# Lecture: P1_Wk2_L4

# Elasticity of Materials

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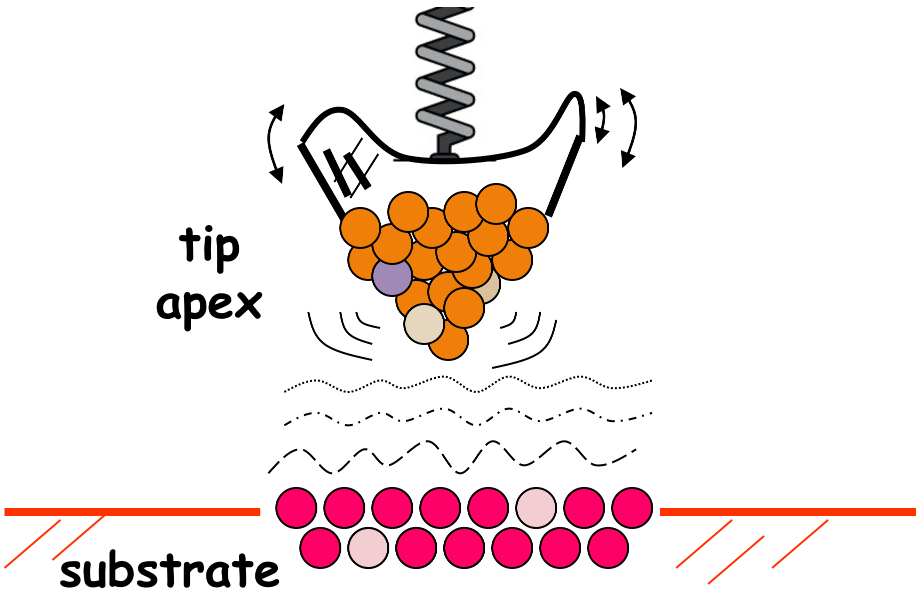
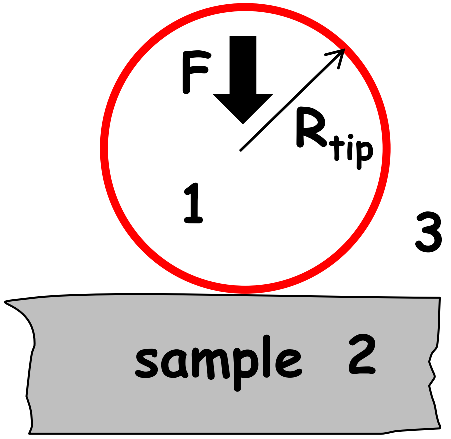
# Nanomechanics - what happens at contact?

Atom-Atom?

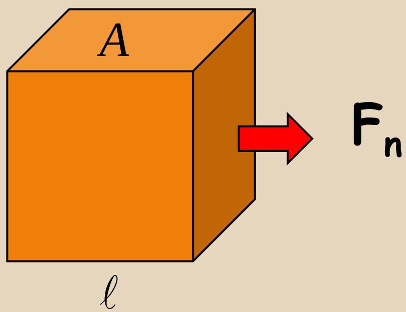
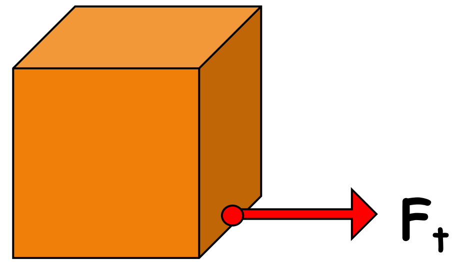
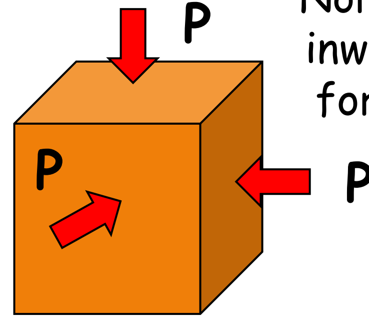
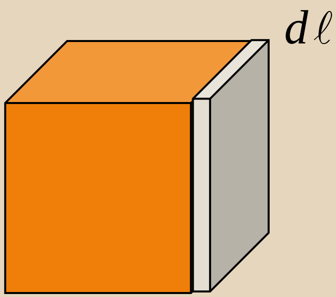
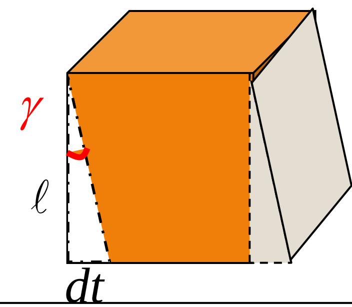
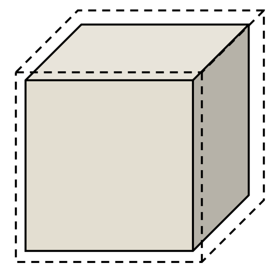



Sphere-Plane?




