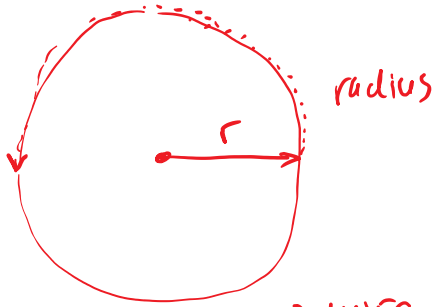


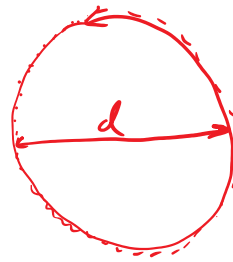
Atomic Packing Factor (APF)

2D



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

circumferences

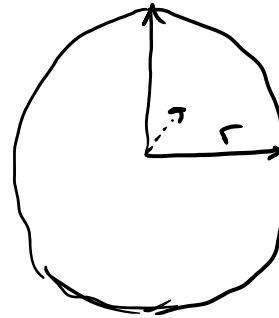


diameter

$$d=1 \quad \pi = 3.1415926535 \\ = 3.14159$$

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

of an atom / 1 atom.



3D

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

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

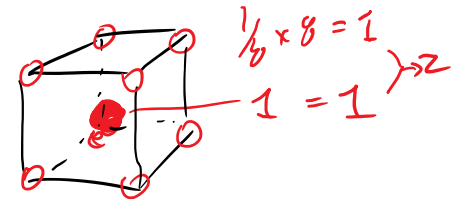
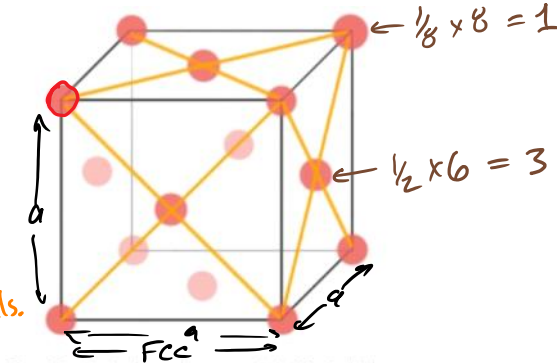
APF - atomic packing factor

