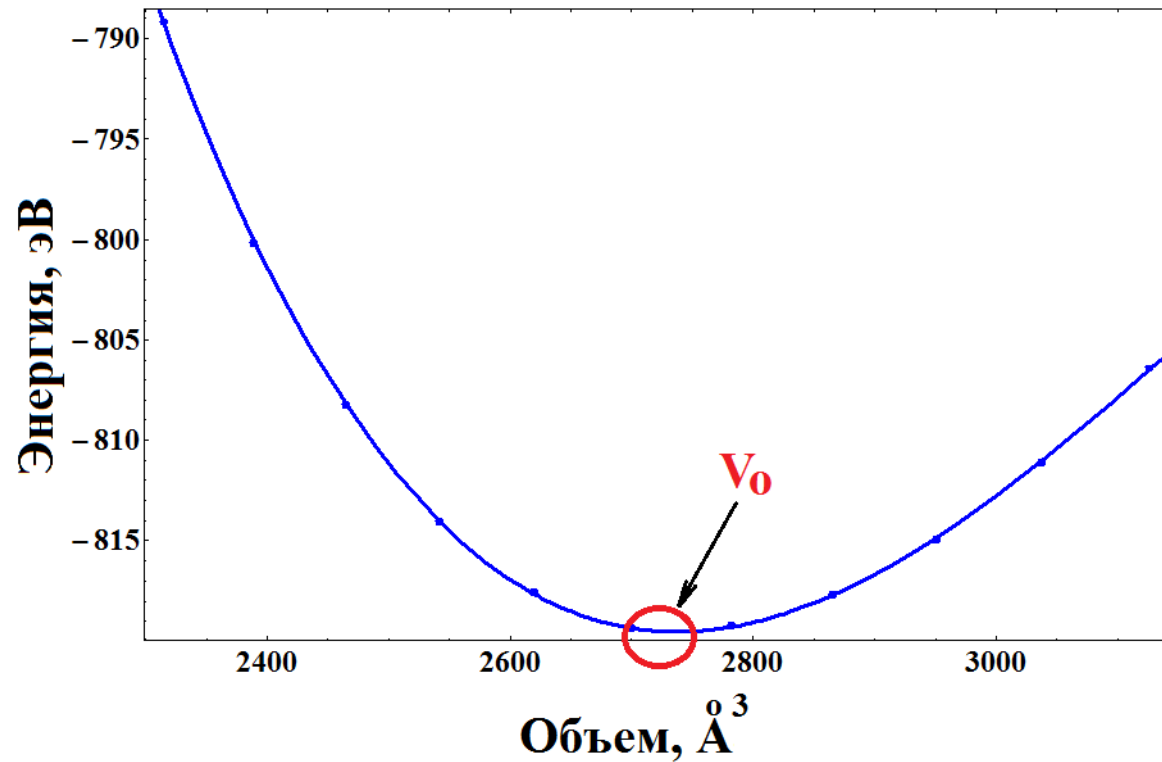
FRANCIS BIRCH

*Harvard University, Cambridge, Massachusetts*

(Received February 24, 1947)

# Birch-Murnaghan equation

$$P(V) = \frac{3B_0}{2} \left[ \left( \frac{V_0}{V} \right)^{\frac{7}{3}} - \left( \frac{V_0}{V} \right)^{\frac{5}{3}} \right] \left\{ 1 + \frac{3}{4} (B'_0 - 4) \left[ \left( \frac{V_0}{V} \right)^{\frac{2}{3}} - 1 \right] \right\}$$



# stress( $\sigma$ ) – strain( $\epsilon$ ) relation

---

PHYSICAL REVIEW B, VOLUME 65, 104104

**Symmetry-general least-squares extraction of elastic data for strained materials  
from *ab initio* calculations of stress**

Yvon Le Page\*

*ICPET, National Research Council of Canada, Ottawa, Canada K1A 0R6*

Paul Saxe†

*Materials Design Incorporated, PMB No. 176, 825 College Boulevard, Suite 102, Oceanside, California 92057*

stress - force per unit area

strain - resulting compression/stretching

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$$\sigma_i = \sum_{j=1,6} C_{ij} \epsilon_j$$

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$$\sigma_i = \sum_{j=1,6} C_{ij} \epsilon_j$$

$$\mathbf{S} = \mathbf{C}^{-1}$$

$$\epsilon_i = \sum_{j=1,6} S_{ij} \sigma_j$$

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$$\Sigma(\mathbf{E} + \mathbf{e}) = \Sigma(\mathbf{E}) + \mathbf{s} = \Sigma(\mathbf{E}) + \mathbf{C}(\mathbf{E}) \mathbf{e}.$$

# stress( $\sigma$ ) – strain( $\epsilon$ ) relation

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$$\underline{\Sigma(\mathbf{E} + \mathbf{e})} = \Sigma(\mathbf{E}) + \mathbf{s} = \underbrace{\Sigma(\mathbf{E})}_{6 \text{ comp.}} + \underbrace{\mathbf{C}(\mathbf{E})}_{21 \text{ comp.}} \underline{\mathbf{e}}.$$