Maybe if the contact area involves tens or hundreds of atoms the description of net repulsive force is best captured by continuum elasticity models

# External Forces Deform Solids

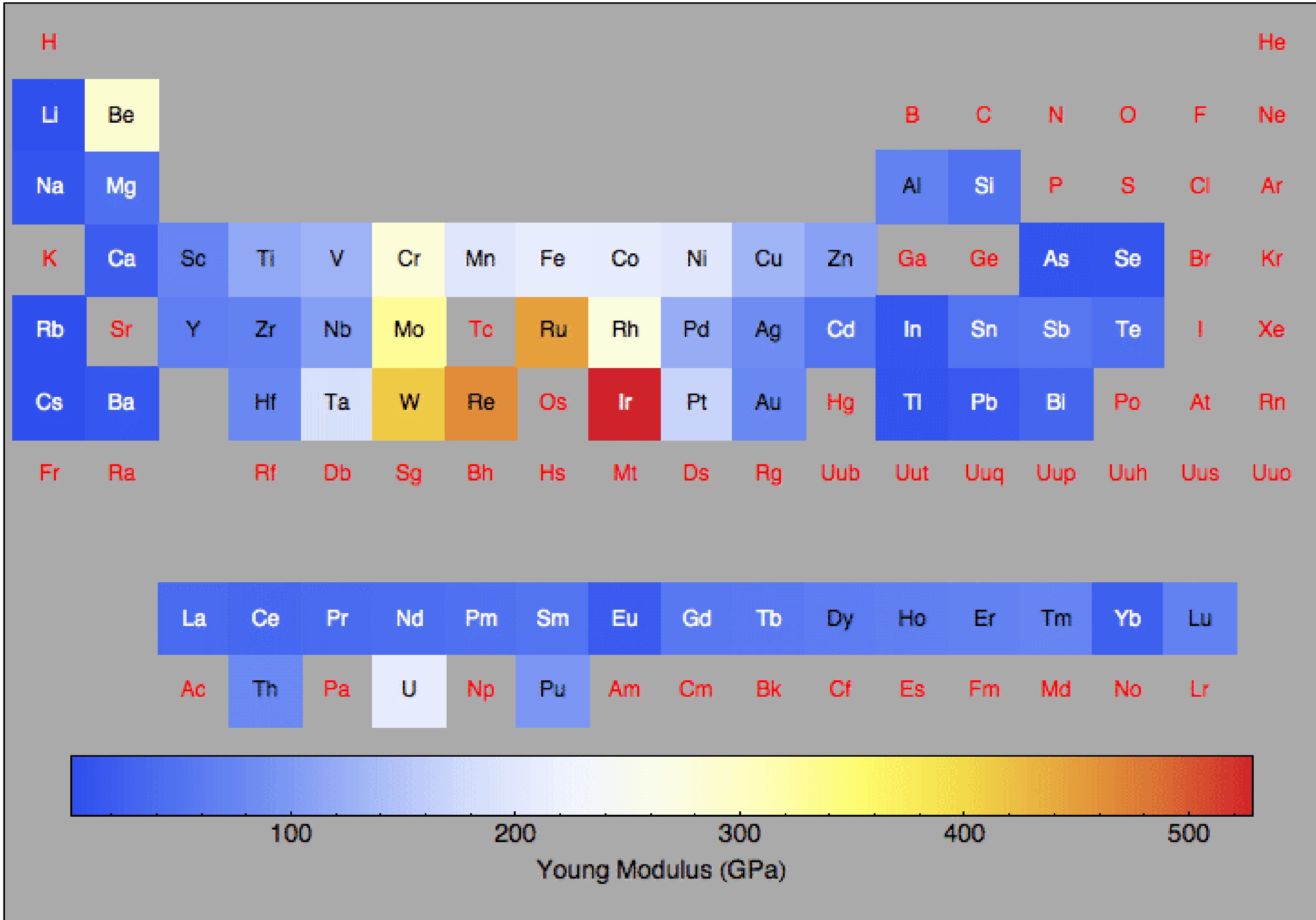
| Normal Stress | Tangential Stress | Bulk Stress |
|---|---|---|
| Normal force  | Tangential force  | Normal inward force  |
|  |  |  |
| Young's Modulus $E = \frac{F/A}{dl/l} \equiv \frac{\text{stress}}{\text{strain}} = \frac{F}{A} \times \frac{l}{dl}$ | Shear Modulus $G = \frac{F_t/A}{dt/l} = \frac{F_t l}{A\,dt} = \frac{1}{\gamma}\frac{F_t}{A}$ | Bulk Modulus $B = \frac{P}{-dV/V} = -\frac{PV}{dV}$ |

$$E \left[ units : \frac{N}{m^2} = Pa \right]$$

(for homogeneous isotropic materials):

