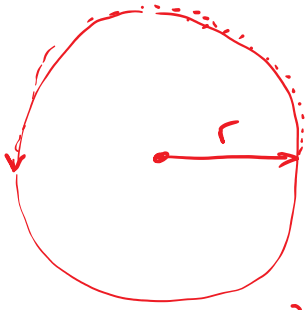
APS110H1f2024 Sept 23 2024

September 23, 2024 9:38 AM

Atomic Packing Factor (APF)

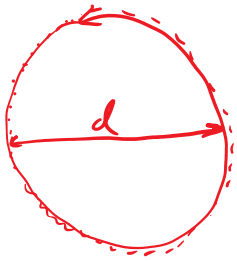
2D



radius

$r = 1$ $\pi = 3.14159 \times 2$

circumferences



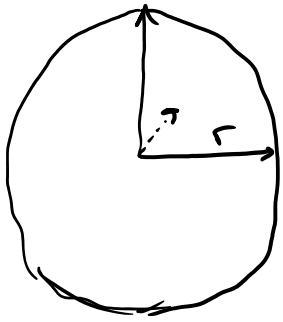
diameter

$d = 1$ $\pi = 3.141592653 5$

$= 3.14159$

$$\text{volume} = \frac{4}{3}\pi R^3$$

of an atom / 1 atom.



3D

$1\ pm = 1e^{-10}\ cm$

$1\ cm = 1e^{10}\ pm$

FCC --> APF

September 23, 2024 10:30 AM

APF - atomic packing factor

$$APF = \frac{\text{volume}_{\text{spheres}}}{\text{volume}_{\text{unit cell}}}$$ (spheres: atoms)

$$APF = \frac{n \frac{4}{3} \pi R^3}{a^3}$$ only metals.

$$= \frac{n \frac{4}{3} \pi R^3}{x \cdot y \cdot z}$$ = only 1 metal

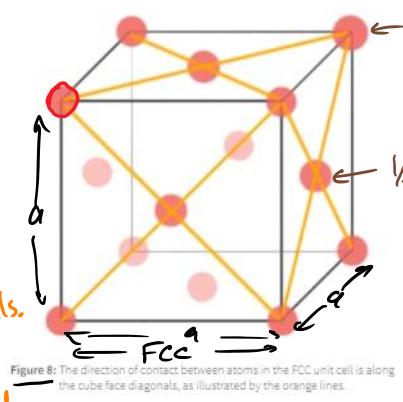
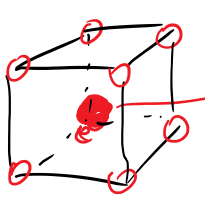


Figure 8: The direction of contact between atoms in the FCC unit cell is along the cube face diagonals, as illustrated by the orange lines.

$\frac{1}{8} \times 8 = 1$

$\frac{1}{2} \times 6 = 3$

$\rightarrow 4 = n$



$\frac{1}{8} \times 8 = 1$

$1 = 1$ $\rightarrow 2$

Fe / iron

↳ 194 pm

FCC - face centred cubic

$$a_{FCC} = 2\sqrt{2}R$$

$$= 548.7096 \text{ pm}$$

$\sqrt{2} = 1.4142$? ✓ Yes is a yes

$\sqrt{4} = 2$? ✓ Yes - is a yes

$$APF = \frac{n \frac{4}{3} \pi R^3}{FCC^3} = \frac{n \frac{4}{3} \pi R^3}{(2\sqrt{2}R)^3}$$

