Miller indices and interplanar spacing, Linear density and Planar density

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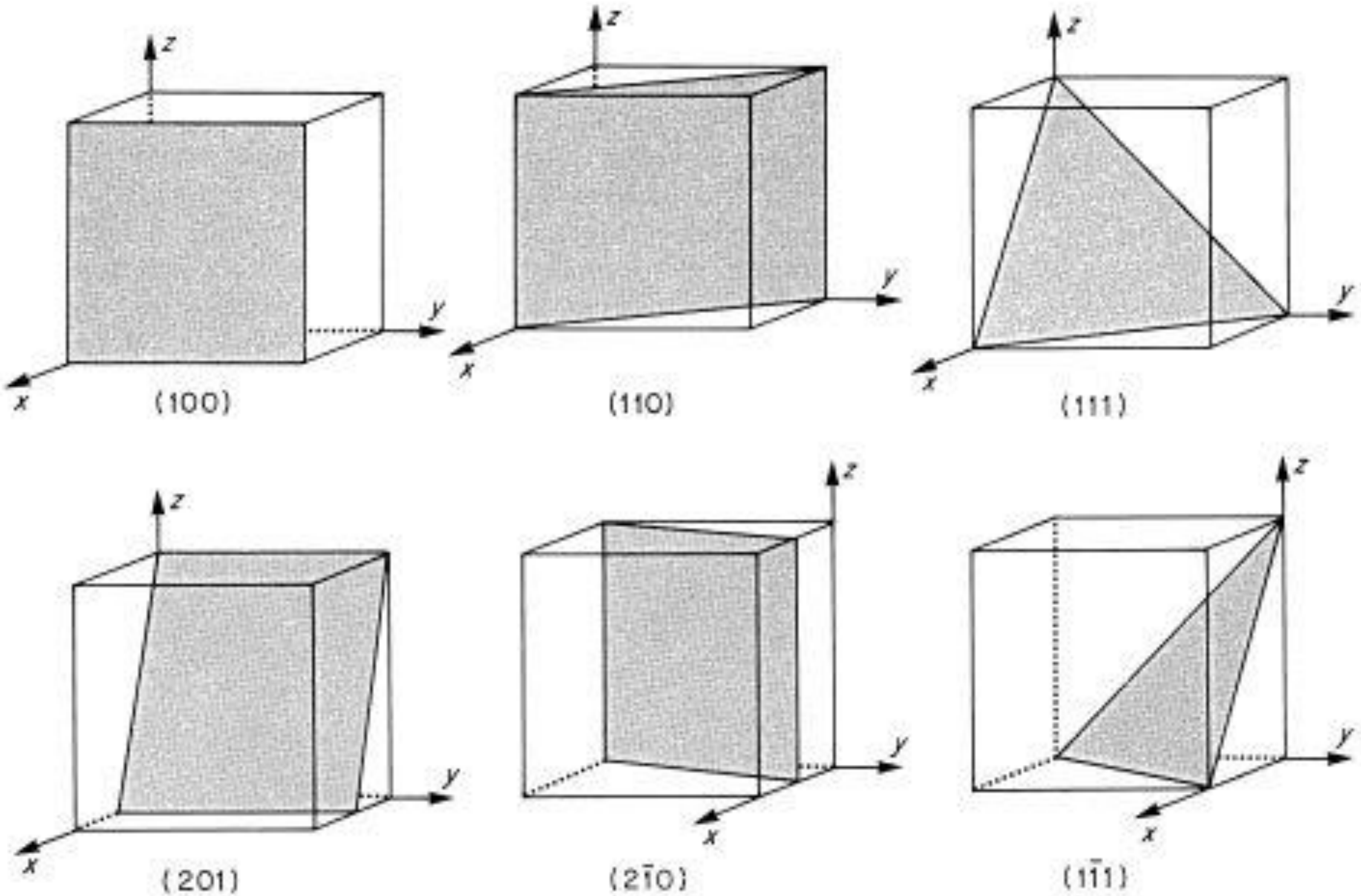
Miller Indices of Cubic Crystals



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.

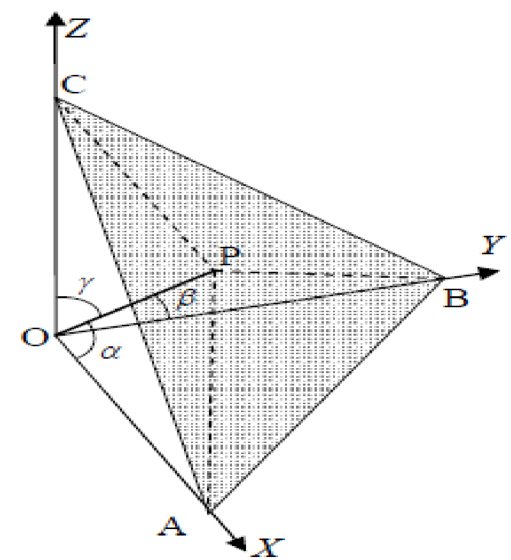
Let OP = d_{hkl}, the interplaner spacing be normal to the plane drawn from the origin and makes angle α, β, and γ with the 3 axes respectively.

