Crystal Directions

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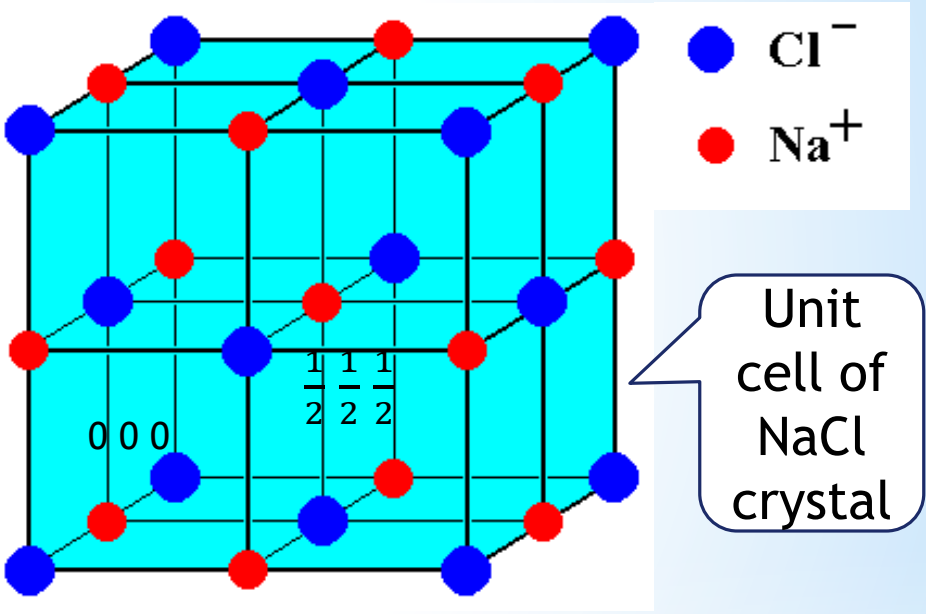
NaCl Structure

- NaCl is a cubic type of ionic crystal.
- FCC type of lattice.

  Cl^-: 8 x 1/8 corner + 6 x ½ faces = 4

  Na^+: 12 x ¼ edges + 1 center = 4
- So, total 4 NaCl molecules, each NaCl is a basis.
- Each Na^+ 6 nearest neighbor Cl^- and vice versa.
- Nearest neighbor distance = a/2.
- 2nd neighbor distance =a/√2
- Each Na^+ 12 2nd nearest neighbor Na^+ and vice versa.



Cl^-: $0\ 0\ 0,\ \frac{1}{2}\ \frac{1}{2}\ 0,\ \frac{1}{2}\ 0\ \frac{1}{2},\ 0\ \frac{1}{2}\ \frac{1}{2}$.

Na^+: $\frac{1}{2}\ \frac{1}{2}\ \frac{1}{2},\ \frac{1}{2}\ 0\ 0,\ 0\ \frac{1}{2}\ 0,\ 0\ 0\ \frac{1}{2}$.