$$E = 2G(1+\nu) \qquad E = 3B(1-2\nu)$$

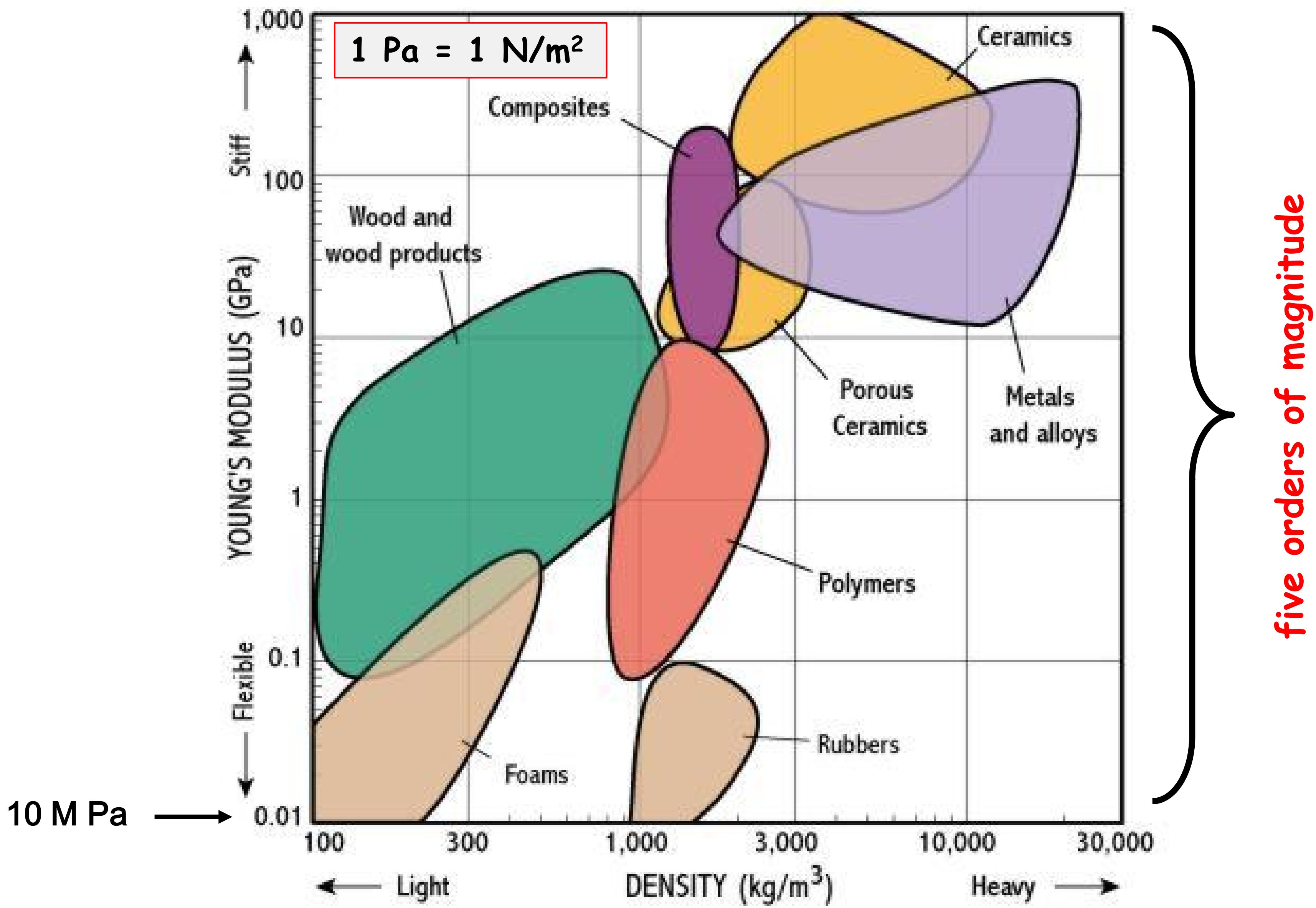
# Young's Modulus of the Elements






Source: http://periodictable.com/Properties/

# Young's Modulus by material class






http://www-materials.eng.cam.ac.uk/mpsite/interactive_charts/stiffness-density/NS6Chart.html