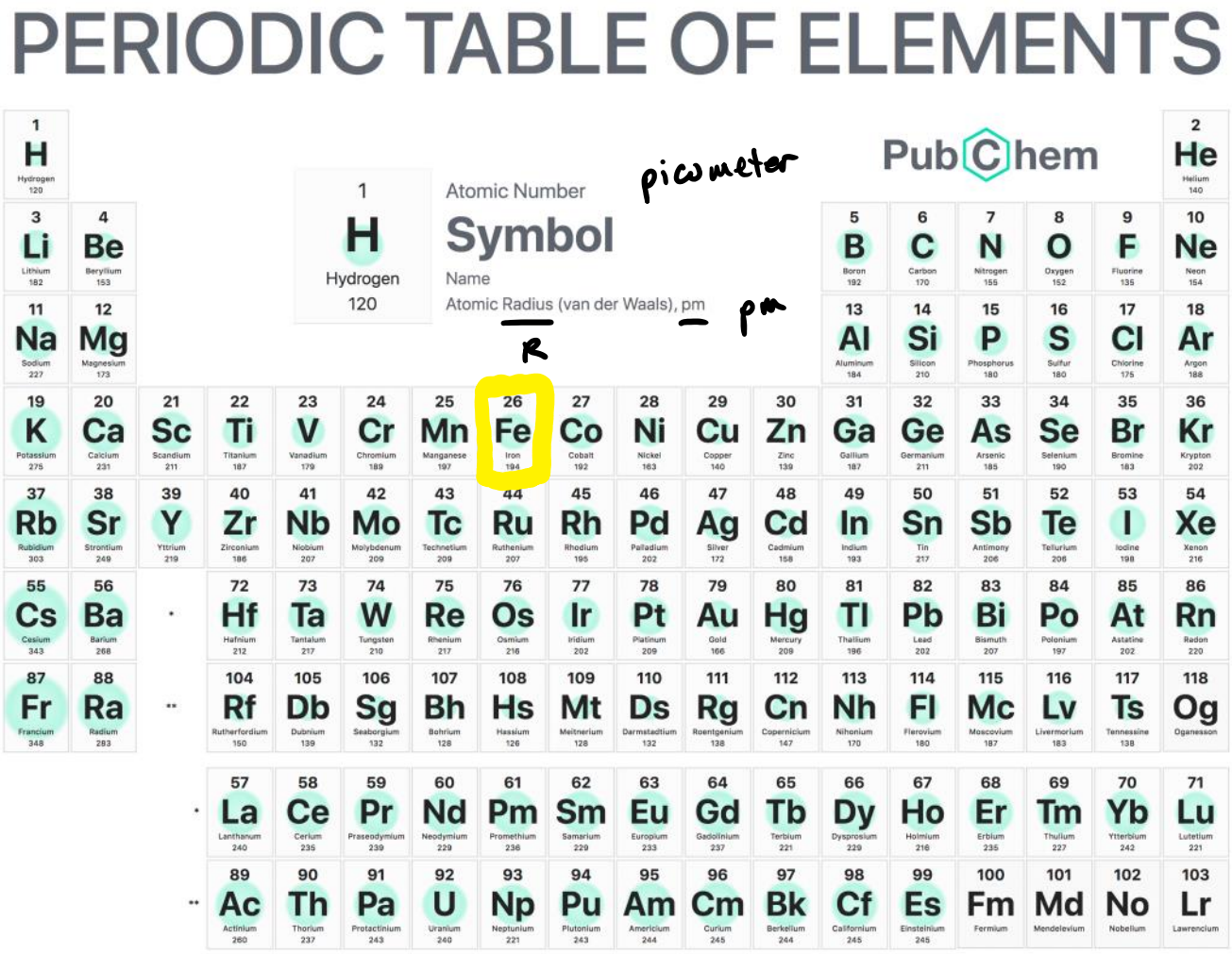
iron

$$APF = \frac{4 \cdot \frac{4}{3} \cdot 3.14159 \cdot (194 \text{ pm})^3}{(548.7096 \text{ pm})^3} = 668451.0380$$

density

Periodic Table

September 23, 2024 10:54 AM



APS110H1f2024 Sept 25 2024

September 24, 2024 4:38 PM

BCC --> FCC

BCC : Body Centred Cubic (Crystal Structure/Nanostructure)

stress + strain

metal only

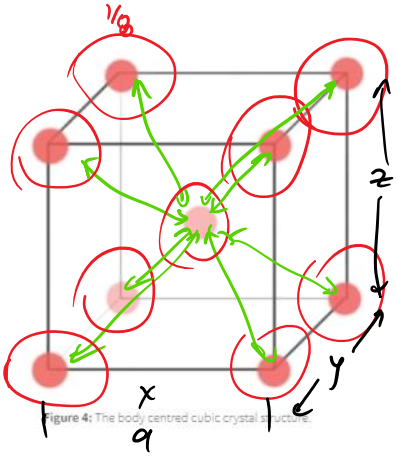


Figure 4: The body centred cubic crystal structure.

$8 \times 1/8$

$CN_{BCC} = 8$

coordination number

$n_{BCC} = 2$

$APF_{BCC} = \frac{n \frac{4}{3}\pi R^3}{a^3}$

$= \frac{n \frac{4}{3}\pi R^3}{\left(\frac{4}{\sqrt{3}}R\right)^3} = 0.68$

R = pm? nm? cm?

