Universidad
Carlos III de Madrid
www.uc3m.es

MATERIALS SCIENCE AND ENGINEERING

TOPIC 2. STRUCTURE OF MATERIALS II

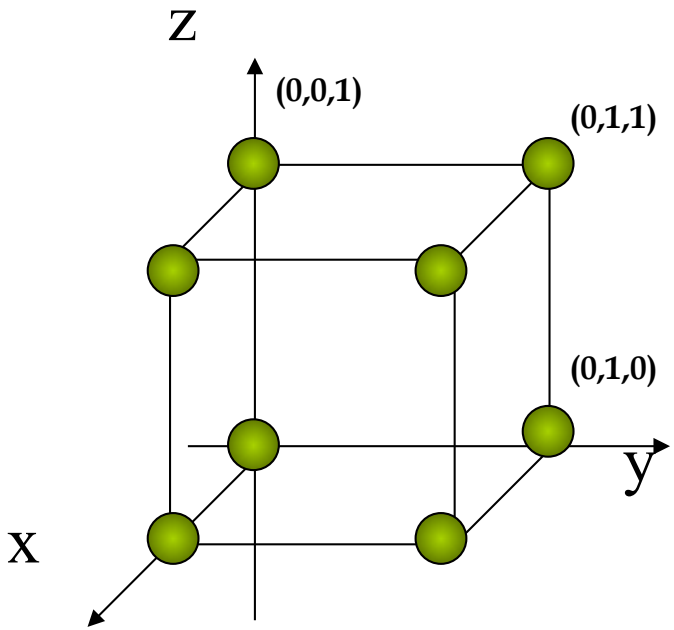
Topic 2.2:

- **Atomic positions.**
- **Directions in the crystalline cells.**
- **Planes in the crystalline cells.**
- **Calculation of the atomic density.**

ATOMIC POSITIONS IN THE CUBIC CELLS

Atomic positions :

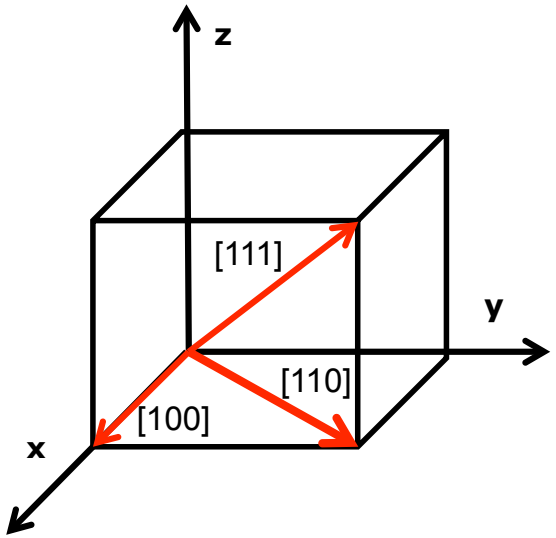
System of axes x,y,z unit distance



DIRECTIONS IN THE CUBIC CELL

The properties of materials depend on the direction in which they are measured ⇒ they deform in the directions in which the atoms are in close contact.

"crystallographic direction indices are the vector components of the directions resolved along each of the coordinate axes and reduced at the smallest integrals"



DIRECTIONS IN THE CUBIC CELL

Procedure for determining crystallographic directions:

1. Choose a vector of appropriate length that passes through the origin (parallelism must be maintained).
2. Determine the length of the projection on each of the three axes *measured in terms of the unit cell dimensions a, b, c.*
3. Multiply or divide by common factor to reduce to the smallest integer value.
4. Notation: enclose the three indices in square brackets, without comma [y v w]

DIRECTIONS IN THE CUBIC CELLS

Individual directions: [uvw]