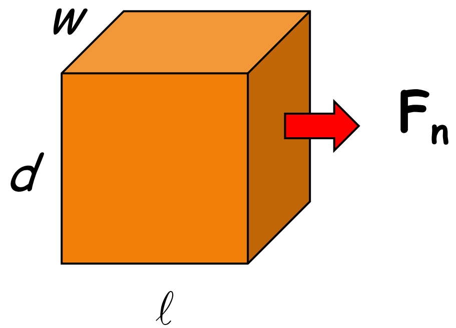
# Young's Modulus – various materials

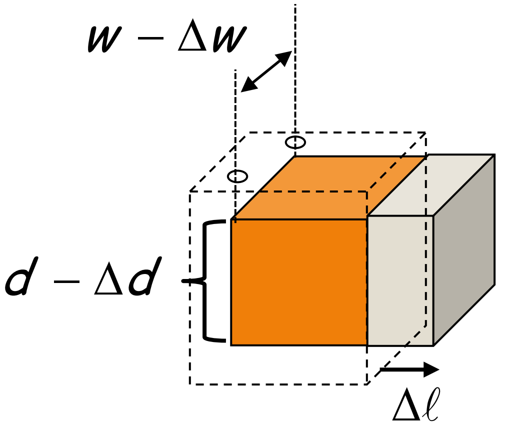
| Material | Young's Modulus (Gpa) |
|---|---|
| Stainless Steel | 190-210 |
| Ti | 116 |
| Al 7075 | 72 |
| Invar 36 | 147 |
| Si | 179 |
| Au | 79 |
| W | 400 |
| Super Invar | 148 |
| Pyrex | 61 |
| Zerodur | 91 |
| $SiO_2$ (crystalline quartz) | 72 |
| Sapphire ($Al_2O_3$) | 345 |
| HOPG | 36 ($\perp$ to basal plane) |
| $SiO_2$ (oxide film) | 66 |
| Muscovite Mica | 48 (parallel to c-axis) |

Higher thermal conductivity (Stainless Steel through Super Invar)

Lower thermal conductivity (Pyrex through Muscovite Mica)