$$APF = \frac{\text{volume spheres}}{\text{volume unit cell}}$$

$$APF = \frac{n \cdot \frac{4}{3} \pi R^3}{a^3}$$

only metals.
= only 1 metal

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



Fe/iron
↳ 194 pm

FCC - face centred cubic

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

$$= 548.7096 \text{ pm}$$

$$\sqrt{2} = 1.4142? \quad \text{Yes is a yes}$$

$$\sqrt{4} = 2? \quad \text{Yes - is a yes}$$

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

iron

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

density

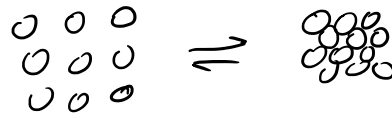
PERIODIC TABLE OF ELEMENTS

1 H Hydrogen 120	Atomic Number Symbol Name Atomic Radius (van der Waals), pm																2 He Helium 140	
3 Li Lithium 182	4 Be Beryllium 153	picometer																10 Ne Neon 154
11 Na Sodium 227	12 Mg Magnesium 173	pm																18 Ar Argon 188
19 K Potassium 375	20 Ca Calcium 231	21 Sc Scandium 211	22 Ti Titanium 187	23 V Vanadium 179	24 Cr Chromium 189	25 Mn Manganese 193	26 Fe Iron 194	27 Co Cobalt 192	28 Ni Nickel 163	29 Cu Copper 140	30 Zn Zinc 139	31 Ga Gallium 187	32 Ge Germanium 211	33 As Arsenic 185	34 Se Selenium 190	35 Br Bromine 183	36 Kr Krypton 202	
37 Rb Rubidium 303	38 Sr Strontium 249	39 Y Yttrium 219	40 Zr Zirconium 186	41 Nb Niobium 207	42 Mo Molybdenum 209	43 Tc Technetium 209	44 Ru Ruthenium 207	45 Rh Rhodium 195	46 Pd Palladium 202	47 Ag Silver 172	48 Cd Cadmium 158	49 In Indium 193	50 Sn Tin 217	51 Sb Antimony 206	52 Te Tellurium 208	53 I Iodine 198	54 Xe Xenon 216	
55 Cs Cesium 343	56 Ba Barium 268	•	72 Hf Hafnium 212	73 Ta Tantalum 217	74 W Tungsten 210	75 Re Rhenium 217	76 Os Osmium 216	77 Ir Iridium 202	78 Pt Platinum 209	79 Au Gold 166	80 Hg Mercury 209	81 Tl Thallium 186	82 Pb Lead 202	83 Bi Bismuth 207	84 Po Polonium 197	85 At Astatine 202	86 Rn Radon 220	
87 Fr Francium 348	88 Ra Radium 283	**	104 Rf Rutherfordium 150	105 Db Dubnium 139	106 Sg Seaborgium 132	107 Bh Bohrium 128	108 Hs Hassium 126	109 Mt Meitnerium 128	110 Ds Darmstadtium 132	111 Rg Roentgenium 138	112 Cn Copernicium 147	113 Nh Nihonium 170	114 Fl Flerovium 180	115 Mc Moscovium 187	116 Lv Livermorium 183	117 Ts Tennessine 138	118 Og Oganesson	
•	57 La Lanthanum 240	58 Ce Cerium 235	59 Pr Praseodymium 239	60 Nd Neodymium 229	61 Pm Promethium 238	62 Sm Samarium 229	63 Eu Europium 233	64 Gd Gadolinium 237	65 Tb Terbium 221	66 Dy Dysprosium 229	67 Ho Holmium 216	68 Er Erbium 235	69 Tm Thulium 227	70 Yb Ytterbium 242	71 Lu Lutetium 221			
**	89 Ac Actinium 260	90 Th Thorium 237	91 Pa Protactinium 243	92 U Uranium 240	93 Np Neptunium 221	94 Pu Plutonium 243	95 Am Americium 244	96 Cm Curium 245	97 Bk Berkelium 244	98 Cf Californium 245	99 Es Einsteinium 245	100 Fm Fermium	101 Md Mendelevium	102 No Nobelium	103 Lr Lawrencium			

BCC --> FCC

BCC : Body Centred Cubic (Crystal Structure/Nanostructure)

stress + strain



metal only

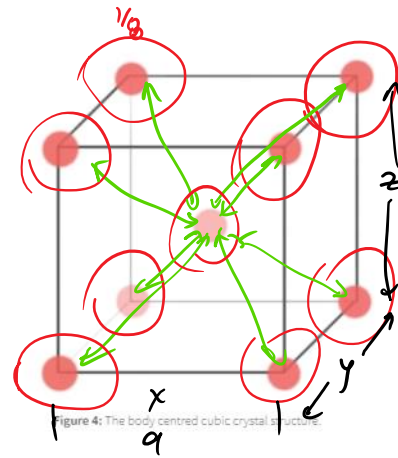


Figure 4: The body-centred cubic crystal structure.

$$CN_{BCC} = 8$$

Coordination number 1

$$n_{BCC} = 2$$

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

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

R = pm? nm? cm?

$$4 \times \frac{1}{4} = 1$$

$$8 \times \frac{1}{2} = 4$$

" 5

metals

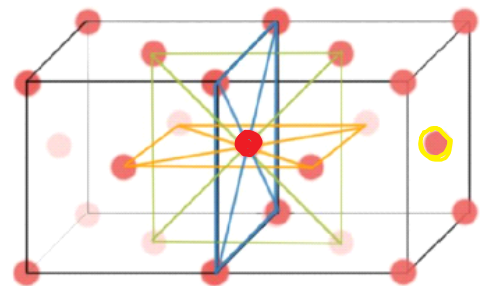
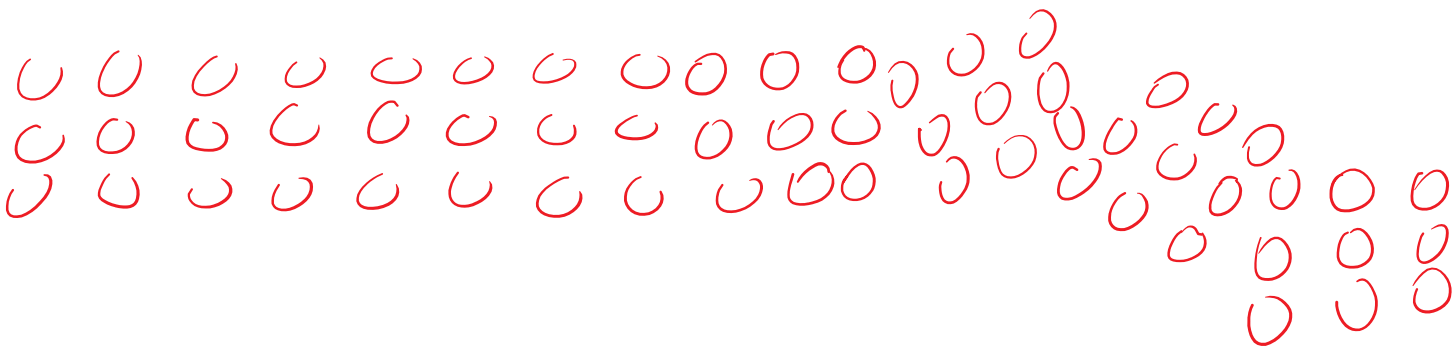