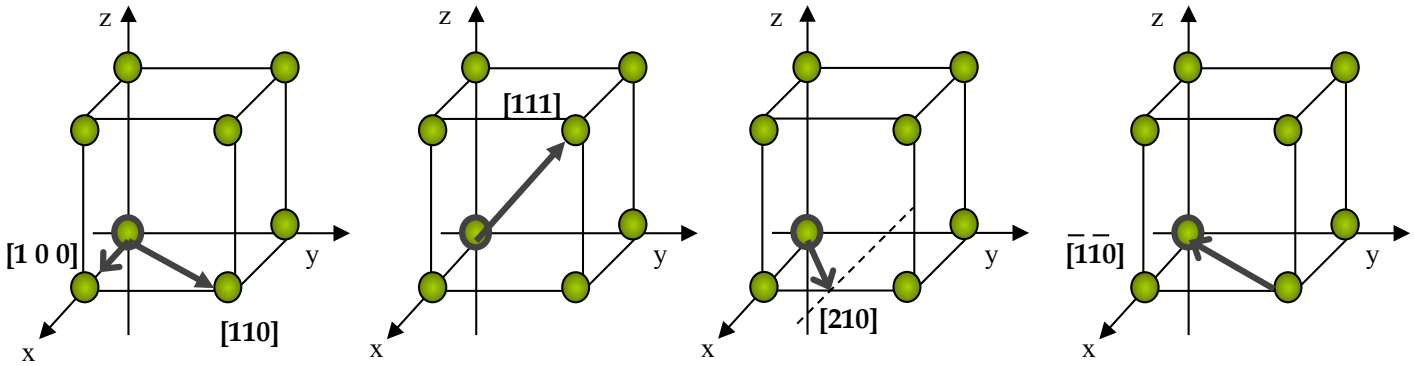
// direction vectors ⇒ the same indexes

Equivalent directions in the network (indices of a family): <uvw>
When the spacing along each direction is the same

Cube axes: [100],[010],[001],[010],[001],[100]=⟨100⟩

Cube diagonals : ⟨111⟩

Cube face diagonals: ⟨110⟩

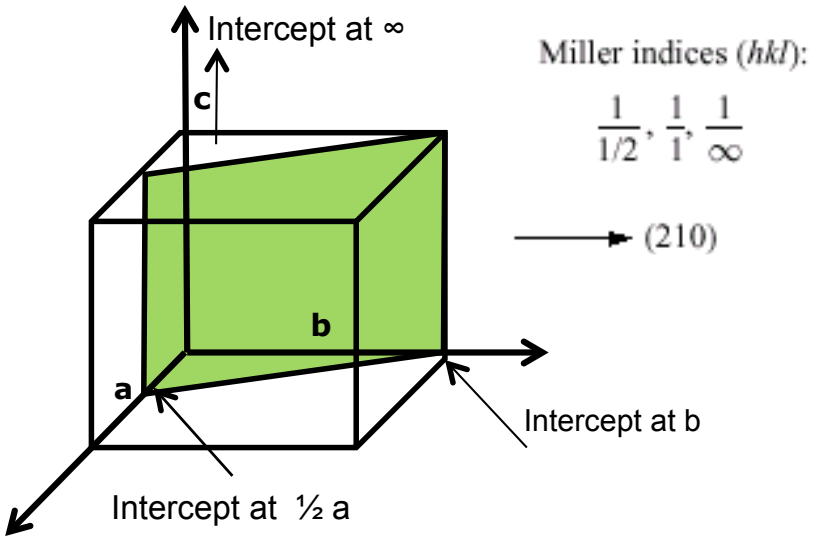


PLANES IN THE CUBIC CELL

Miller indices are used: "reciprocal of the intersections of the plane with the axes determine x,y,z"

Procedure :

1. Choose a plane that does not pass from the origin
2. Determine the length of intercepts of the plane with the 3 axes
3. Obtain the reciprocals of these intersections
4. Determine the smaller set of integers that have the same ratio as the intercepts
5. Notation: enclose them in parenthesis without coma (h k l)