# A normal stress produces strains in lateral directions

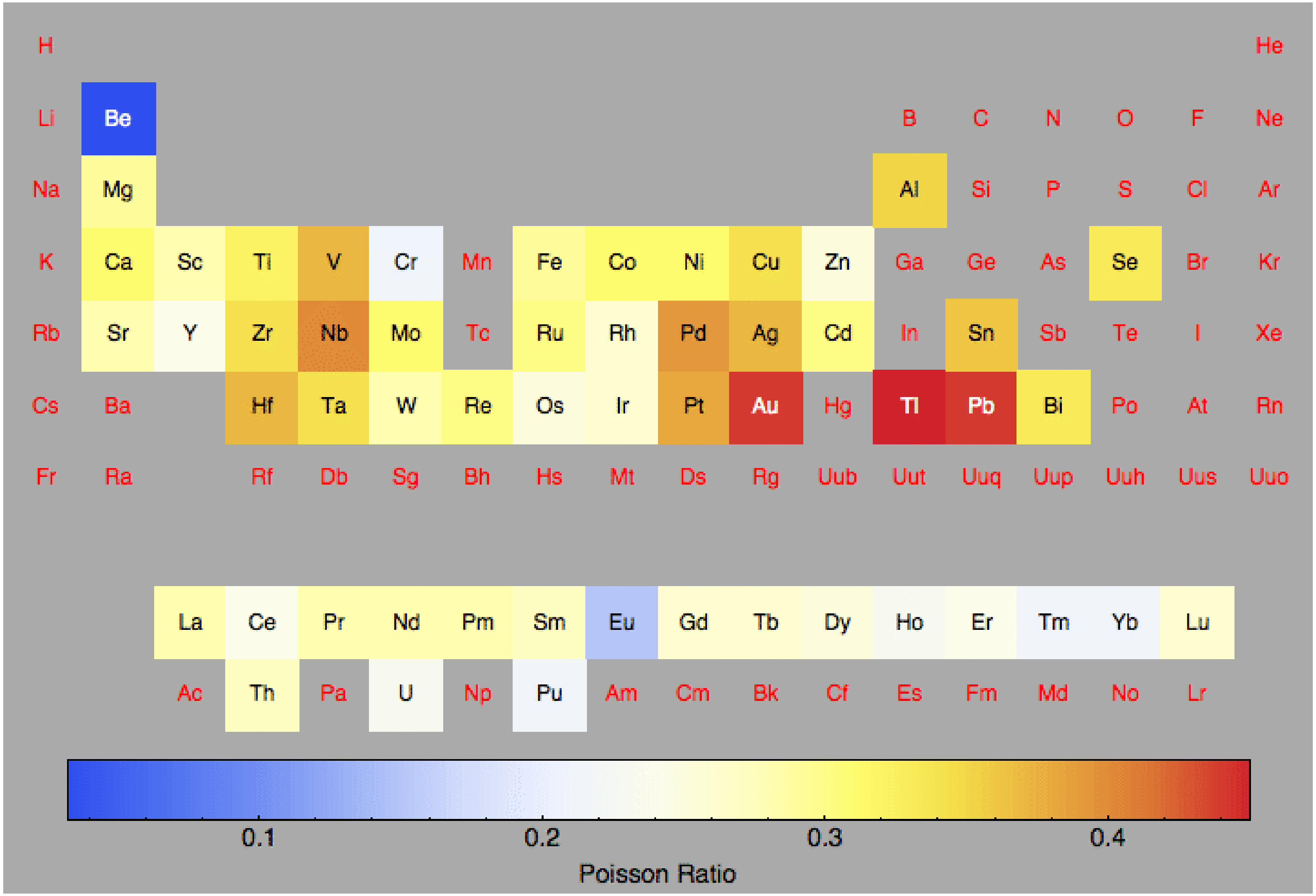



longitudinal elongation,
lateral contraction

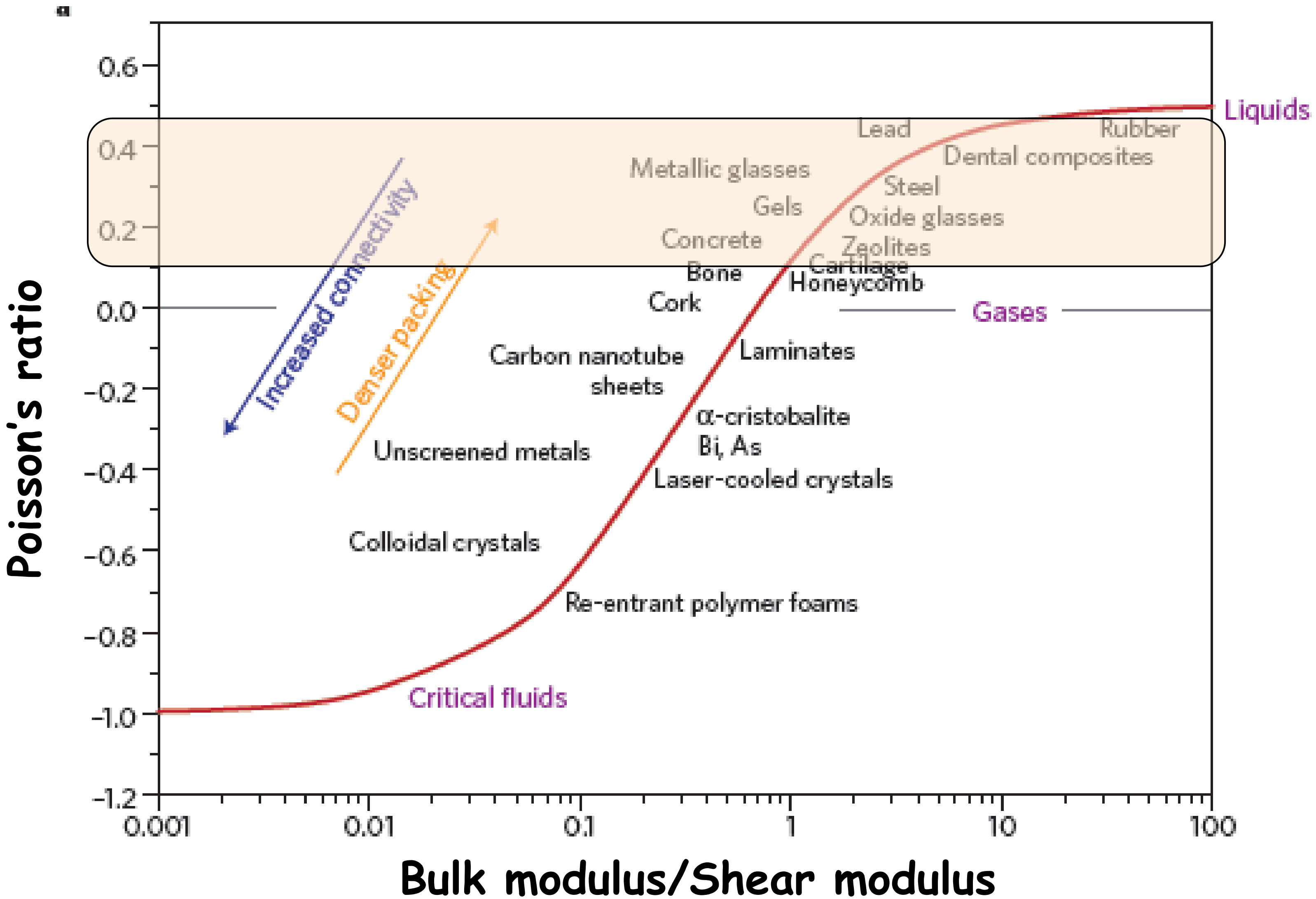
$$\text{Poisson ratio} = \nu = \frac{-\Delta d / d}{\Delta \ell / \ell} = \frac{-\Delta w / w}{\Delta \ell / \ell}$$

# Poisson's Ratio for the Elements



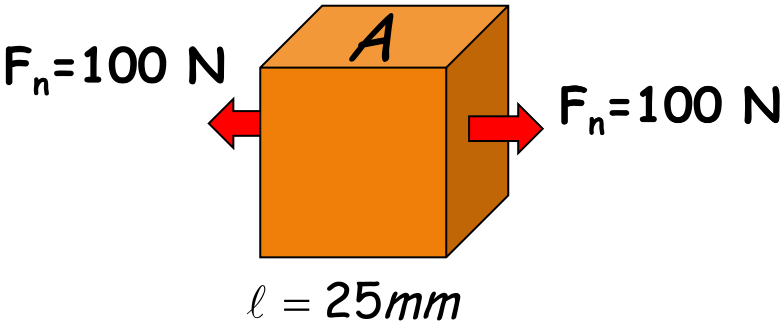

 Source: http://periodictable.com/Properties/

# Poisson's Ratio by material class




G. N. Greaves, et al. Nature Materials **10**, 823 (2011)

**Example:** A cube of material 25 mm on a side has a Poisson ratio of 0.3. An outward force of 100 N is applied to opposite faces, causing an extension of 200 nm.




a) What is the normal stress on the cube?

$$Stress = \frac{F_n}{A} = \frac{100N}{(0.025m)^2} = 1.6 \times 10^5\,Pa \simeq 1.6\ atmospheres$$

b) What is the normal strain in the cube?

$$Strain = \frac{\Delta\ell}{\ell} = \frac{200nm}{(0.025m)} = 8 \times 10^{-6}$$

c) What is Young's modulus?