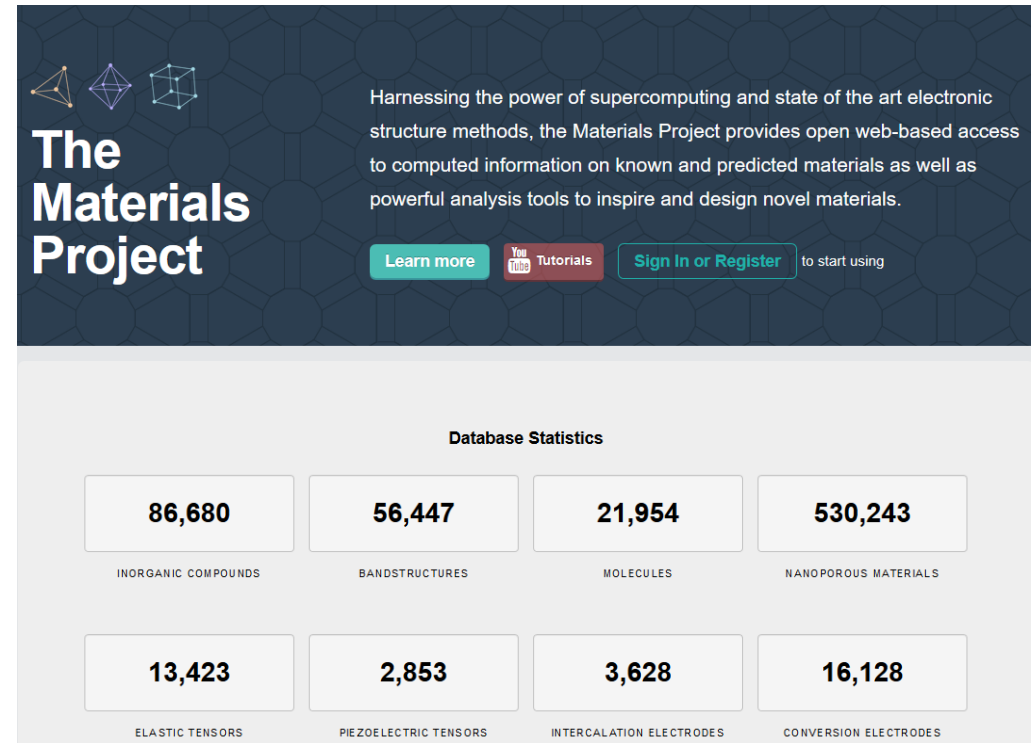
6 comp.

21 comp.

# DFT calculations of elastic properties

M. J. Mehl, J. E. Osburn, D. A. Papaconstantopoulos, and B. M. Klein, *Phys. Rev. B* **41**, 10 311 (1990).

M. J. Mehl, J. E. Osburn, D. A. Papaconstantopoulos, and B. M. Klein, in *Alloy Phase Stability and Design*, edited by G. M. Stocks, D. P. Pope, and A. F. Giamei, MRS Symposia Proceedings No. 186 (Materials Research Society, Pittsburgh, 1991), pp. 277–282.



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### Database Statistics

86,680	56,447	21,954	530,243
INORGANIC COMPOUNDS	BANDSTRUCTURES	MOLECULES	NANOPOROUS MATERIALS
13,423	2,853	3,628	16,128
ELASTIC TENSORS	PIEZOELECTRIC TENSORS	INTERCALATION ELECTRODES	CONVERSION ELECTRODES

# VASP code & elastic constants

---

INCAR

KPOINTS

POTCAR

POSCAR

# VASP code & elastic constants

---

INCAR

KPOINTS

POTCAR

POSCAR

IBRION = 6

ISIF  $\geq$  3

POTIM = **0.015** +/-

NFREE = Integer (usually 2 / 4 )

