① Classification - amorphous or crystalline, discrete or extended molecular or atomic, ionic covalent or metallic

② Structures

a) Crystallographic descriptions

- unit cell - a b c, α β γ
- centering, P F I C, essential symmetry
- point symmetry
- translational symmetry - glide plane
  screw axis
- 95% of all crystalline structures exist
  monoclinic triclinic orthorhombic
- 83% of all structures
  $P2_1/c$ monoclinic
  $P\bar{1}$ triclinic
  $P2_12_12_1$ orthorhombic
  $C2/c$ monoclinic
  $P2$ monoclinic
  $Pbca$ - orthorhombic

③ Close packed structures -

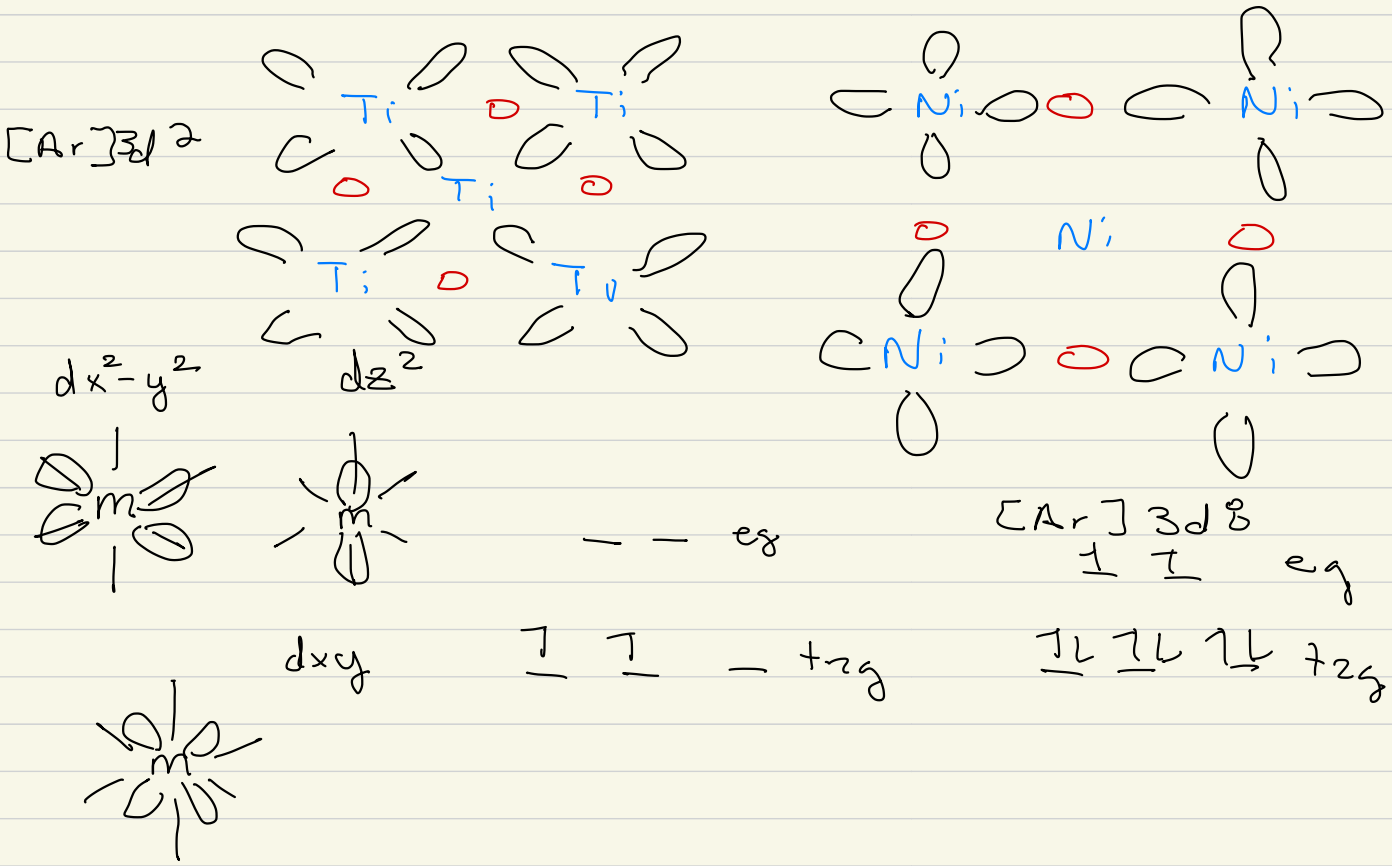
ccp - ABC