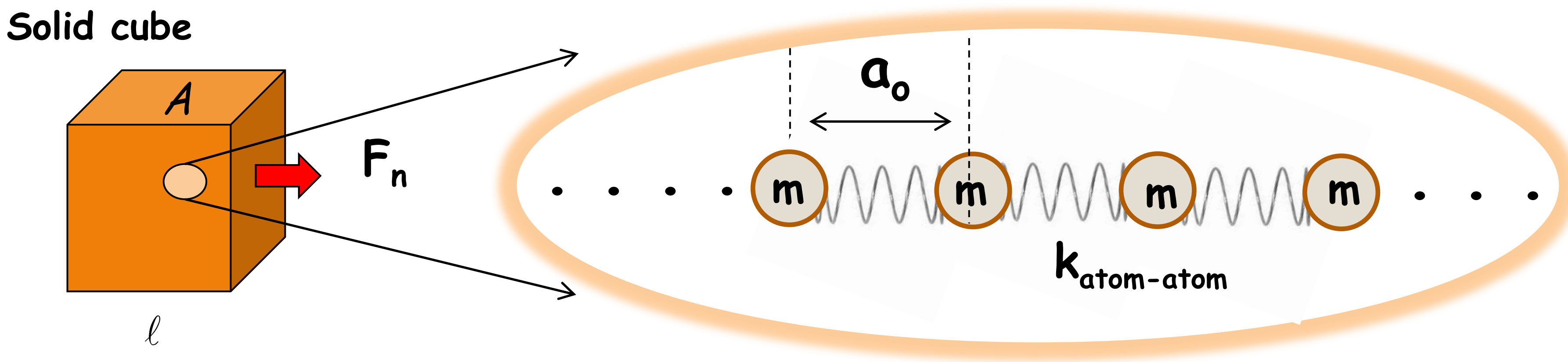
$$E = \frac{stress}{strain} = \frac{1.6 \times 10^5\,Pa}{8 \times 10^{-6}} = 20\,GPa$$

d) What is the lateral displacement on the sides of the cube?

$$\nu = -\frac{\Delta d / d}{\Delta\ell / \ell} \Rightarrow \Delta d = -\nu\left(\Delta\ell / \ell\right) d$$

$$\Delta d = -0.3\left(8 \times 10^{-6}\right)(0.025m) = -60nm$$

# Microscopic Model for Young's Modulus




$$\text{define} \quad dF \equiv -\frac{F_n}{\text{No. atoms in area } A} = -\frac{F_n}{(\text{No. atoms in length } \ell)^2}$$

$$= -\frac{F_n}{(\ell/a_o)^2} = -\left(\frac{F_n}{\ell^2}\right)\cdot a_o^2$$

$$\text{by definition,} \quad \text{Stress} \equiv \frac{F_n}{A} = \left(\frac{F_n}{\ell^2}\right) \qquad \text{Strain} \equiv \frac{\Delta\ell}{\ell} = \frac{da_o}{a_o}$$

$$dF = -\left(\frac{F_n}{\ell^2}\right)\cdot a_o^2 = -\text{Stress}\times a_o\left(\frac{da_o}{\text{Strain}}\right)$$