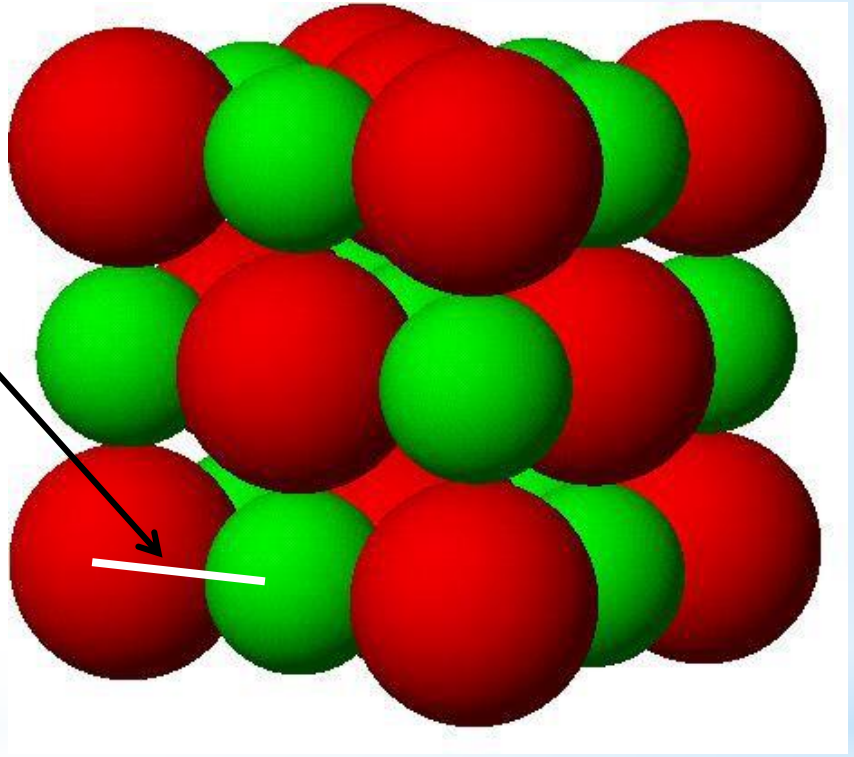
Packing Factor of NaCl structure

Closest packing along nearest neighbor distance, a/2= $r_{Na^+} + r_{Cl^-}$

$$PF = \frac{4 \times \frac{4}{3}\pi[(r_{Na^+})^3 + (r_{Cl^-})^3]}{[2\,(r_{Na^+} + r_{Cl^-}]^3}$$

$$= 0.67$$

Example: LiH, NaCl, KBr, KCl, PbS, NH_4I, AgBr, MgO, MnO, BaO, etc.

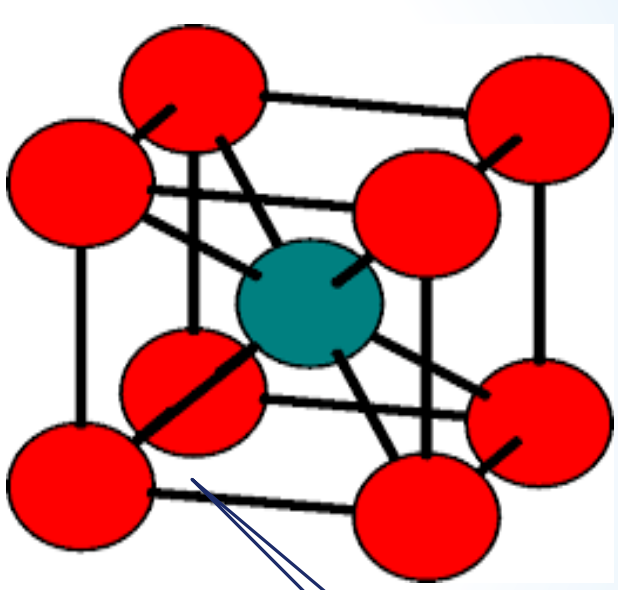


CsCl Structure

- CsCl is a simple cubic type of ionic crystal.

  Cs^+: 8 x 1/8 corner = 1

  Cl^-: 1 body center = 1
- So, total 1 CsCl molecule (basis).
- Each Cs^+ 8 nearest neighbor Cl^- and vice versa.
- Nearest neighbor distance = $\sqrt{3}a/2$.
- 2^{nd} neighbor distance = a
- Each Cs^+ 6 2^{nd} nearest neighbor Cs^+ and vice versa.
- Cs^+: 0 0 0; Cl^-: $\frac{1}{2}\frac{1}{2}\frac{1}{2}$.

