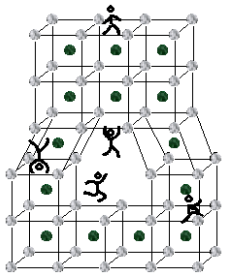
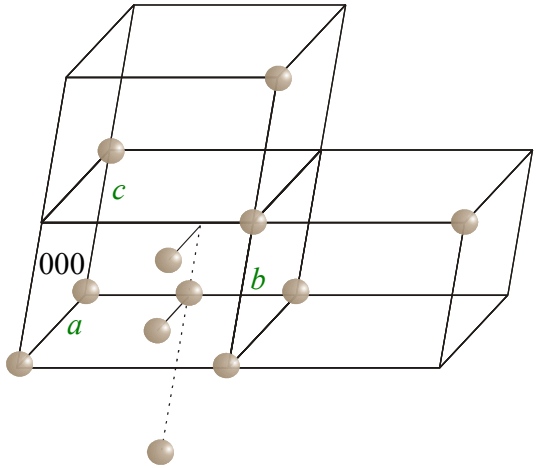
Building A Crystal



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

Wednesday
Sept. 3, 2003

Example of Atomic Positions

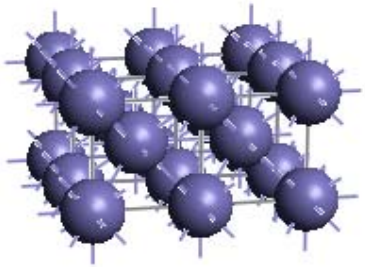


BCC

- 2 atom basis

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

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



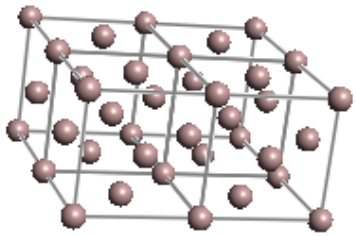
- CN = 8
- Ex) Cr, Fe, Mo, V

FCC

- 4 atom basis

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

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



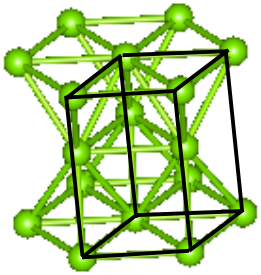
- CN = 12
- Ex) Al, Cu, Au, Ag

HCP

- 2 atom basis

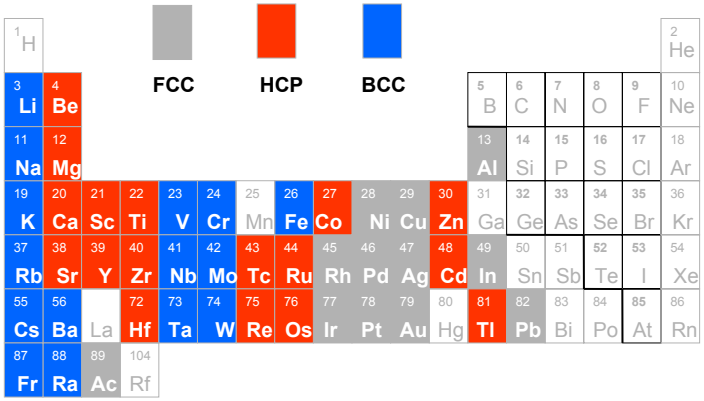
$$(0,0,0)\left(\frac{1}{3},\frac{2}{3},\frac{1}{2}\right)$$

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

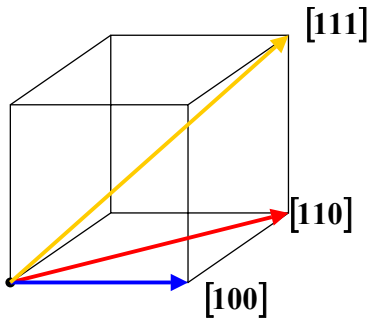


- CN = 12
- Ex) Cd, Mg, Ti, Zn

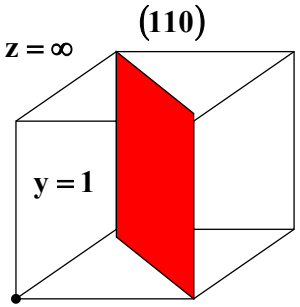
Metal Crystal Structures…



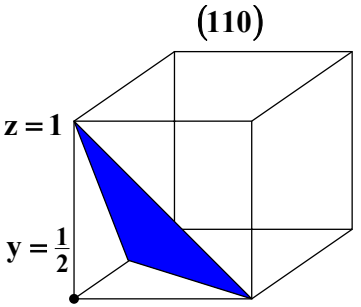
Miller Indices Directions



Miller Indices



$$\left(\frac{1\,1\,1}{1\,1\,\infty}\right)=(110)$$



$$\left(\frac{1\,2\,1}{1\,1\,1}\right)=(121)$$

Miller Indices

- Directions
  - specific $[hkl]$
  - families $\langle hkl \rangle$
- Planes
  - specific (hkl)
  - families $\{hkl\}$

Miller Indices
Hexagonal Systems

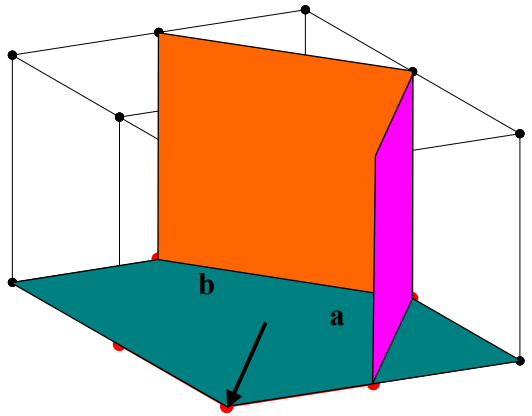
$(hkil)$

$i = -(h+k)$

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

Miller Indices
Spacing Between Planes

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

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

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

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