# VASP code & elastic constants

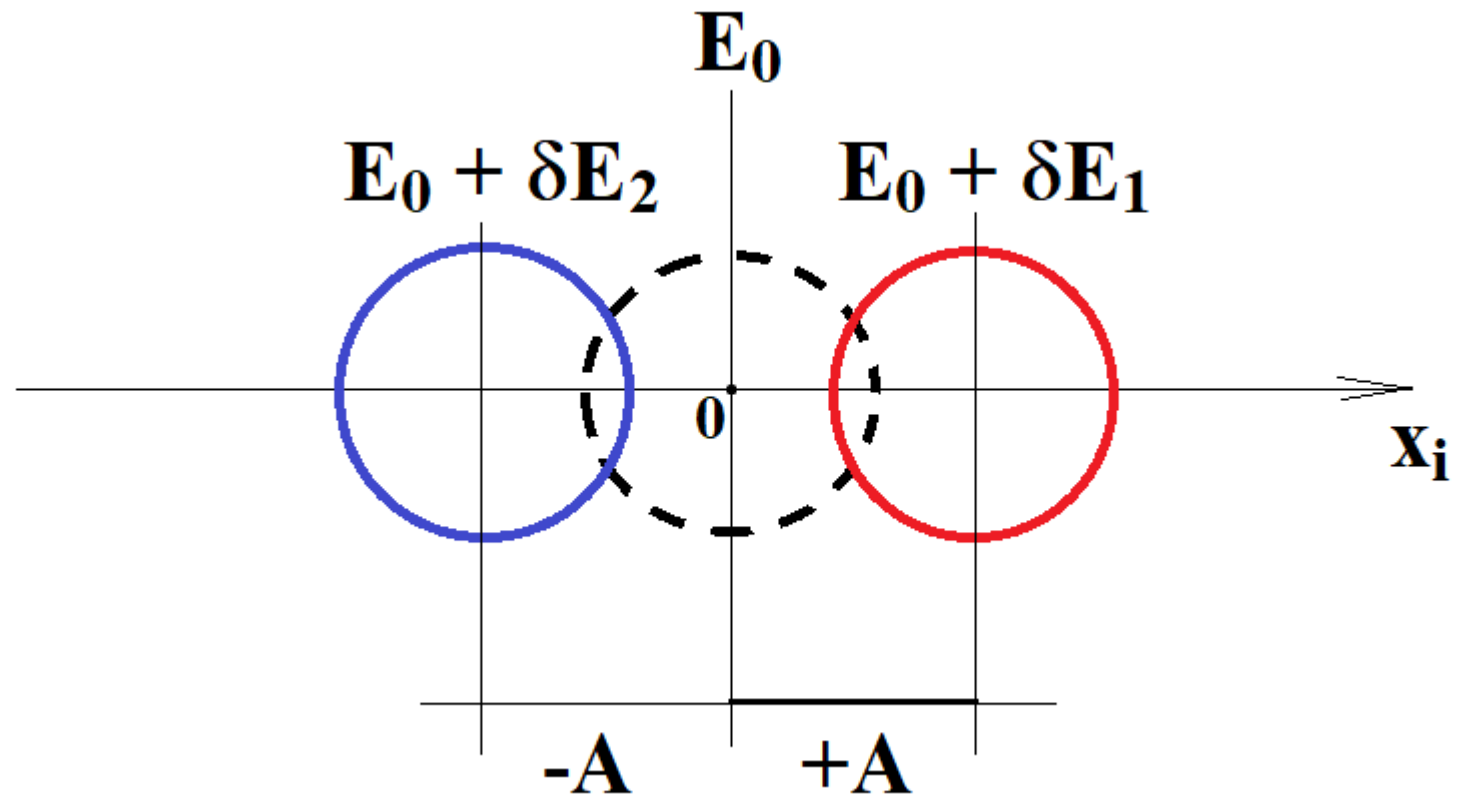
IBRION = 6

ISIF  $\geq 3$

POTIM = 0.015

NFREE = 2

POTIM = A