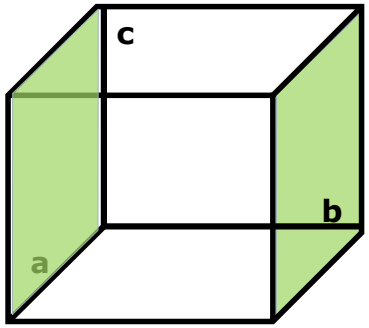
PLANES IN THE CUBIC CELL

$x=\frac{1}{2}$, $y=1$, $z=\infty$ } (210)

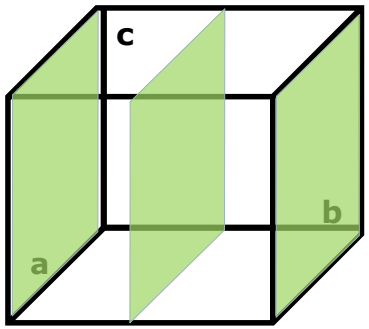
$x=1$, $y=1$, $z=\infty$ } (110)

$x=1$, $y=1$, $z=1$ } (111)

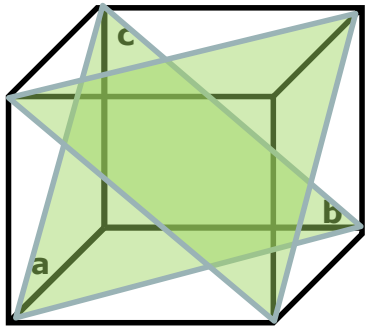
$x=1$, $y=\infty$, $z=\infty$ } (100)



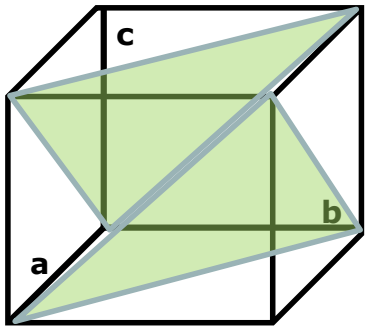
(010)



(020)



(111)