hcp - ABA

Rock salt type structure

Fcc anion array Na are found in octahedral

① Early TM oxides, TiO, exhibit metallic like conductivity, & this is not the case for late TMO, like NiO.

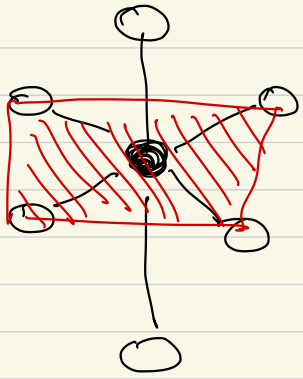
Rocksalt

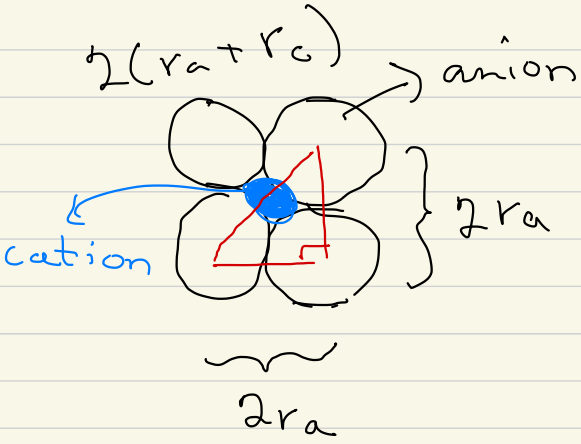


Radius Ratio Rule: minimum radius ratio (r_c/r_a) it tells you what coordination environment is preferred

coord. env:	R_m (r_c/r_a)
trigonal, 3	0.155
tetrahedral, 4	0.225
octahedral, 6	0.414
Cubic, 8	0.732
dodecahedral, 12	1.00

When calculating R_{min}
① cations must be in contact.
② Anions may or may not be in contact