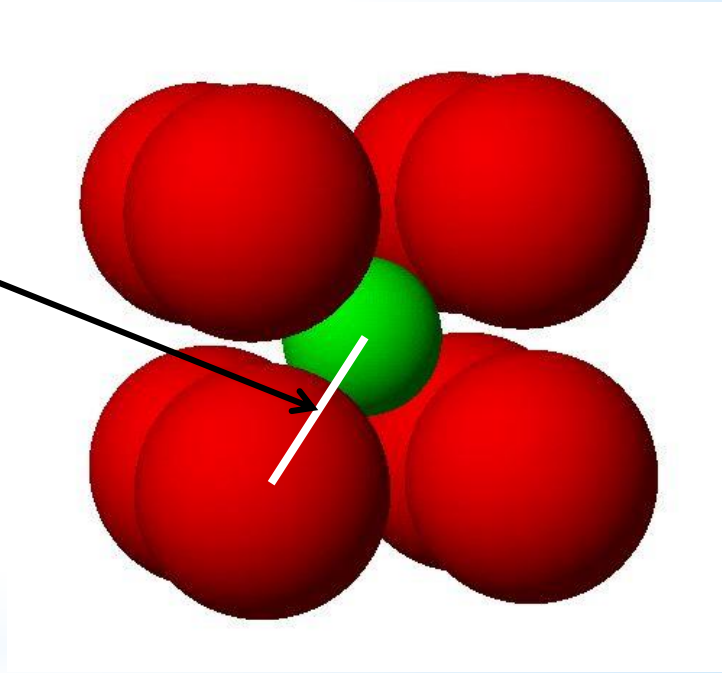


Packing Factor of CsCl structure

Closest packing along nearest neighbor distance, $\sqrt{3}a/2 = r_{Cs^+} + r_{Cl^-}$

$$PF = \frac{1 \times \frac{4}{3}\pi[(r_{Cs^+})^3 + (r_{Cl^-})^3]}{[2/\sqrt{3}\,(r_{Cs^+} + r_{Cl^-}]^3}$$

$$= 0.684$$

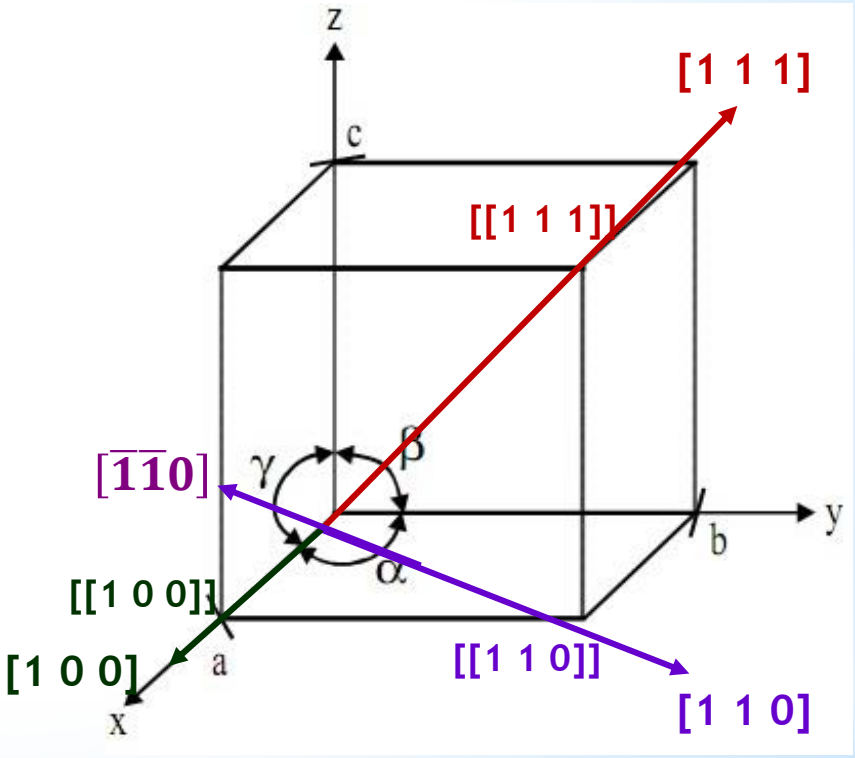


Example: CsCl, CsBr, NH_4Cl, CuZn, TlI, TlBr, etc.

Miller Indices

1. Indices of Site, [[m n p]]
2. Indices of Direction, [m n p]
3. Indices of Plane, (h k l)

* Indices of negative directions are indicated by " ¯ " bar sign.
  Example: $[\bar{1}00]$, $[\bar{1}\bar{1}0]$, etc.
* Intercepts of the planes are used describe a plane.