$(11\bar{1})$

- directions are ⊥ to the plane with the same Miller indices

PLANES IN THE HEXAGONAL CELL

In this case there are 4 axes: 3 in the basal plane and the c axis

Basal plane (a_1, a_2, a_3) +Axis c

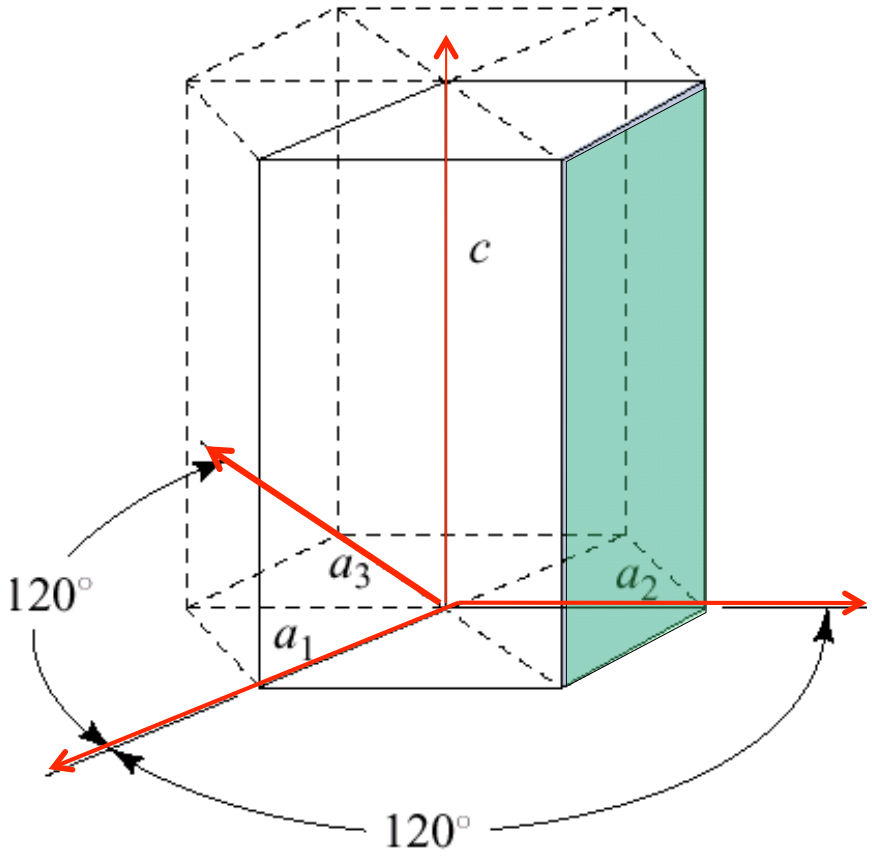
↓ ↓

uvt w

They can be expressed in 3 taking

t= -(u+v)

(u'v'w')=(uvtw)