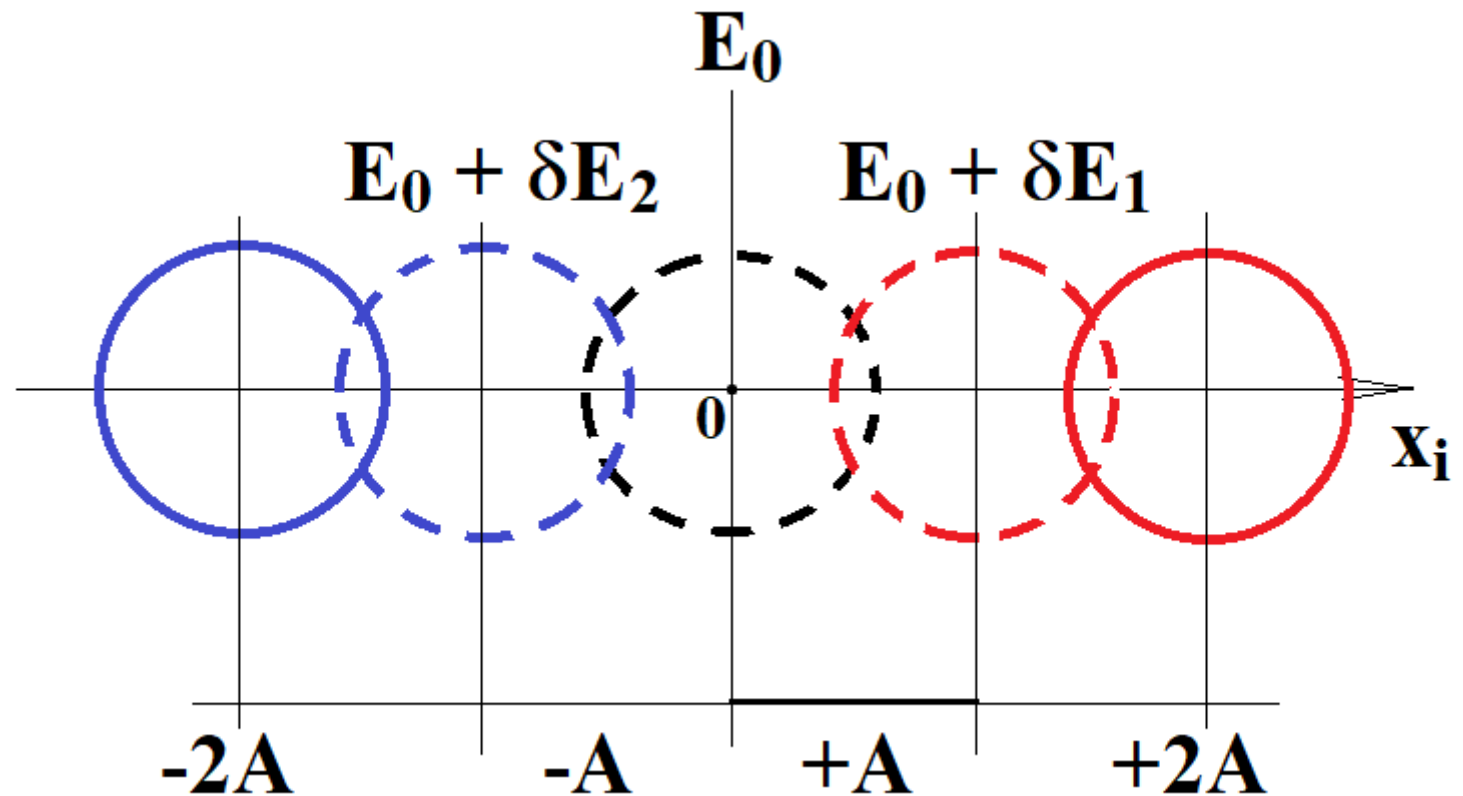
# VASP code & elastic constants

IBRION = 6

ISIF  $\geq 3$

POTIM = 0.015

NFREE = 4



# VASP code & elastic constants

