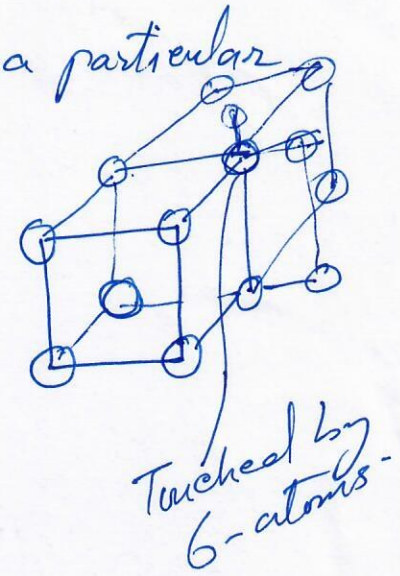
29.3.2012.

Coordination number – No. of atoms touching a particular atom. C.N for S.C = 6

C.N for B.C.C – 8

F.C.C = 12

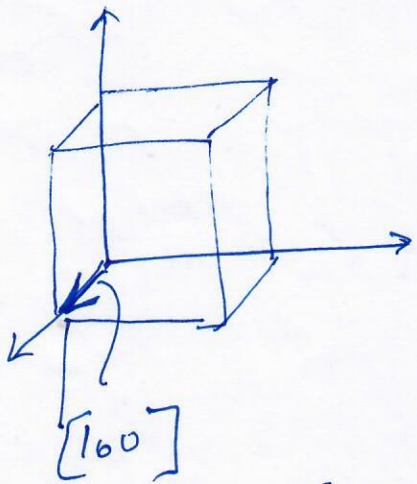


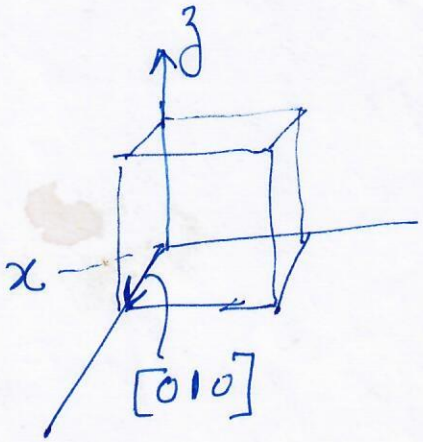
REPEAT DISTANCE

Equivalent directions.

Important Points about Miller indices

1. A direction and its –ve are not identical
   => [1 0 0] is not equal to [$\bar{1}$ 0 0]
   => same line but opposite direction
2. A direction and its multiple are identical;
   => [1 0 0] & [2 0 0] are identical



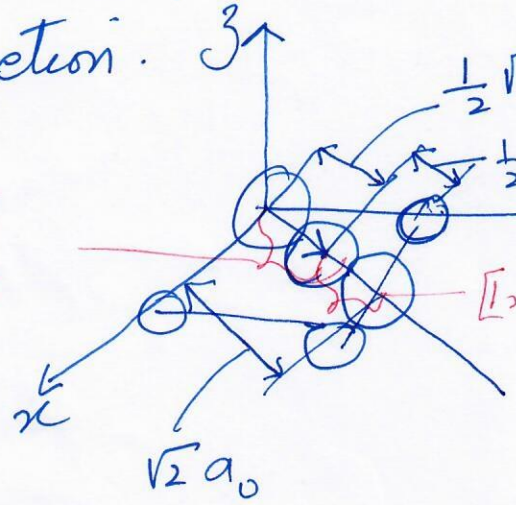


$\langle 1\,1\,0 \rangle = \begin{cases} [1\,1\,0] \\ [1\,0\,1] \\ [0\,1\,1] \end{cases}$

$[\bar{1}\,\bar{1}\,0]$
$[\bar{1}\,0\,\bar{1}]$
$[0\,\bar{1}\,\bar{1}]$

Linear Density

It is the number of lattice points per unit length (repeat distances) along a particular direction.



In copper there are two repeat distances

linear density along [1,1,0] in copper $= \frac{2 \text{ repeat distances}}{\sqrt{2}a_0}$

$= \frac{2}{5.1125 \times 10^{-8}}$

$= 3.9 \times 10^7$ lattice points/cm.

Packing Fraction = (linear density) × distance / repeat

for copper $= 3.9 \times 10^7 \times (2R)$

$= 3.9 \times 10^7 \times 2 \times 1.2781 \times 10^{-8}$

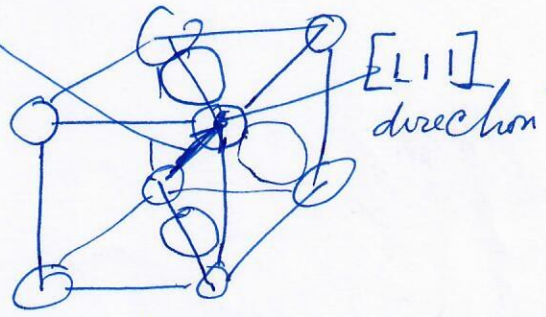
$= 1$

EXAMPLE

Calculate the repeat distance, linear density and packing fraction for the [1 1 1] direction in FCC copper.

Answer

repeat distance $= \sqrt{3}a_0$



Repeat distance, linear density and packing fraction for [1 1 1] direction in FCC Copper.

Repeat distance $= \sqrt{3}\, a_0$

$= \sqrt{3}(3.6151 \times 10^{-8})$

$= 6.262 \times 10^{-8}$ cm

Linear density

$= \dfrac{\text{no. of ~~repeat distance~~ lattice points}}{\text{length of the distance}}$

$= \dfrac{1}{6.262 \times 10^{-8}} = 1.597 \times 10^{7}$ lattice points/cm

2.5562
3.9
22.5658
76686
9.9191
= 10.

Packing fraction of a particular direction [1 1 1]

= Fraction covered by atoms = Linear density × 2r

$= \dfrac{\text{No. of ~~repeat distances~~ lattice points}}{\text{length of direction}} \times$ length of repeat distance

in FCC Copper

$= 2 \times 2r = 2r = \dfrac{2 \times 1.278 \times 10^{-8}}{\sqrt{2}} = 0.408$

Planes in the Unit Cell

Metals deform along planes of atoms that are tightly packed together. Miller indices can be used to identify these important planes, as described:

(a) Indentify the points at which the plane intercepts the x, y, and z coordinates in terms of the number of lattice parameters. If plane passes through origin then coordinate system may be shifted.

(b) Take reciprocals of these intercepts

(c) Clear fractions but do not reduce to lower integers

(d) Enclose numbers in parantheses.
-ve numbers should be written under bar

EXAMPLE

Determine Miller indices of plane A, B, C

Plane A

(a) $x = 1$, $y = 1$, $z = 1$

(b) $\frac{1}{x} = 1$, $\frac{1}{y} = 1$, $\frac{1}{z} = 1$

(c) No fractions to clear

(d) (111)