$4 \times 1/4 = 1$

$8 \times 1/2 = 4$

$= 5$

metals

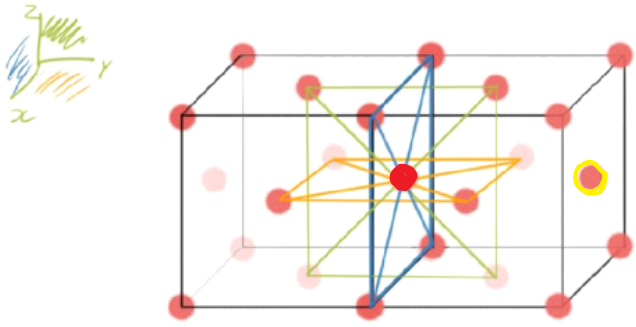
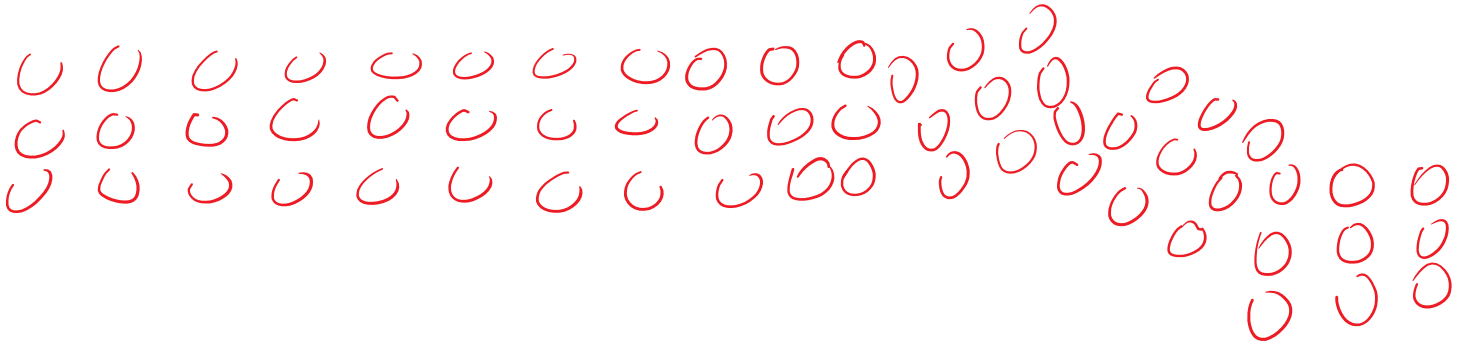


Figure 6: The coordination number for atoms in FCC. The right side face-centred atom makes contact with four atoms in the right side plane, with four atoms in the face-centred positions in the original unit cell, and with four atoms in teh face-centred positions in the unit cell to the right.



Octahedron

September 25, 2024 9:43 AM

6 = coordinate number

$CN_{bcc} = 6$

$12 \times 1/4 = 3$

$+ 1 = 4$

$8 \times 1/8 = 1$

$6 \times 1/2 = 3$

" 4

Cationic 1+ anionic 1-

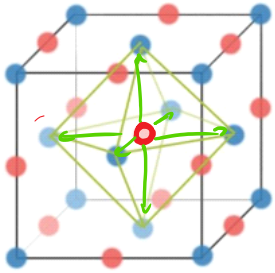


Figure 7: The octahedral interstitial site. Note that all cations, not just the central one, occupy octahedral interstitial sites within rock salt.

4 = 4

balance

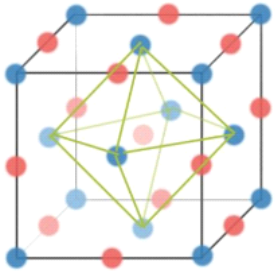


Figure 7: The octahedral interstitial site. Note that all cations, not just the central one, occupy octahedral interstitial sites within rock salt.