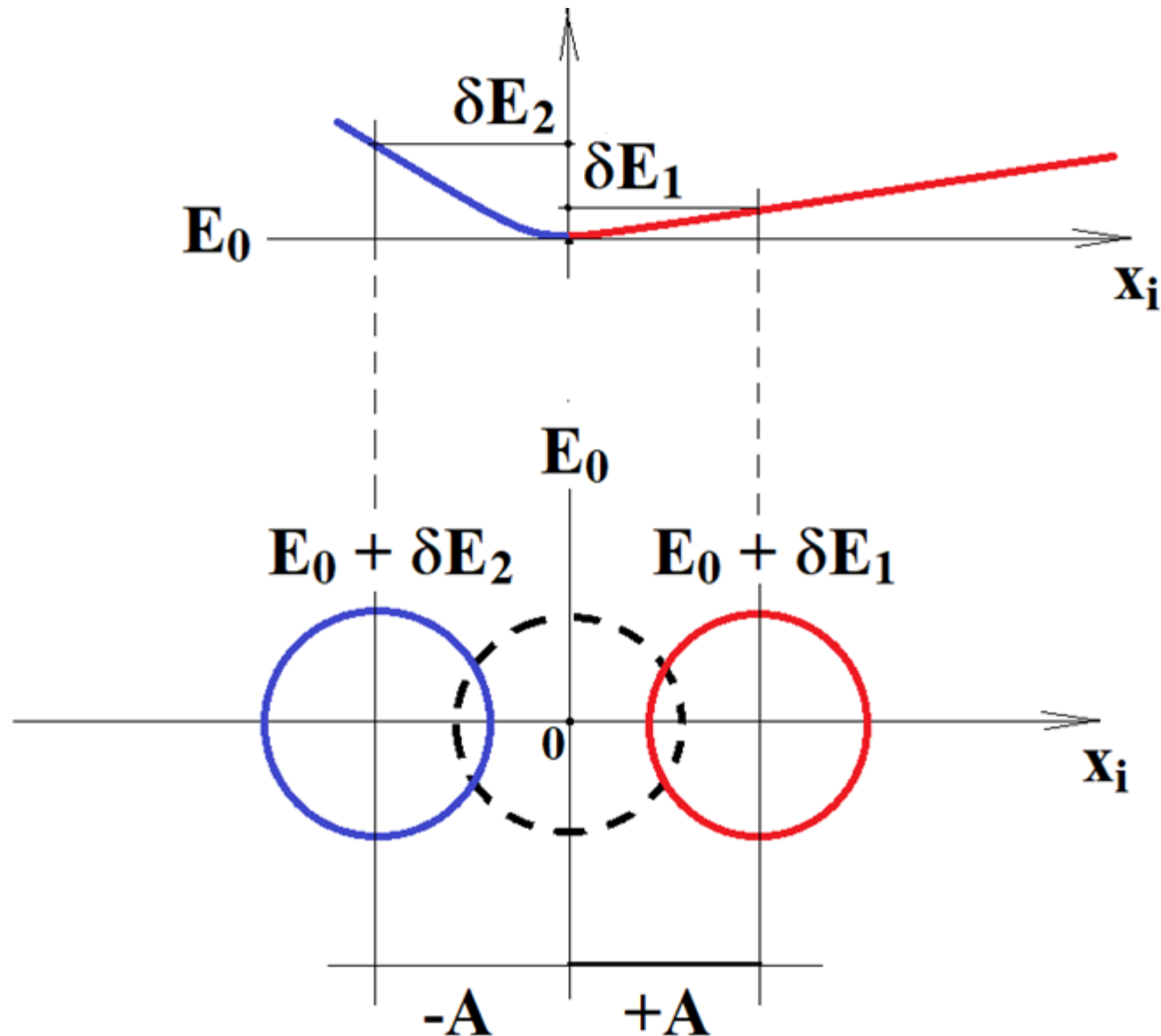
IBRION = 6

ISIF >= 3

POTIM = 0.015

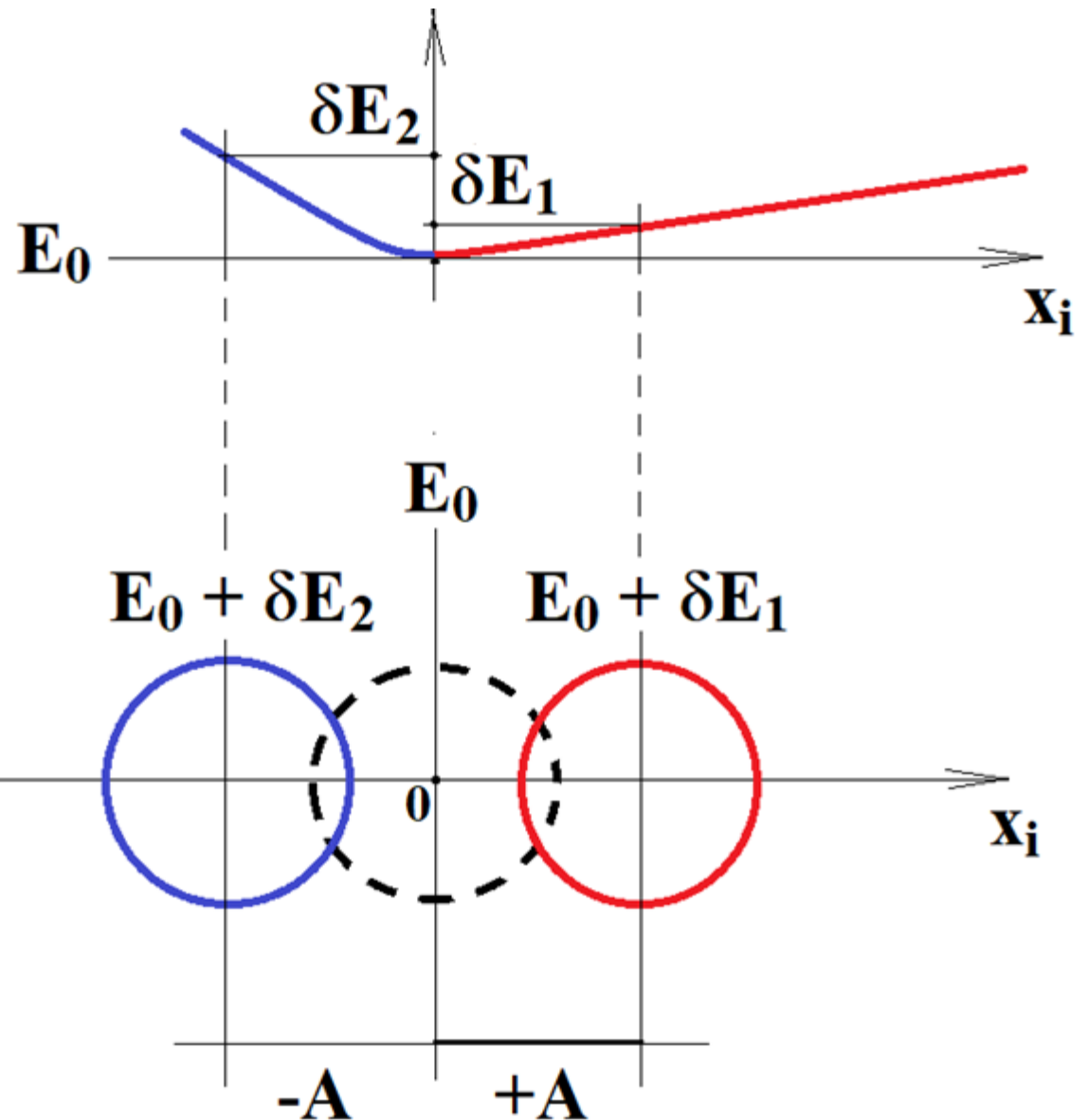
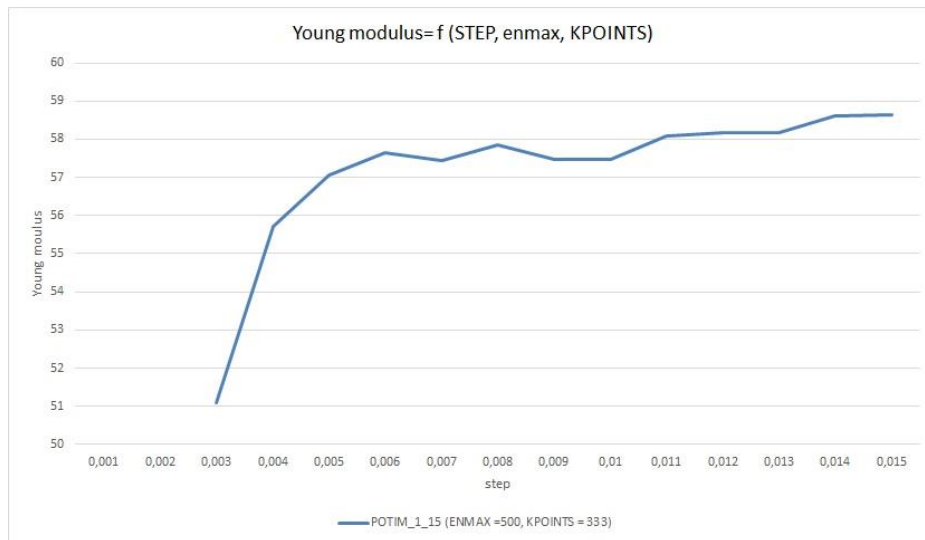
NFREE = 2