Figure 6: The coordination number for atoms in FCC. The right side face-centred atom makes contact with four atoms in the right side plane, with four atoms in the face-centred positions in the original unit cell, and with four atoms in the face-centred positions in the unit cell to the right.



Octahedron

September 25, 2024 9:43 AM

6 = coordinate number
CN_{bcc} = 6

$12 \times \frac{1}{4} = 3$
 $+ 1 = 4$
 $8 \times \frac{1}{8} = 1$
 $6 \times \frac{1}{2} = 3$
" 4

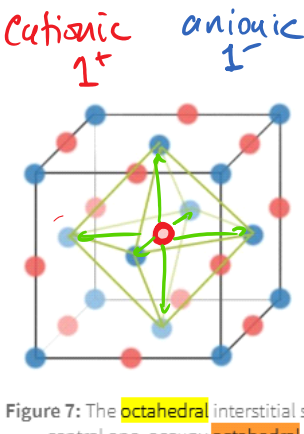


Figure 7: The octahedral interstitial site. Note that all cations, not just the central one, occupy octahedral interstitial sites within rock salt.

4 = 4
balance

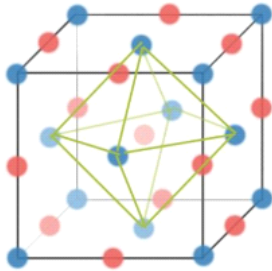


Figure 7: The octahedral interstitial site. Note that all cations, not just the central one, occupy octahedral interstitial sites within rock salt.

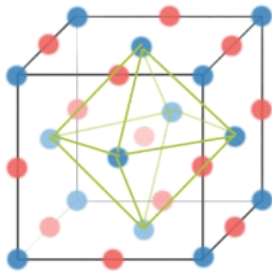


Figure 7: The octahedral interstitial site. Note that all cations, not just the central one, occupy octahedral interstitial sites within rock salt.

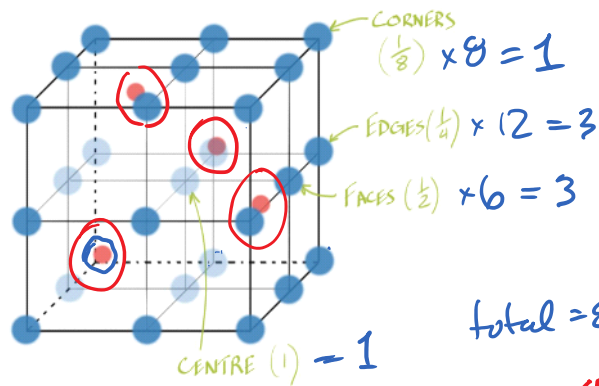


Figure 8. There are 8 anions within the calcium fluoride ceramic crystal structure. The fraction of an atom for each position type is shown here.

$$\text{Ca} = 231 \text{ pm} = 2.31 \times 10^{-8} \text{ cm} = 0.231 \text{ nm}$$

$$\text{F} = 135 \text{ pm} = 1.35 \times 10^{-8} \text{ cm} = 0.135 \text{ nm}$$

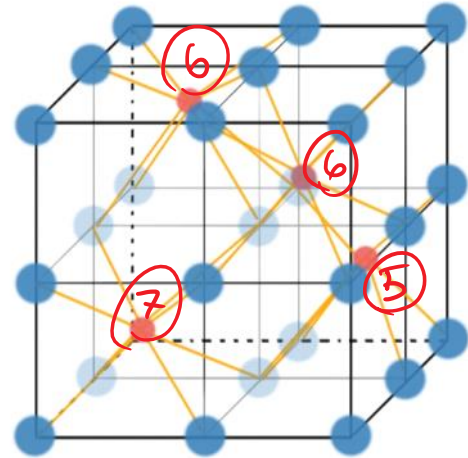


Figure 6. The calcium fluoride ceramic crystal structure. Anions represented as blue dots are in a simple cubic lattice with half of the simple cubic interstitial sites occupied by cations. Cations touch their 8 nearest neighbour anions along the cube diagonals, as illustrated by the orange lines.