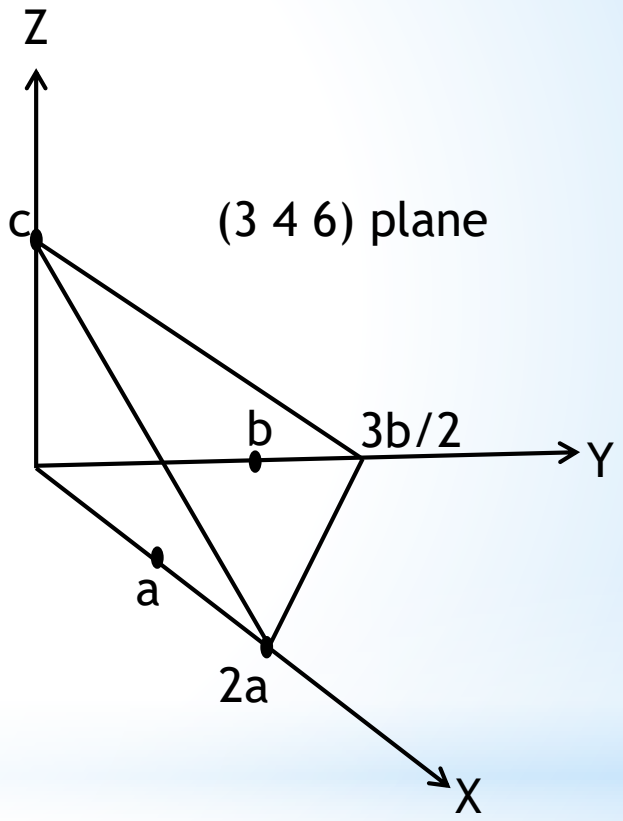


How to find Miller Indices

1. First we have to find the intercepts with the axes along the basis vector $\vec{a}$, $\vec{b}$ and $\vec{c}$. Let these intercepts of the plane be x, y, z. We form the fractional triplet $\left(\frac{x}{a}, \frac{y}{b}, \frac{z}{c}\right)$.
2. Take reciprocal to this set $\left(\frac{a}{x}, \frac{b}{y}, \frac{c}{z}\right)$.
3. Then reduce this set to a similar one having the smallest integers multiplying by common factor.
4. This last set is enclosed in parentheses (h k l), is called the index of the plane or Miller Indices.

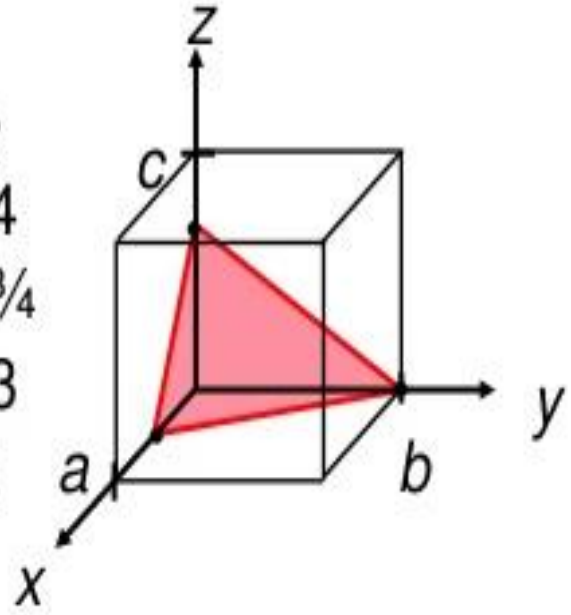
Example:

1. Let the intercepts are x = 2a, y = 3b/2, z = c.
2. We first form the set, $\left(\frac{x}{a},\frac{y}{b},\frac{z}{c}\right)$= $\left(\frac{2a}{a},\frac{3b}{2b},\frac{c}{c}\right)$= $\left(2,\frac{3}{2},1\right)$
3. Taking the reciprocal, $\left(\frac{1}{2},\frac{2}{3},1\right)$
4. Finally, multiply by a common (factor) denominator. Which is 6, to obtain the miller indices (h k l) = (3 4 6).