$$W = \frac{E}{V} = \frac{1}{2} C_{ijkl} \varepsilon_{ij} \varepsilon_{kl}$$



# VASP code & elastic constants

POTIM = 0.001÷0.015



# VASP input/output as an example

```
general:  
IBRION=6  
ISIF=3  
ENCUT=400  
ISMear=0;  
SIGMA=0.1  
EDIFF=1.d-4
```

```
TOTAL ELASTIC MODULI (kBar)  
Direction    XX          YY          ZZ          XY          YZ          ZX  
-----  
XX           11346.3730    48.4982    609.9718    -0.0000    0.0000    292.7267  
YY            48.4982   10185.3108   1435.5444    -0.0000    0.0000   -201.0226  
ZZ            609.9718   1435.5444  12664.2312    0.0000   -0.0000    93.5947  
XY           -0.0000    -0.0000    0.0000   3423.7069   397.8546    0.0000  
YZ           -0.0000    0.0000   -0.0000   397.8546  5052.2823    0.0000  
ZX           292.7267   -201.0226    93.5947    0.0000    0.0000   4910.2493  
-----
```

**The Born criterion**

# VASP input/output as an example

## Al. LDA results

TOTAL ELASTIC MODULI (kBar)						
Direction	XX	YY	ZZ	XY	YZ	ZX
XX	919.3255	588.6109	588.5349	0.0309	-0.0143	-0.0000
YY	588.6109	918.7531	588.3125	0.0271	-0.0022	0.0016
ZZ	588.5349	588.3125	918.7523	0.0886	-0.0100	0.0056
XY	0.0309	0.0271	0.0886	316.7230	-0.1000	-0.0250
YZ	-0.0143	-0.0022	-0.0100	-0.1000	316.3742	-0.0743
ZX	-0.0000	0.0016	0.0056	-0.0250	-0.0743	316.5473

## Al. GGA results

TOTAL ELASTIC MODULI (kBar)						
Direction	XX	YY	ZZ	XY	YZ	ZX
XX	1001.0323	629.9660	629.8624	-0.0394	0.0261	0.0103
YY	629.9660	1000.2397	629.5681	-0.0189	0.0051	0.0264
ZZ	629.8624	629.5681	1000.2403	0.0258	0.0112	0.0017
XY	-0.0394	-0.0189	0.0258	359.4068	-0.4186	-0.0766
YZ	0.0261	0.0051	0.0112	-0.4186	358.5990	-0.4874
ZX	0.0103	0.0264	0.0017	-0.0766	-0.4874	358.5127

T, °K	C <sub>11</sub> , 10 <sup>10</sup> Pa	C <sub>12</sub> , 10 <sup>10</sup> Pa	C <sub>44</sub> , 10 <sup>10</sup> Pa
300	10,73	6,08	2,83
77	11,42	6,31	3,06
4	11,63	6,48	3,09

# Bulk & Shear moduli

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**Cubic phase ( $C_{11}$ ,  $C_{44}$ , and  $C_{12}$ )**

$$B_V = B_R = (C_{11} + 2C_{12})/3,$$

$$G_V = (C_{11} - C_{12} + 3C_{44})/5,$$

$$G_R = 5(C_{11} - C_{12})C_{44}/[4C_{44} + 3(C_{11} - C_{12})]$$

**Tetragonal phase ( $C_{11}$ ,  $C_{33}$ ,  $C_{44}$ ,  $C_{66}$ ,  $C_{12}$ , and  $C_{13}$ )**

$$B_V = (1/9)[2(C_{11} + C_{12}) + C_{33} + 4C_{13}],$$

$$G_V = (1/30)(M + 3C_{11} - 3C_{12} + 12C_{44} + 6C_{66}),$$

$$B_R = C^2/M,$$

$$G_R = 15\{(18B_V/C^2) + [6/(C_{11} - C_{12})] + (6/C_{44}) + (3/C_{66})\}^{-1},$$

$$M = C_{11} + C_{12} + 2C_{33} - 4C_{13},$$

$$C^2 = (C_{11} + C_{12})C_{33} - 2C_{13}^2.$$

# Bulk & Shear moduli

Monoclinic phase ( $C_{11}, C_{22}, C_{33}, C_{44}, C_{55}, C_{66}, C_{12}, C_{13}, C_{23},$   
 $C_{15}, C_{25}, C_{35},$  and  $C_{46}$ )

$$B_V = (1/9)[C_{11} + C_{22} + C_{33} + 2(C_{12} + C_{13} + C_{23})],$$

$$G_V = (1/15)[C_{11} + C_{22} + C_{33} + 3(C_{44} + C_{55} + C_{66}) \\ - (C_{12} + C_{13} + C_{23})],$$

$$B_R = \Omega[a(C_{11} + C_{22} - 2C_{12}) + b(2C_{12} - 2C_{11} - C_{23}) \\ + c(C_{15} - 2C_{25}) + d(2C_{12} + 2C_{23} - C_{13} - 2C_{22}) \\ + 2e(C_{25} - C_{15}) + f]^{-1},$$