The Size of Interstitial Sites

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

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

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

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

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

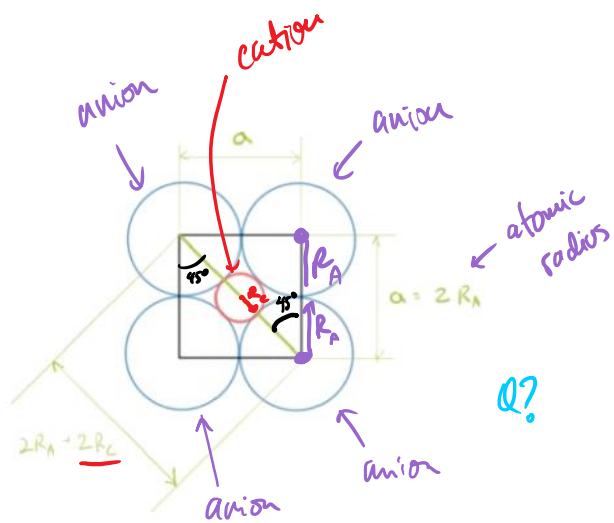
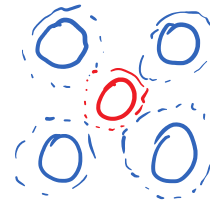


Figure 9: A 2D slice through the octahedral interstitial site at the geometrically ideal radius ratio when the anions are touching one another and the cation is just big enough to fit into the site without pushing the anions apart.



Hexagonal

September 26, 2024 7:53 PM

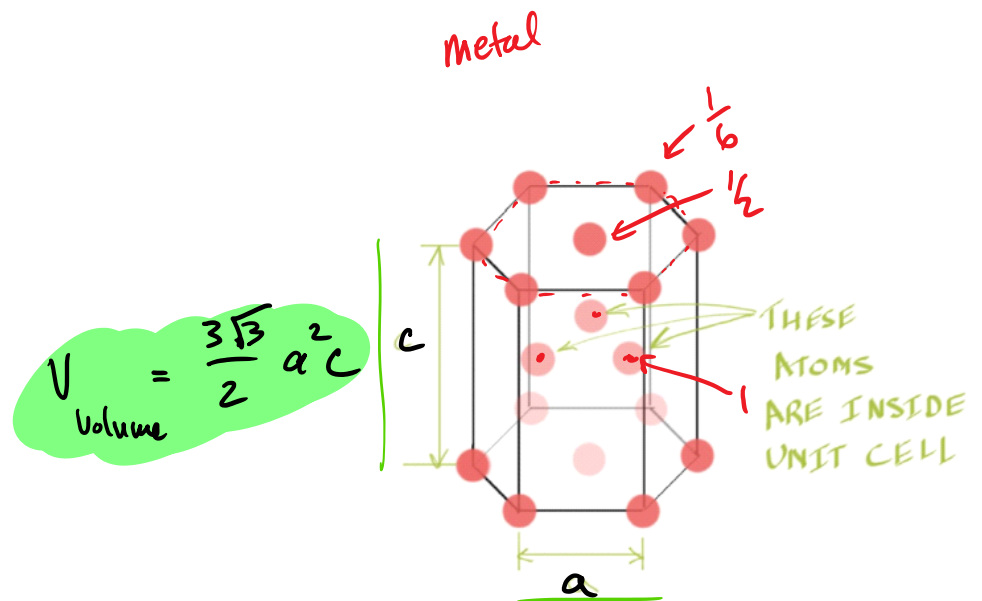


Figure 11: A hexagonal close packed unit cell. Note that the three atoms in the middle are inside the unit cell and are part of a close packed plane that is identical to the top and bottom planes.

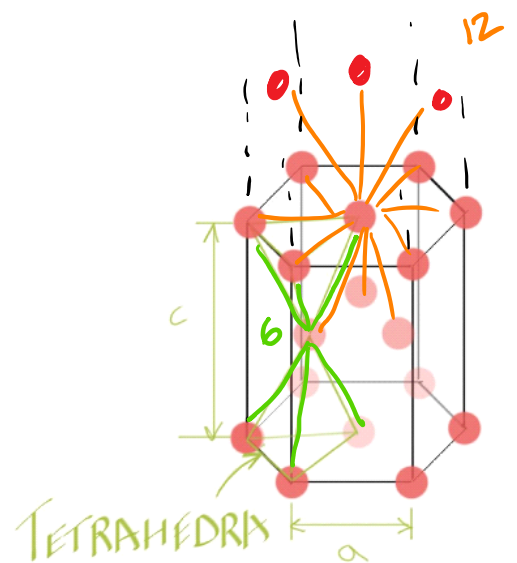


Figure 12: A hexagonal close packed unit cell showing the positioning of the three middle atoms nestled into the low spots between three atoms on the bottom plane.