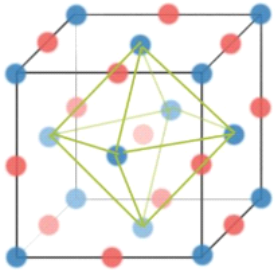


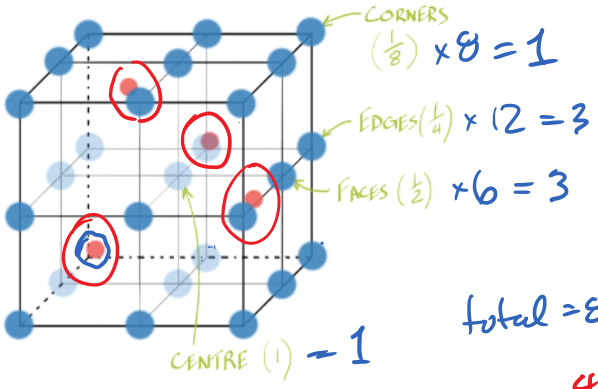
Figure 7: The octahedral interstitial site. Note that all cations, not just the central one, occupy octahedral interstitial sites within rock salt.

CaF_2

September 25, 2024 10:27 AM

Ca^{2+}

F^{1-}



total = 8. = F^{1-}

4 = Ca^{2+}

CaF_2

Figure 8. There are 8 anions within the calcium fluorite ceramic crystal structure. The fraction of an atom for each position type is shown here.

Ca = 231 pm = 2.31×10^{-8} cm = 0.231 nm

F = 135 pm = 1.35×10^{-8} cm = 0.135 nm

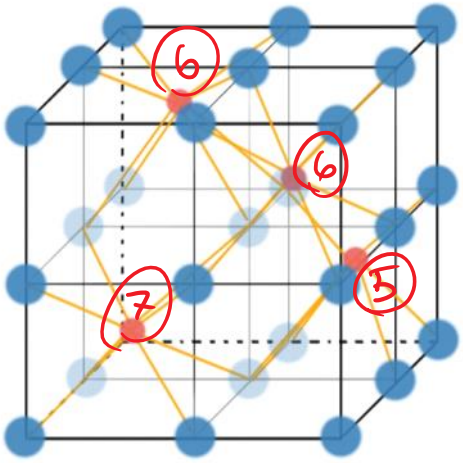


Figure 6. The calcium fluorite ceramic crystal structure. Anions represented as blue dots are in a simple cubic lattice with half of the simple cubic interstitial sites occupied by cations. Cations touch their 8 nearest neighbour anions along the cube diagonals, as illustrated by the orange lines.

APS110H1f2024 Sept 27 2024

September 26, 2024 7:52 PM

The Size of Interstitial Sites

$$\sin 45^\circ = \frac{1}{\sqrt{2}} = \frac{1}{1.414}$$

$$\sin 45 = \frac{2R_A}{2R_A + 2R_c}$$

$$\frac{R_c}{R_A} = \frac{1 - \sin 45}{\sin 45}$$

$$= \frac{1 - \frac{1}{1.414}}{\frac{1}{1.414}}$$

$$\frac{R_c}{R_A} = 0.414$$

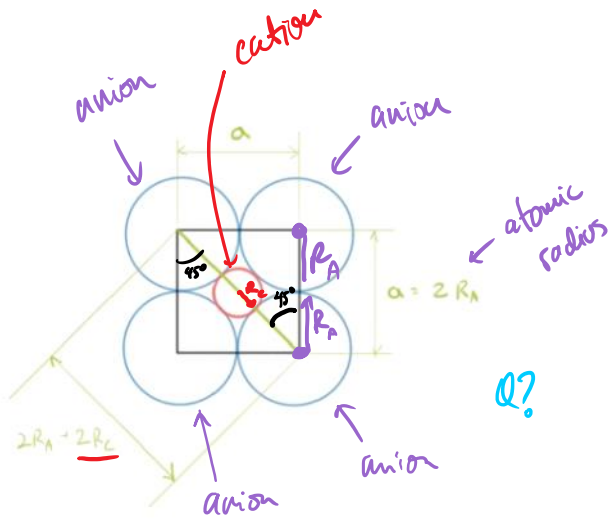
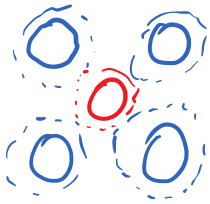


Figure 9: A 2D slice through the octahedral interstitial site at the geometrically ideal radius ratio when the anions are touching one another and the cation is just big enough to fit into the site without pushing the anions apart.