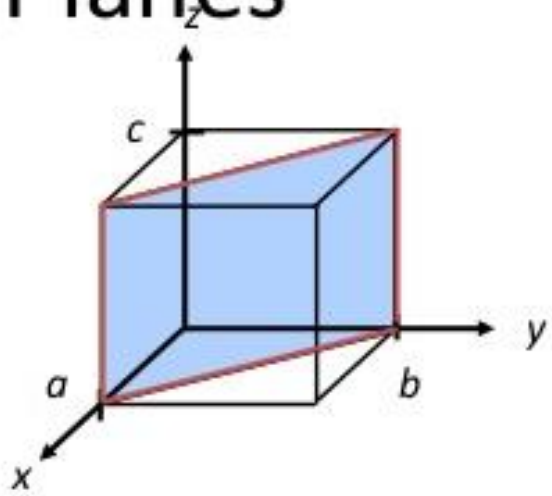
Crystallographic Planes

example	a	b	c
1. Intercepts	1/2	1	3/4
2. Reciprocals	1/½	1/1	1/¾
	2	1	4/3
3. Reduction	6	3	4
4. Miller Indices	(634)		

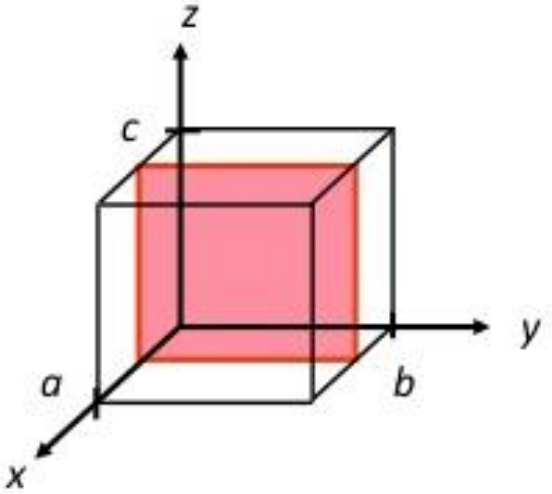


Crystallographic Planes

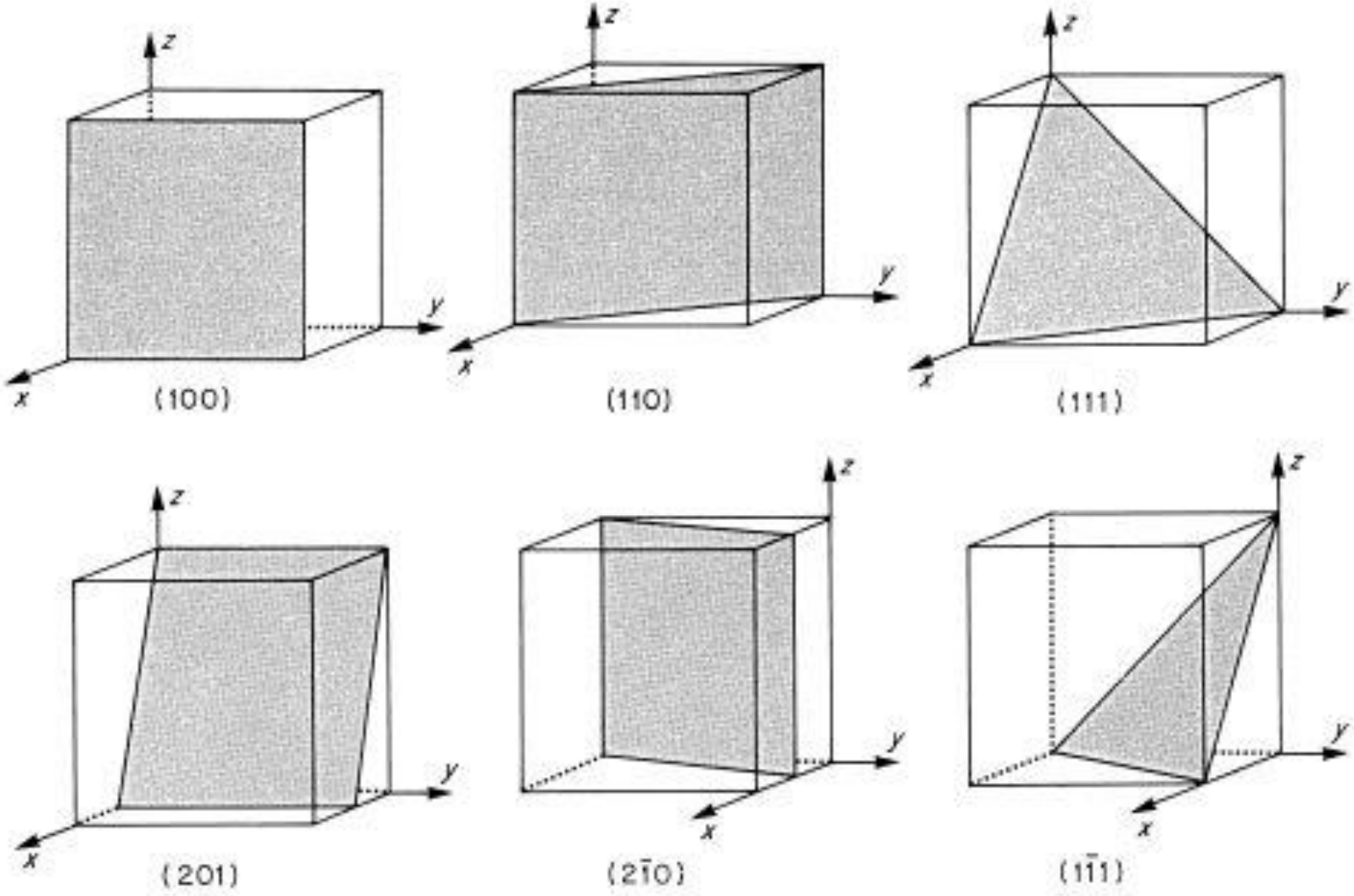
example		*a*	*b*	*c*
1.	Intercepts	1	1	∞
2.	Reciprocals	1/1	1/1	1/∞
		1	1	0
3.	Reduction	1	1	0
4.	Miller Indices	(110)		