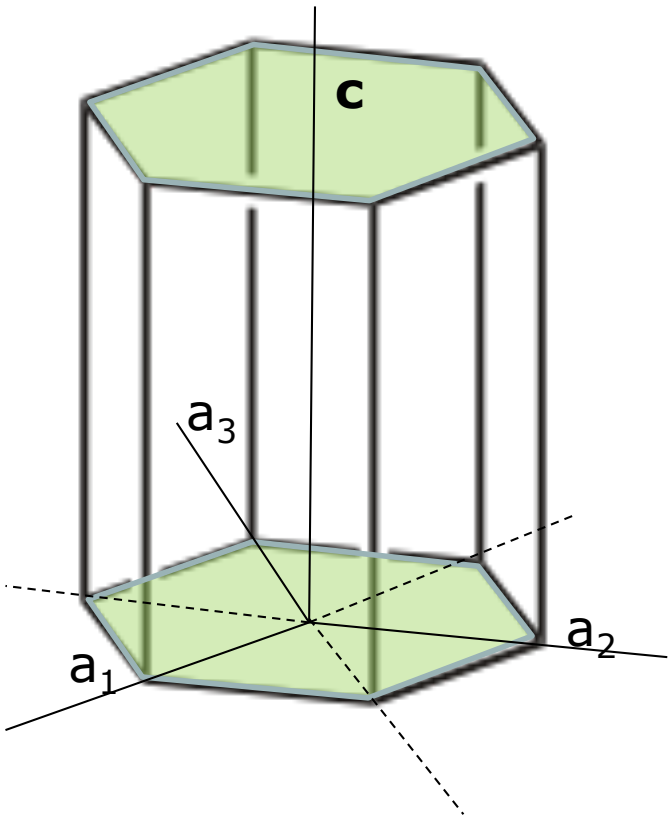
PLANES IN THE HEXAGONAL CELL

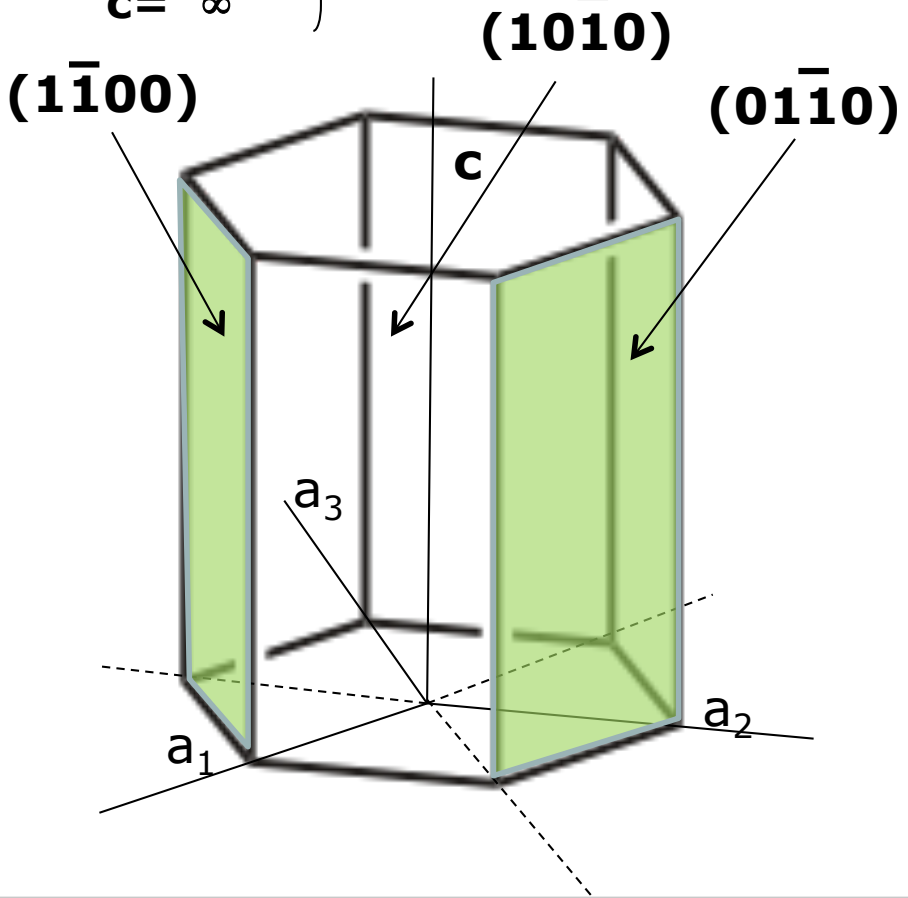
$a_1 = \infty$
$a_2 = \infty$
$a_3 = \infty$
$c = 1$

(0001) Basal plane

$a_1 = \infty$
$a_2 = 1$
$a_3 = -1$
$c = \infty$

$(01\bar{1}0)$ prism plane





DIRECTIONS IN THE HEXAGONAL CELL

In this case there are 4 axes: 3 in the basal plane and the c axes for the height