Hexagonal

September 26, 2024 7:53 PM

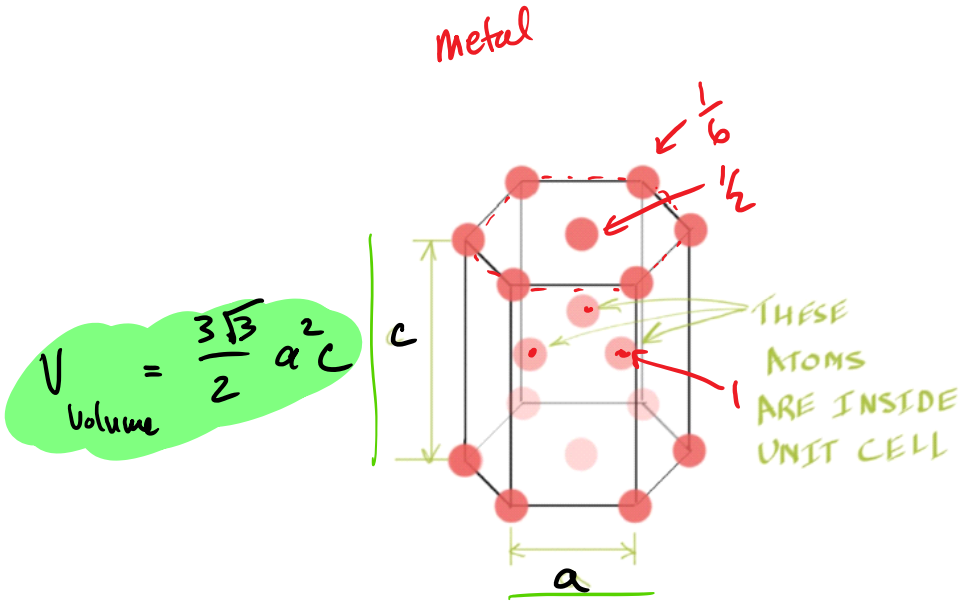


Figure 11: A hexagonal close packed unit cell. Note that the three atoms in the middle are inside the unit cell and are part of a close packed plane that is identical to the top and bottom planes.

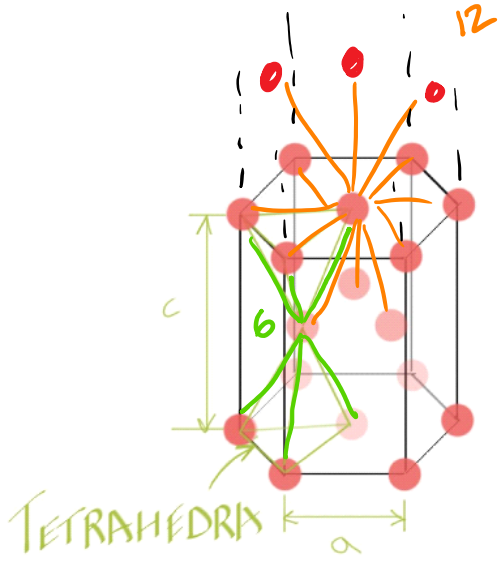
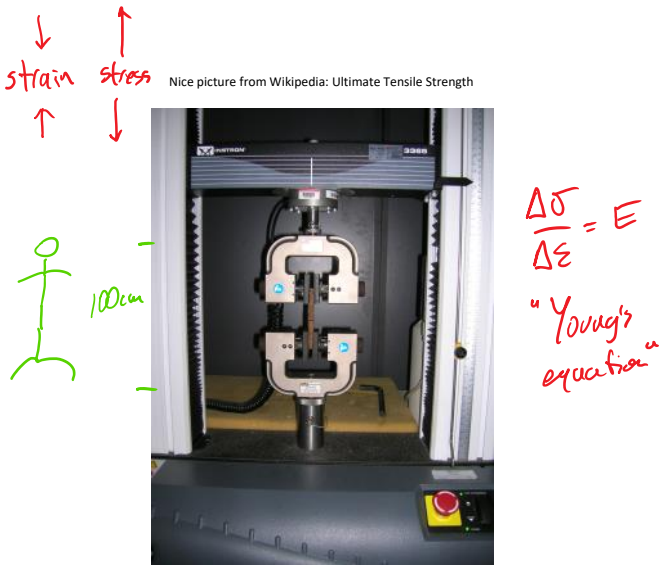


Figure 12: A hexagonal close packed unit cell showing the positioning of the three middle atoms nestled into the low spots between three atoms on the bottom plane.