example		*a*	*b*	*c*
1.	Intercepts	1/2	∞	∞
2.	Reciprocals	1/½	1/∞	1/∞
		2	0	0
3.	Reduction	2	0	0
4.	Miller Indices	(200)		



Miller Indices of Cubic Crystals



Relation between interplanar spacing and Miller indices:

Let us consider three mutually perpendicular coordinate axis, OX, OY, and OZ and assume that a plane (hkl) parallel to the plane passing through the origin makes intercepts a/h, b/k and c/l on the three axes at A. B and C respectively as shown in figure.

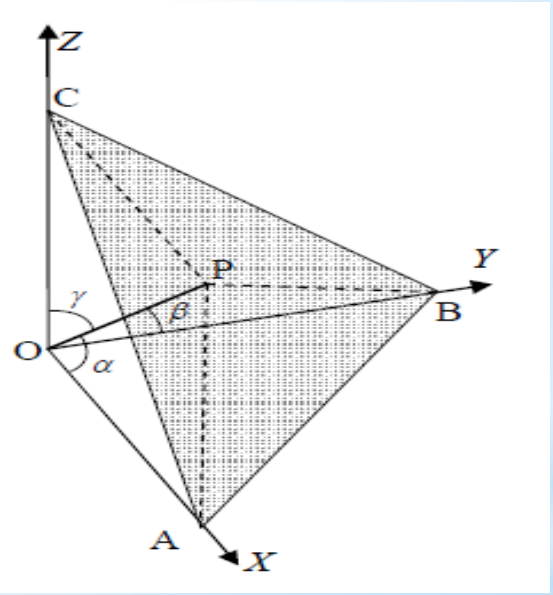
Let OP = d_{hkl}, the interplaner spacing be normal to the plane drawn from the origin and makes angle $\alpha, \beta, \text{and } \gamma$ with the 3 axes respectively.

Therefore, OA= $\frac{a}{h}$, OB= $\frac{b}{k}$, OC= $\frac{c}{l}$.