$$G_R = 15\{4[a(C_{11} + C_{22} + C_{12}) + b(C_{11} - C_{12} - C_{23}) + c(C_{15} \\ + C_{25}) + d(C_{22} - C_{12} - C_{23} - C_{13}) + e(C_{15} - C_{25}) + f]/\Omega \\ + 3[g/\Omega + (C_{44} + C_{66})/(C_{44}C_{66} - C_{46}^2)]\}^{-1},$$

$$a = C_{33}C_{55} - C_{35}^2,$$

$$b = C_{23}C_{55} - C_{25}C_{35},$$

$$c = C_{13}C_{35} - C_{15}C_{33},$$

$$d = C_{13}C_{55} - C_{15}C_{35},$$

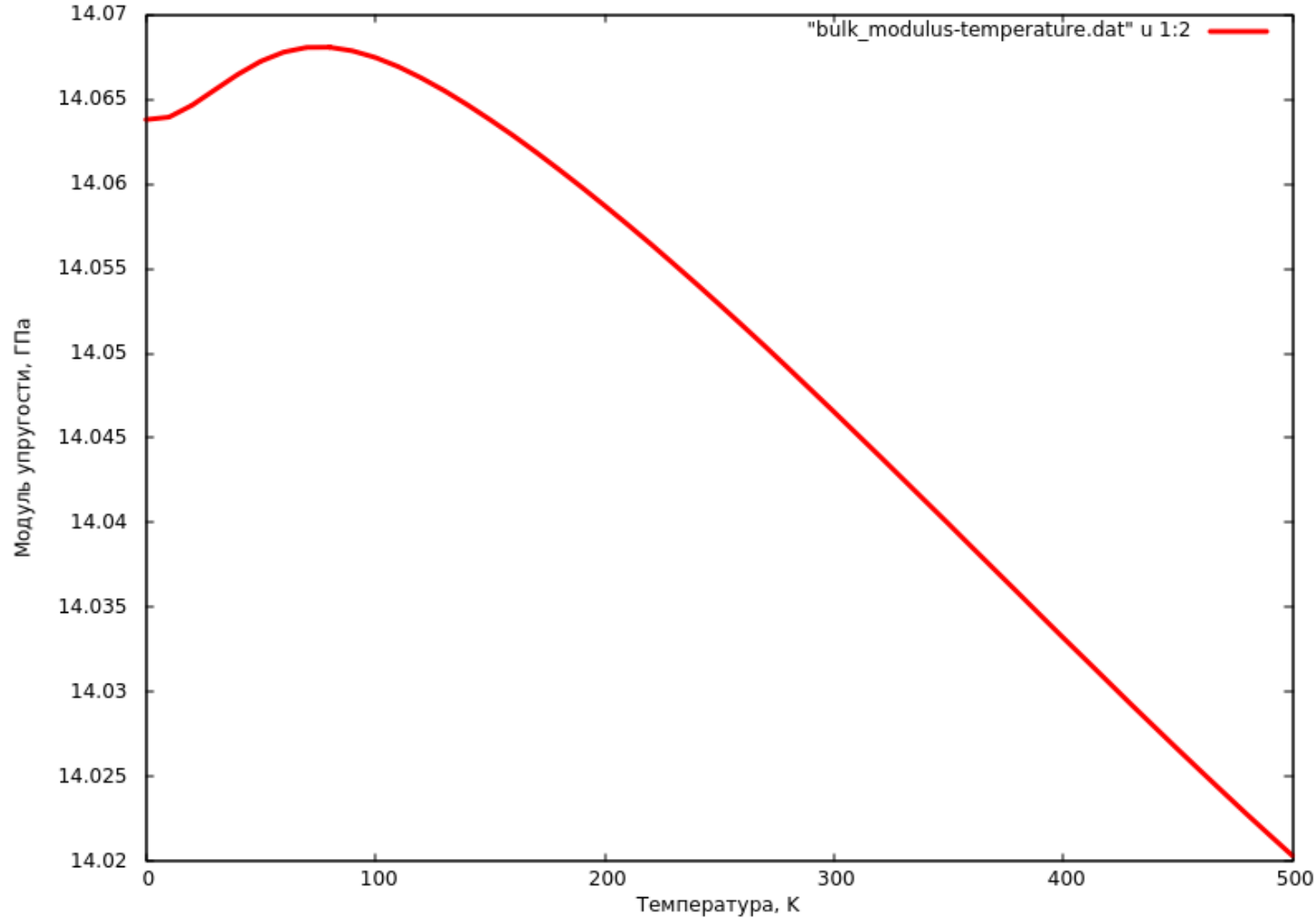
$$e = C_{13}C_{25} - C_{15}C_{23},$$

$$f = C_{11}(C_{22}C_{55} - C_{25}^2) - C_{12}(C_{12}C_{55} - C_{15}C_{25}) \\ + C_{15}(C_{12}C_{25} - C_{15}C_{22}) + C_{25}(C_{23}C_{35} - C_{25}C_{33}),$$

$$g = C_{11}C_{22}C_{33} - C_{11}C_{23}^2 - C_{22}C_{13}^2 - C_{33}C_{12}^2 + 2C_{12}C_{13}C_{23},$$

$$\Omega = 2[C_{15}C_{25}(C_{33}C_{12} - C_{13}C_{23}) + C_{15}C_{35}(C_{22}C_{13} - C_{12}C_{23}) \\ + C_{25}C_{35}(C_{11}C_{23} - C_{12}C_{13})] - [C_{15}^2(C_{22}C_{33} - C_{23}^2) \\ + C_{25}^2(C_{11}C_{33} - C_{13}^2) + C_{35}^2(C_{11}C_{22} - C_{12}^2)] + gC_{55}.$$