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

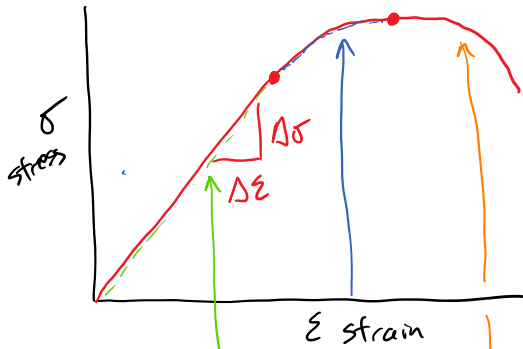
↓ strain
 ↑ stress
 ↑ strain
 ↓ stress

Nice picture from Wikipedia: Ultimate Tensile Strength

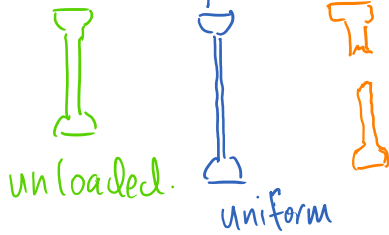


$$\frac{\Delta \sigma}{\Delta \epsilon} = E$$

"Young's equation"



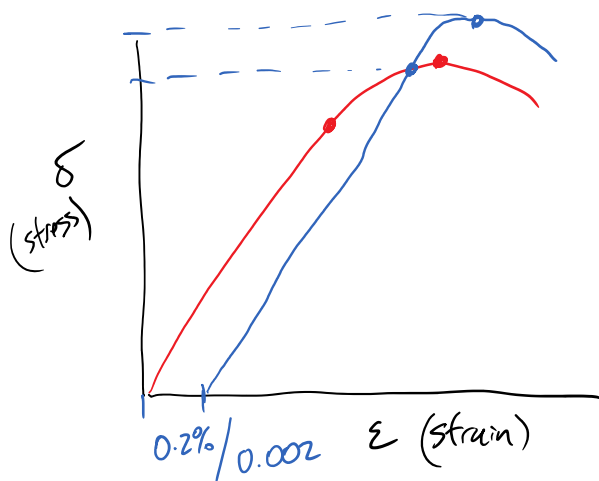
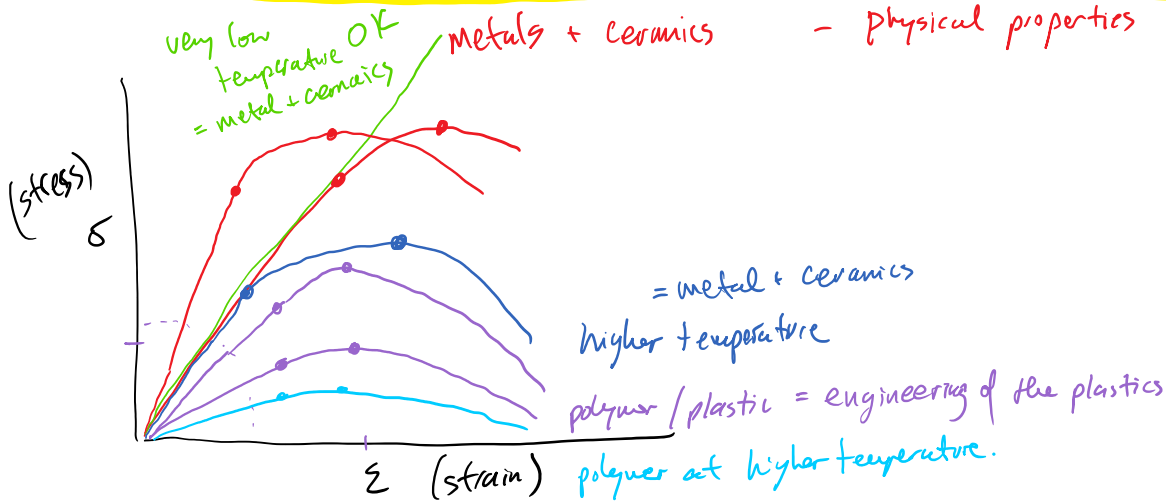
"stress"



non-uniform



another example.



"fracture" → "ductile" (6.1)
 see this visible
 "brittle"
 can not see this

name
structure