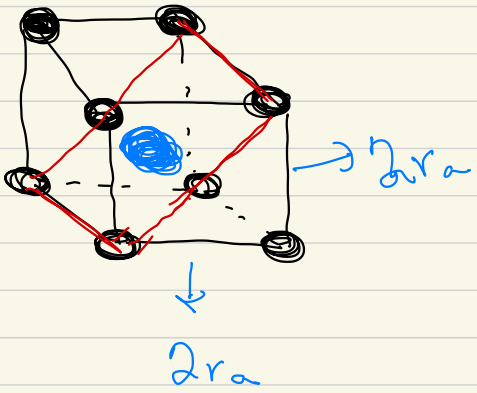


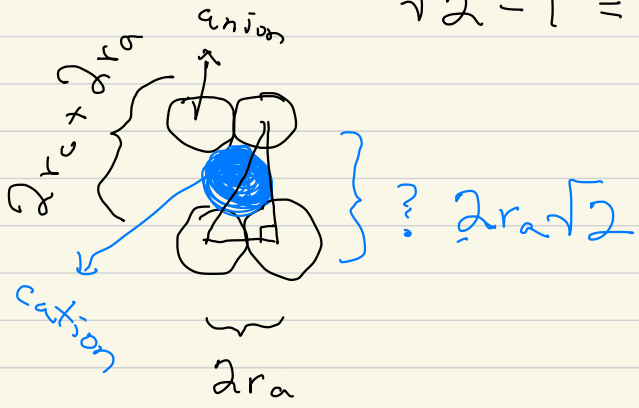
$a^2 + b^2 = c^2$

$\sqrt{4r_a^2 + 4r_a^2} = \sqrt{(2(r_a + r_c))^2}$

$2r_a\sqrt{2} = 2(r_c + r_a)$

$\sqrt{2} - 1 = \frac{r_c}{r_a} = 0,414$





$4r_a^2 + 4r_a^2 = x^2$

$x = 2r_a\sqrt{2}$

$8r_a^2 + 4r_a^2 = [2(r_c + r_a)]^2$

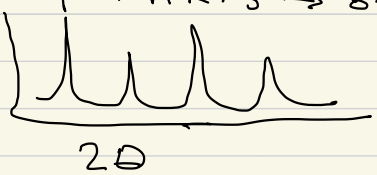
$2r_a\sqrt{3} = 2r_c + 2r_a$

$\sqrt{3} - 1 = \frac{r_c}{r_a}$

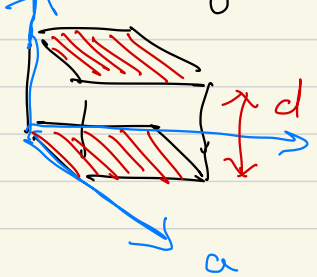
$= 0.732$

Lattice planes Miller Indices indices of direction

$n\lambda = 2d\sin\theta$



d-spacing → distance planes



d → defines your c-axis

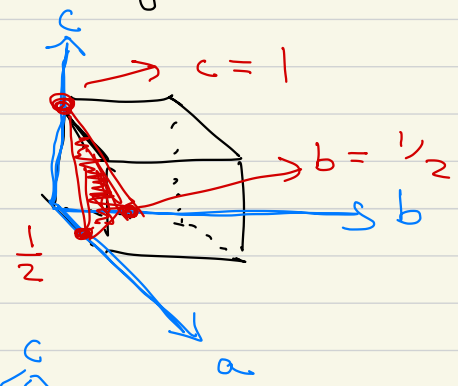
Miller Indices

① Identify Plane of atoms

② Identify where plane intersects the a, b, c axis

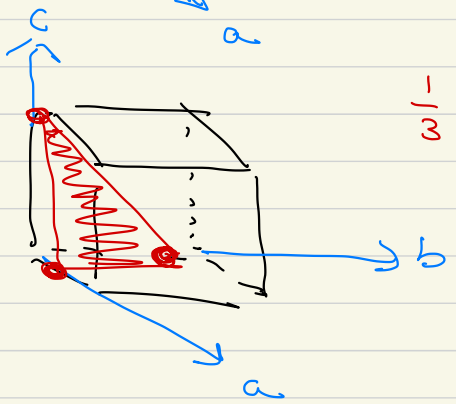
③ Take reciprocal of the intersection

④ if there are fractions you must multiply by denominator.



$(\frac{1}{2} \quad \frac{1}{2} \quad 1) \rightarrow$ reciprocal

$(2 \quad 2 \quad 1)$



$\frac{1}{3} \quad \frac{2}{3} \quad 1$ intercept $\rightarrow$ reciprocal

$(3 \quad \frac{3}{2} \quad 1) \cdot 2 = (6 \; 3 \; 2)$

miller index

Indices of direction

① Draw x y z axes if # > 1 divide by that #

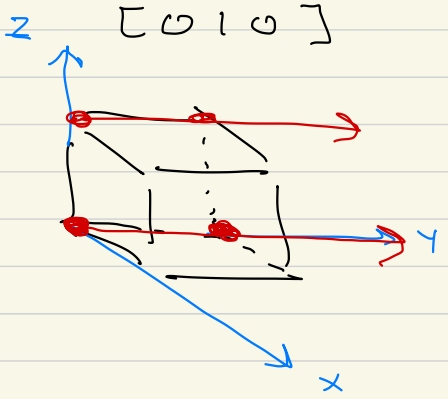
② Choose a point of origin.. if there is a negative # then move the origin in a positive direction

③ Move your pencil along the u v w direction

④ Label end point

⑤ Draw your vector

[0 1 0]



[1 1 0]