Basal plane (a_1, a_2, a_3) + c Axis

↓ ↓

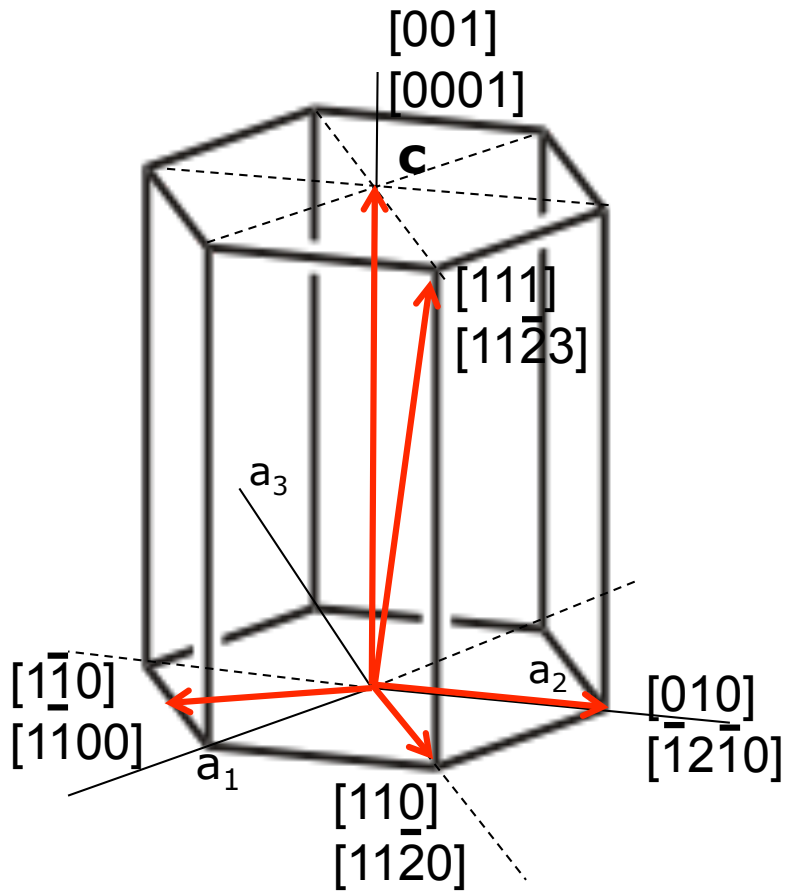
uvt w

They can be expressed in 3 taking $t = -(u+v)$

$[u'\ v'\ w] \equiv [u\ v\ t\ w]$

$[1\ 0\ 0] \equiv [2\ \bar{1}\ \bar{1}\ 0]$

$[1\ 1\ 0] \equiv [1\ 1\ \bar{2}\ 0]$



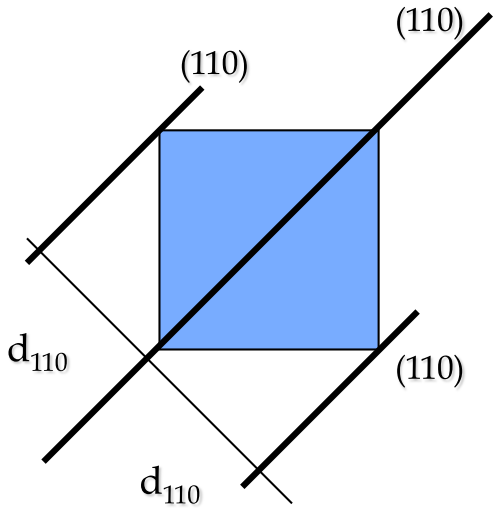
Bragg´s law

The magnitude of the distance between two adjacent parallel planes (i.e. the interplanar spacing d_{hkl} is a function of the Miller indices (h, k, l) as well as the lattice paremeter(s)

Cubic Crystals:

- Distance between // planes in cubic crystals : d_{hkl}

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



- For orthogonal crystals, in general:

$$\frac{1}{d_{hkl}^2} = \frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2}$$

ATOMIC DENSITY IN CRYSTALS

Volume density of a crystal

Rigid spheres model

$R_{atomic} \Rightarrow$ X-ray diffraction

$$\rho_V = \frac{\text{mass of unit cell}}{\text{volume of unit cell}} = \frac{\text{nº atoms per cell} \cdot \text{mass of atom}}{\text{volume of unit cell}}$$

ATOMIC DENSITY IN CRYSTALS: examples

Volumetric density of Cu, knowing:

R=0.1278 nm M=63.54 g/mol FCC

$$\rho = \frac{n \cdot M}{V_C N_A}$$

n: number of atoms /unit cell

M: atomic weight

V_C: volume of the unit cell

N_A: Avogadro number (6.023×10^{23} atoms/mol)

$$V_C = a^3 = (2R\sqrt{2})^3 = 16\sqrt{2}R^3$$

$$\rho = \frac{(4)(63.5)}{[16\sqrt{2}(1.28\times10^{8})^3 \times 6.023\times10^{23}]} = 8.98 g/cm^3$$

8.94 ***g/cm³ from the bibliography***

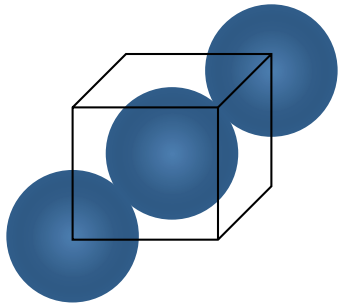
ATOMIC DENSITY IN CELLS

Linear Atomic Density:

$$\rho_l = \frac{\text{Nº .atoms intersected diametrically by the line}}{\text{length of line}} = \frac{atoms}{m}$$