# Bulk & Shear moduli



B(T) for Li

**VASP+PHONOPY**

# Bulk & Shear moduli

TABLE I. Calculated lattice constants (in Å) and bulk modulus  $B_0$  (in GPa) and its pressure derivative  $B'_0$  of  $\text{KMgF}_3$  at the theoretical equilibrium volume compared with the experiment and other theoretical calculations. The bulk moduli have been calculated both at the experimental and theoretical volumes [ $B_0(V_0^{\text{exp}})$  and  $B_0(V_0^{\text{th}})$ , respectively].

	Lattice constant	$B_0(V_0^{\text{th}})$	$B_0(V_0^{\text{exp}})$	$B'_0$
GGA <sup>a</sup>	4.0809	72.01	97.85	4.65
LDA <sup>a</sup>	3.9630	91.47	83.23	4.79
LDA, LAPW <sup>b</sup>	3.91	90.97		4.64
Experiment	4.0060(2), <sup>a</sup> 3.973, <sup>c</sup> 3.978±0.05, <sup>d</sup> 3.9897, <sup>e</sup> 3.993, <sup>f</sup> 3.9839 <sup>g</sup>		71.2(2), <sup>a</sup> 70.4, <sup>h</sup> 75.1, <sup>i</sup> 75.6 <sup>j</sup>	4.7(3) <sup>a</sup>

<sup>a</sup>Present work.

<sup>b</sup>Reference 19.

<sup>c</sup>Reference 10.

<sup>d</sup>Reference 34.

<sup>e</sup>Reference 36.

<sup>f</sup>Reference 35.

<sup>g</sup>Reference 29.

<sup>h</sup>Reference 12.

<sup>i</sup>Reference 13.

<sup>j</sup>Reference 14.

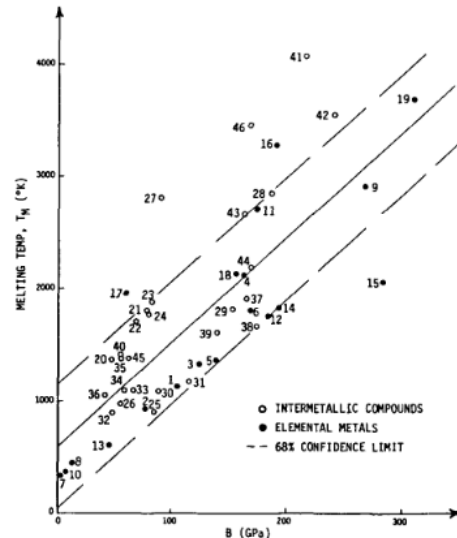
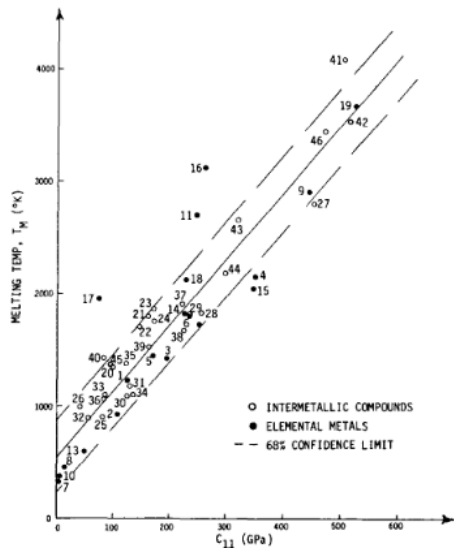
# Some useful relations

Newton-Laplace equation:

$$c_{\text{solid,p}} = \sqrt{\frac{B_0 + \frac{4}{3}G}{\rho}} = \sqrt{\frac{E(1-\nu)}{\rho(1+\nu)(1-2\nu)}}$$

$$c_{\text{solid,s}} = \sqrt{\frac{G}{\rho}}$$

Correlations with melting point:



Soft and fragile materials:

$$\frac{B}{G} < \sim 1.75 - \text{fragile}$$

$$\frac{B}{G} > \sim 1.75 - \text{soft}$$

Young's modulus:  $E = 2G(1 + \nu) = 3B(1 - 2\nu)$

Poisson's ratio: For isotropic materials

$$\nu \approx \frac{1}{2} - \frac{E}{6B}$$

percentage of elastic anisotropy:

$$A = \frac{2c_{44}}{c_{11} - c_{12}} \quad (\text{Zener})$$

$$A^C = \frac{G_V - G_R}{G_V + G_R} \quad (\text{Chung-Buessem})$$

Thank you for attention

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