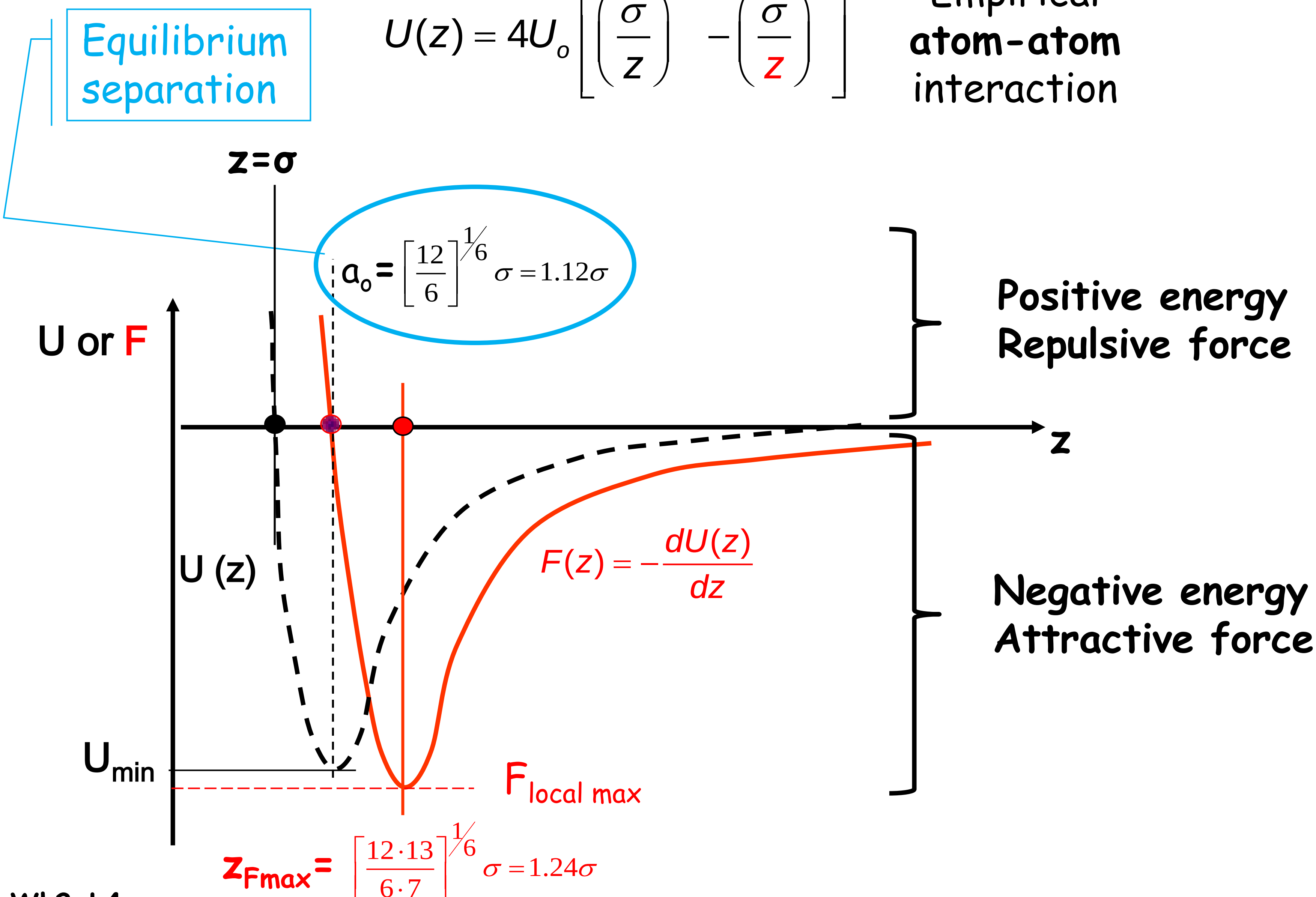
$$= -\left(\frac{\text{Stress}}{\text{Strain}}\times a_o\right)da_o$$

$$= -(E\times a_o)da_o = -k_{atom-atom}da_o \quad \Rightarrow k_{atom-atom} = Ea_o$$

# Correlation with atomic interaction potentials (Lennard-Jones)

$$U(z) = 4U_o\left[\left(\frac{\sigma}{z}\right)^{12} - \left(\frac{\sigma}{z}\right)^{6}\right]$$

Empirical **atom-atom** interaction



# Near z=a$_o$, an atom will obey Hook's Law

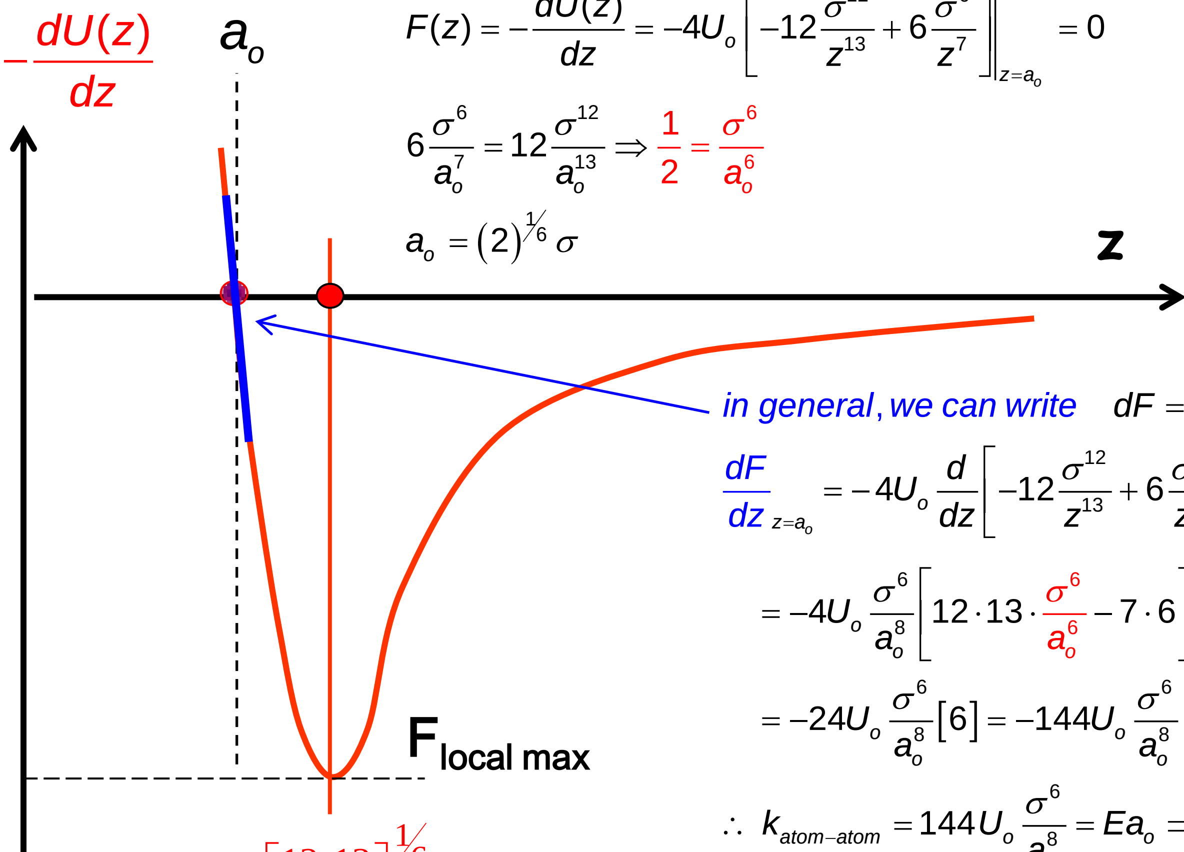
$$U(z) = 4U_o\left[\left(\frac{\sigma}{z}\right)^{12} - \left(\frac{\sigma}{z}\right)^{6}\right]$$

