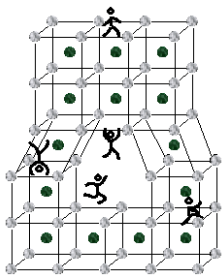


Building A Crystal

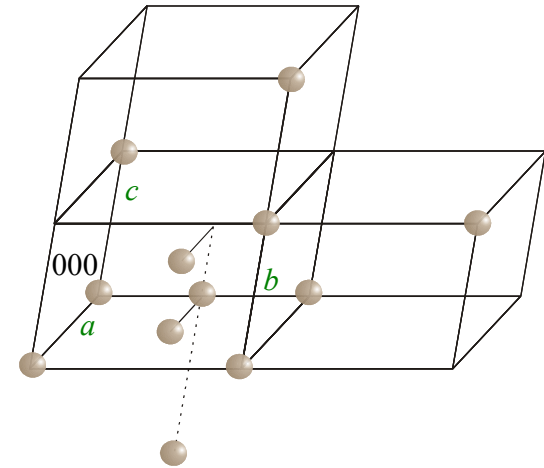


- Typical Crystal Lattices
 - BCC
 - FCC
 - HCP
- Miller Indices
 - Atomic Positions
 - Directions
 - Planes
- Interplanar Spacing

Wednesday
Sept. 3, 2003

MATS275: INTRODUCTION
TO MATERIALS SCIENCE

Example of Atomic Positions



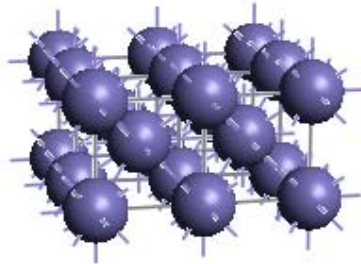
BCC

- 2 atom basis

$$(0,0,0)\left(\frac{1}{2},\frac{1}{2},\frac{1}{2}\right)$$

$$d = \sqrt{\left(\frac{1}{2}a_0\right)^2 + \left(\frac{1}{2}a_0\right)^2 + \left(\frac{1}{2}a_0\right)^2} = \frac{\sqrt{3}}{2}a_0$$

- CN = 8
- Ex) Cr, Fe, Mo, V



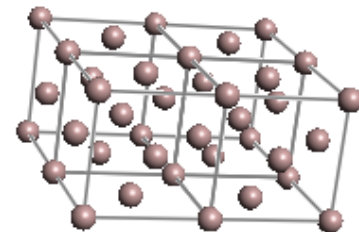
FCC

- 4 atom basis

$$(0,0,0)\left(\frac{1}{2},\frac{1}{2},0\right)\left(\frac{1}{2},0,\frac{1}{2}\right)\left(0,\frac{1}{2},\frac{1}{2}\right)$$

$$d = \sqrt{\left(\frac{1}{2}a_0\right)^2 + \left(\frac{1}{2}a_0\right)^2 + (0a_0)^2} = \frac{\sqrt{2}}{2}a_0$$

- CN = 12
- Ex) Al, Cu, Au, Ag



HCP

- $$(0,0,0)\left(\frac{1}{3},\frac{2}{3},\frac{1}{2}\right)$$

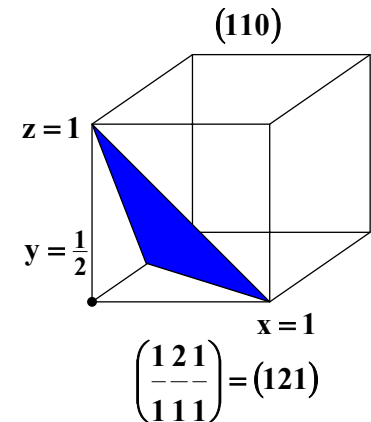
- # Miller Indices Directions



1 H																	2 He						
3 Li	4 Be																	5 B	6 C	7 N	8 O	9 F	10 Ne
11 Na	12 Mg																	13 Al	14 Si	15 P	16 S	17 Cl	18 Ar
19 K	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr						
37 Rb	38 Sr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe						
55 Cs	56 Ba	57 La	58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb	71 Lu	72 Hf						
73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn										
87 Fr	88 Ra	89 Ac	90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No	103 Lr	104						

Miller Indices

Diagram illustrating the Miller indices for a crystal plane. The plane is shown in a 3D coordinate system with axes labeled $x=1$, $y=1$, and $z=\infty$. The plane is labeled (110) . The formula for determining the Miller indices is shown below the diagram:

$$\left(\begin{array}{ccc} 1 & 1 & 1 \\ \hline 1 & 1 & \infty \end{array} \right) = (110)$$


Miller Indices

- Directions

- specific $[hkl]$
- families $\langle hkl \rangle$

- Planes

- specific (hkl)
- families $\{hkl\}$

Miller Indices Hexagonal Systems

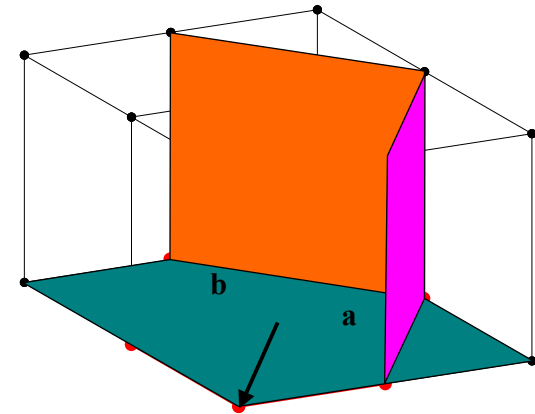
$$(hkil)$$

$$i = -(h + k)$$

$$(0001)$$

$$(11\bar{2}0)$$

$$(1\bar{1}00)$$



Miller Indices Spacing Between Planes

Cubic

$$d_{hkl} = \frac{a}{\sqrt{h^2 + k^2 + l^2}}$$

Hexagonal

$$d_{hkil} = \frac{a}{\sqrt{(h^2 + hk + k^2) + l^2 \left(\frac{a}{c}\right)^2}}$$

Miller Indices Spacing Between Planes

- What is the spacing between $\{100\}$ planes in a cubic crystal? Between $\{110\}$? Between $\{111\}$?

$$d_{100} = \frac{a}{\sqrt{1^2 + 0^2 + 0^2}} = a$$

$$d_{110} = \frac{a}{\sqrt{1^2 + 1^2 + 0^2}} = \frac{a}{\sqrt{2}}$$

$$d_{111} = \frac{a}{\sqrt{1^2 + 1^2 + 1^2}} = \frac{a}{\sqrt{3}}$$