BCC

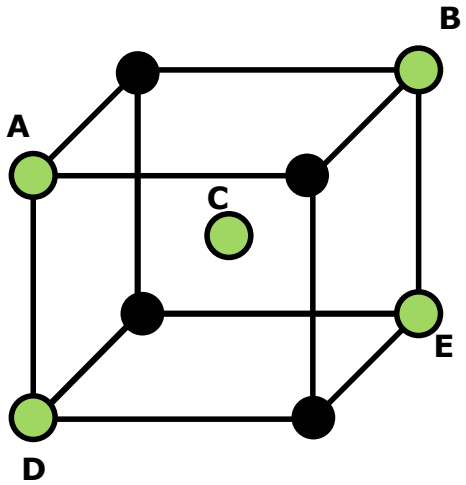
$$\rho_{[111]} = \frac{1\,\text{central atom} + 2\cdot \frac{1}{2}\,\text{vertices}}{\sqrt{3}\cdot a} = \frac{2\sqrt{3}}{3a}\,\frac{atoms}{m}$$

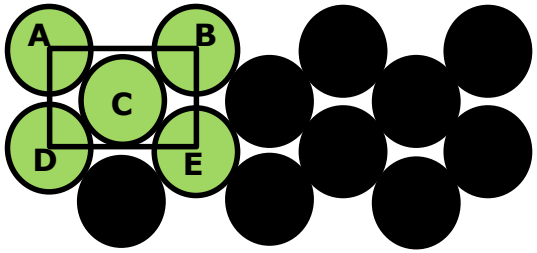


ATOMIC PLANAR DENSITY IN CELLS

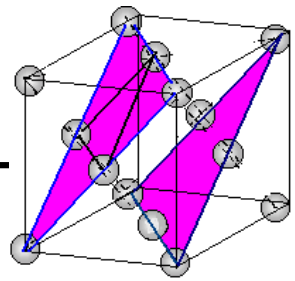
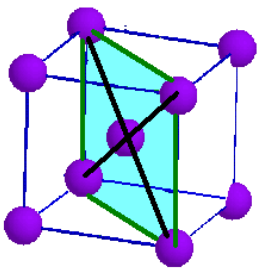
$$\rho_p = \frac{\text{Nº atoms intersected by the area/plane}}{\text{area of plane}} = \frac{atomss}{m^2}$$

$$\rho_p = \frac{1\,\text{central atom} + 4 \cdot {}^{1}\!/_{4}\,\text{vertices}}{\text{a} \cdot \sqrt{2} \cdot a} = \frac{\sqrt{2}}{a^2}\frac{atoms}{m^2}$$





Summary

Type of lattice	FCC	BCC	HCP
Nº atoms/cell	$\bullet 8\cdot{}^1/_8+6\cdot{}^1/_2=4$	$\bullet 8\cdot{}^1/_8+1=2$	$\bullet 12\cdot{}^1/_6+2\cdot{}^1/_2+3=6$
Atomic Radius	$r=\frac{a}{2\sqrt{2}}$	$r=\frac{a\sqrt{3}}{4}$	$r=\frac{\sqrt{\frac{a^2}{3}+\frac{c^2}{4}}}{2}$
V_{cell} and $V_{interstices}$	$V_{cell}=a^3$ $V_h=V_c-4(\frac{4}{3}\pi r^3)=5{,}872r^3$	$V_{cell}=a^3$ $V_h=V_c-2(\frac{4}{3}\pi r^3)=3{,}94r^3$	$V_{cell}=a^2\cdot c\cdot\frac{3\sqrt{3}}{2}$ $V_h=V_c-6(\frac{4}{3}\pi r^3)=8{,}808r^3$
Volume relative of interstitials	$V_r=\frac{V_h}{V_c}=0{,}26$	$V_r=0{,}32$	$V_r=0{,}26$
Octahedral Interstitials	Nº=4 R=½(a-2r)=0,41r	Nº=6 R=½(a-2r)=0,15r	Nº=6 R=0,41r
Tetrahedral Interstitials	Nº=8 $R_t=\left[\sqrt{\frac{3}{2}}-1\right]r=0{,}225r$	Nº=12 $R_t=\left[\sqrt{\frac{5}{3}}-1\right]r=0{,}291r$	Nº=12 R_t=0,225r
Close packed planes	{111} there are 4	{110} there are 6	{0001} there is 1
Closed packed directions	<110> there are 6 	<111> there are 4 	<2$\bar{1}\bar{1}$0> there are 3