From ΔOPA, $\cos\alpha = \frac{OP}{OA} = \frac{d_{hkl}}{a/h}$

Similarly, from ΔOPB, $\cos\beta = \frac{OP}{OB} = \frac{d_{hkl}}{b/k}$

And from ΔOPC, $\cos\gamma = \frac{OP}{OC} = \frac{d_{hkl}}{c/l}$



But, for a rectangular coordinate system, using directional cosine we have, $\cos^2\alpha + \cos^2\beta + \cos^2\gamma = 1$ ----------(1)

Substituting the values of $\cos\alpha$, $\cos\beta$ and $\cos\gamma$ in the equation (1) we get,

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

$$d_{hkl} = \frac{1}{\sqrt{\left[\frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2}\right]}} \text{ ----------(2)}$$

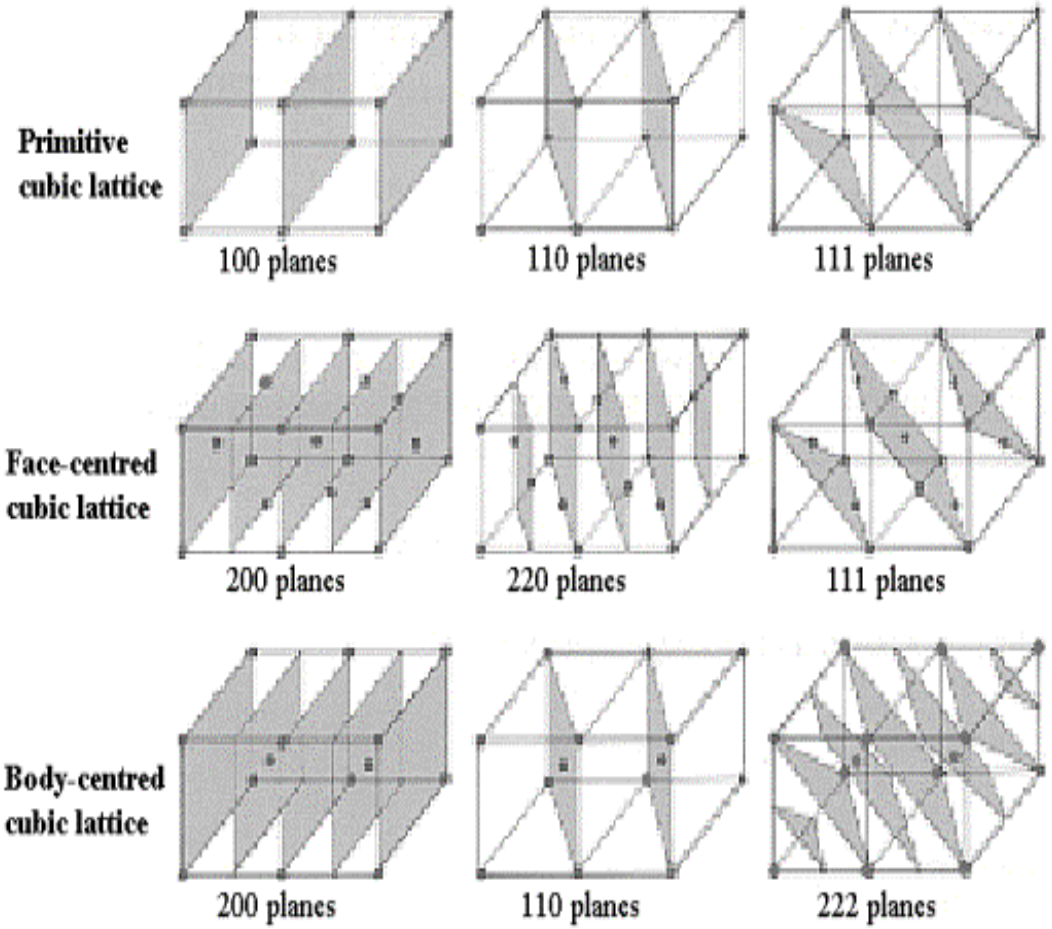
This is the general formula and is applicable to the primitive lattice of orthorhombic, tetragonal and cubic systems.

i. Orthorhombic system: a ≠ b ≠ c $d_{hkl} = \frac{1}{\sqrt{\left[\frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2}\right]}}$

ii. Tetragonal system: a = b ≠ c

iii. Cubic system: a = b = c $d_{hkl} = \frac{a}{\sqrt{h^2 + k^2 + l^2}}$

Miller Indices of Cubic Crystals



$d_{100}: d_{110}: d_{111} = 1: \frac{1}{\sqrt{2}}: \frac{1}{\sqrt{3}}$

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