APS110H1f2024 Sept 30 2024

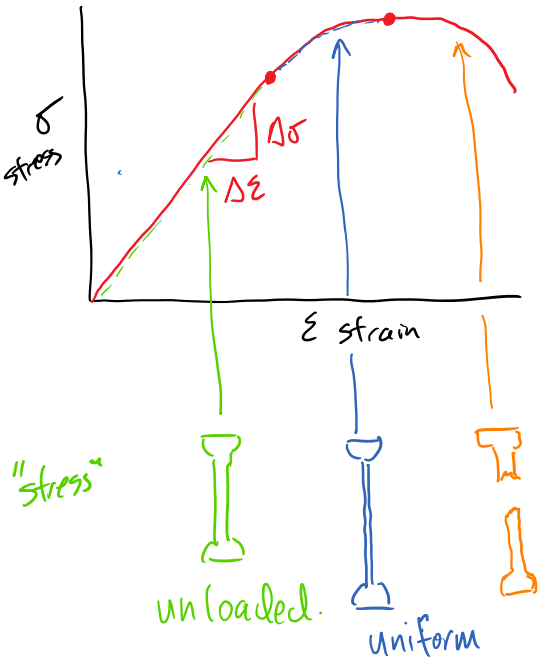
September 29, 2024 1:00 PM

...back from 09-09-2024 --> 09-16-2024 onto mechanical

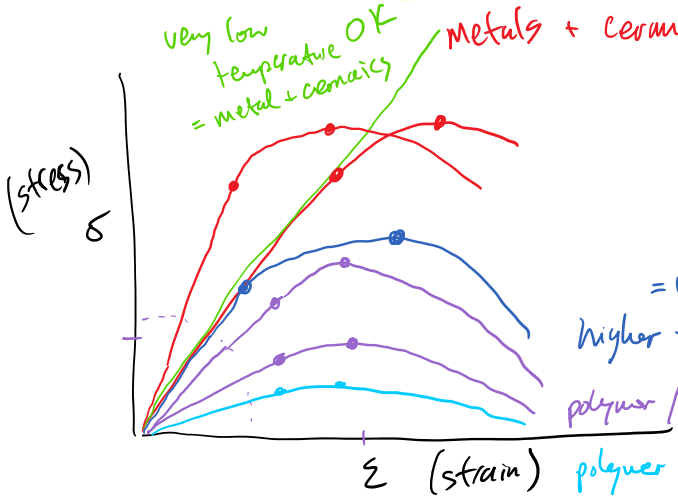


Nice picture from Wikipedia: Ultimate Tensile Strength

$\frac{\Delta\sigma}{\Delta\varepsilon} = E$ "Young's equation"



non-uniform another example.

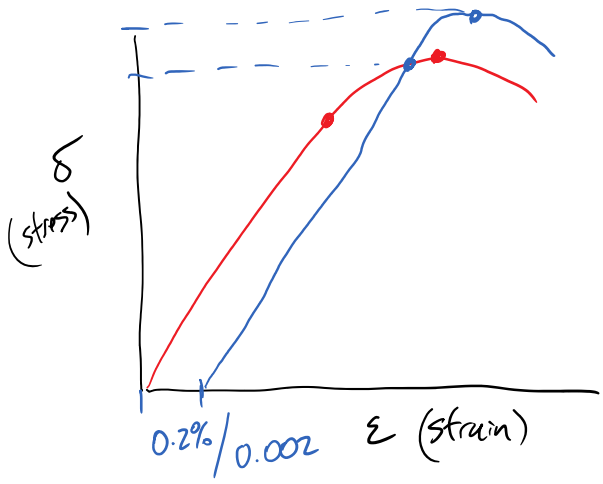


- physical properties

= metal + ceramics higher temperature

polymer / plastic = engineering of the plastics

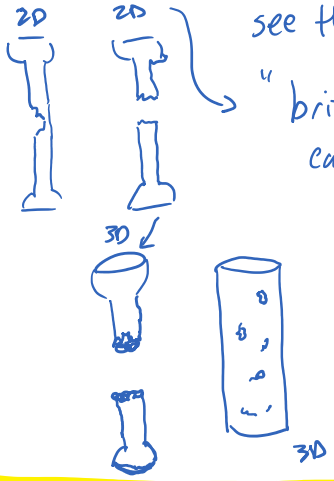
polymer at higher temperature.



6.1

"fracture" → "ductile" see this visible

"brittle" can not see this



nano structure