$$F(z) = -\frac{dU(z)}{dz} = -4U_o\left[-12\frac{\sigma^{12}}{z^{13}} + 6\frac{\sigma^{6}}{z^{7}}\right]\Bigg|_{z=a_o} = 0$$

$$6\frac{\sigma^6}{a_o^7} = 12\frac{\sigma^{12}}{a_o^{13}} \Rightarrow \frac{1}{2} = \frac{\sigma^6}{a_o^6}$$

$$a_o = (2)^{1/6}\sigma$$

$$F(z) = -\frac{dU(z)}{dz}$$




$$z_{Fmax} = \left[\frac{12\cdot 13}{6\cdot 7}\right]^{1/6}\sigma = 1.24\sigma$$

$$\text{in general, we can write} \quad dF = -k_{atom-atom}\,dz$$

$$\frac{dF}{dz}\bigg|_{z=a_o} = -4U_o\frac{d}{dz}\left[-12\frac{\sigma^{12}}{z^{13}} + 6\frac{\sigma^{6}}{z^{7}}\right]\Bigg|_{z=a_o} = -4U_o\left[12\cdot 13\frac{\sigma^{12}}{a_o^{14}} - 7\cdot 6\frac{\sigma^{6}}{a_o^{8}}\right]$$

$$= -4U_o\frac{\sigma^6}{a_o^8}\left[12\cdot 13\cdot\frac{\sigma^6}{a_o^6} - 7\cdot 6\right] = -24U_o\frac{\sigma^6}{a_o^8}\left[2\cdot 13\cdot\frac{1}{2} - 7\right]$$

$$= -24U_o\frac{\sigma^6}{a_o^8}[6] = -144U_o\frac{\sigma^6}{a_o^8}$$

$$\therefore\ k_{atom-atom} = 144U_o\frac{\sigma^6}{a_o^8} = Ea_o \Rightarrow E = 144U_o\frac{\sigma^6}{a_o^9}$$

$$= 144U_o\left(\frac{\sigma^6}{a_o^6}\right)\frac{1}{a_o^3} = \frac{72U_o}{a_o^3}$$

$$U_o = \frac{Ea_o^3}{72}$$ perhaps too simplistic?

Example: for Au atoms, Lenard-Jones parameters*: σ=0.216 nm, $U_o$=4.46 eV; $E_{Au}$=80 Gpa (from handbooks)

$$a_o = (2)^{1/6}\sigma$$

$$k_{atom-atom} = Ea_o = \left(80\times10^9 Pa\right)\cdot\left(2^{1/6}\cdot 0.216\times10^{-9} m\right) = 20\ N/m$$

$$U_o\Big|_{\substack{simple\\theory}} = \frac{Ea_o^3}{72} = \frac{\left(80\times10^9 Pa\right)\cdot\left(2^{1/6}\cdot 0.216\times10^{-9} m\right)^3}{72}$$

$$= 1.58\times10^{-20} J\cdot\left(\frac{1eV}{1.6\times10^{-19} J}\right)\approx 0.1eV$$

$U_o$ is about a factor of 45 too small compared to the 4.46 eV value found in the literature.

*See for example, de Bas et al., J. Molec. Structure (Theochem) **686**, 193 (2004).

## Up Next: An Introduction to Contact Mechanics