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,

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

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

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

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

Interplanar Spacing

Cubic:

$$\frac{1}{d^2} = \frac{h^2 + k^2 + l^2}{a^2}$$

Tetragonal:

$$\frac{1}{d^2} = \frac{h^2 + k^2}{a^2} + \frac{l^2}{c^2}$$

Hexagonal:

$$\frac{1}{d^2} = \frac{4}{3}\left(\frac{h^2 + hk + k^2}{a^2}\right) + \frac{l^2}{c^2}$$

Rhombohedral:

$$\frac{1}{d^2} = \frac{(h^2 + k^2 + l^2)\sin^2\alpha + 2(hk + kl + hl)(\cos^2\alpha - \cos\alpha)}{a^2(1 - 3\cos^2\alpha + 2\cos^3\alpha)}$$

Orthorhombic:

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

Monoclinic:

$$\frac{1}{d^2} = \frac{1}{\sin^2\beta}\left(\frac{h^2}{a^2} + \frac{k^2\sin^2\beta}{b^2} + \frac{l^2}{c^2} - \frac{2hl\cos\beta}{ac}\right)$$

Triclinic:

$$\frac{1}{d^2} = \frac{1}{V^2}\left(S_{11}h^2 + S_{22}k^2 + S_{33}l^2 + 2S_{12}hk + 2S_{23}kl + 2S_{13}hl\right)$$

where

$$S_{11} = b^2c^2\sin^2\alpha$$
$$S_{22} = a^2c^2\sin^2\beta$$
$$S_{33} = a^2b^2\sin^2\gamma$$
$$S_{12} = abc^2(\cos\alpha\cos\beta - \cos\gamma)$$
$$S_{23} = a^2bc(\cos\beta\cos\gamma - \cos\alpha)$$
$$S_{13} = ab^2c(\cos\gamma\cos\alpha - \cos\beta)$$

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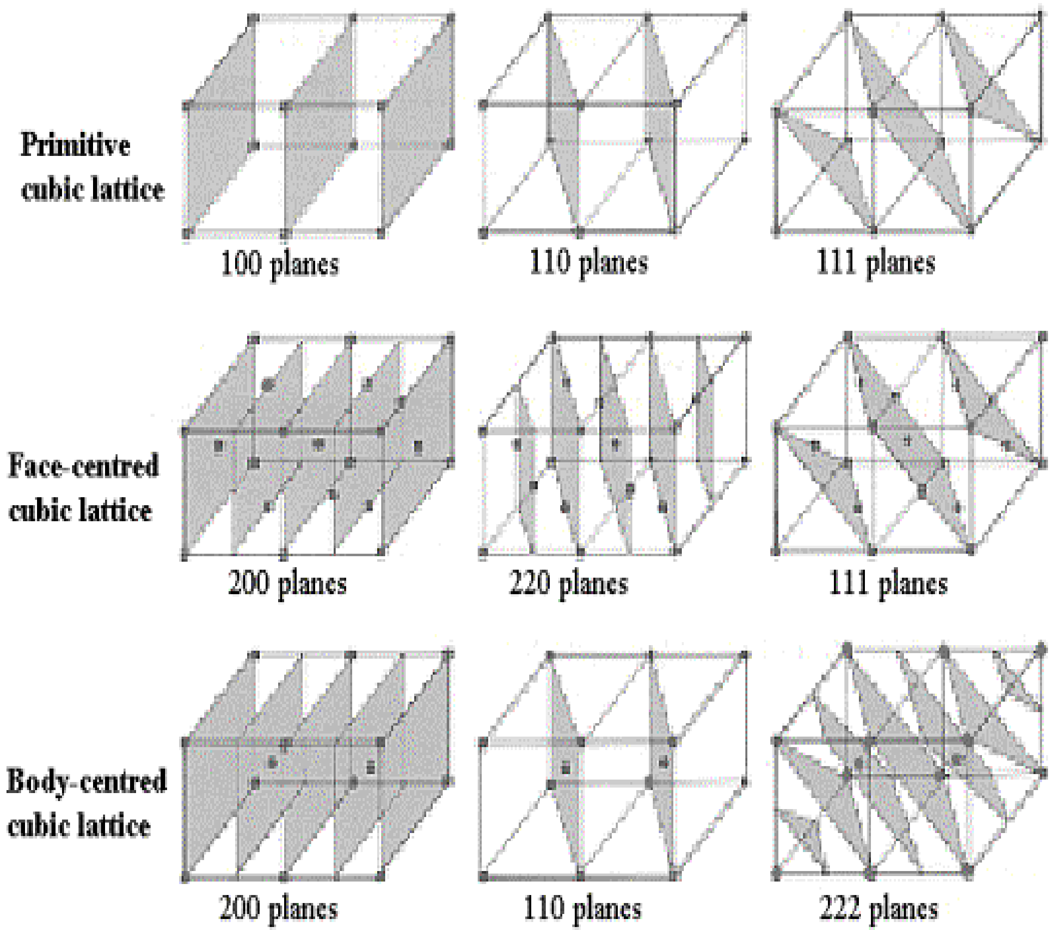

$$d_{100}: d_{110}: d_{111} = 1: \frac{1}{\sqrt{2}}:\frac{1}{\sqrt{3}}$$

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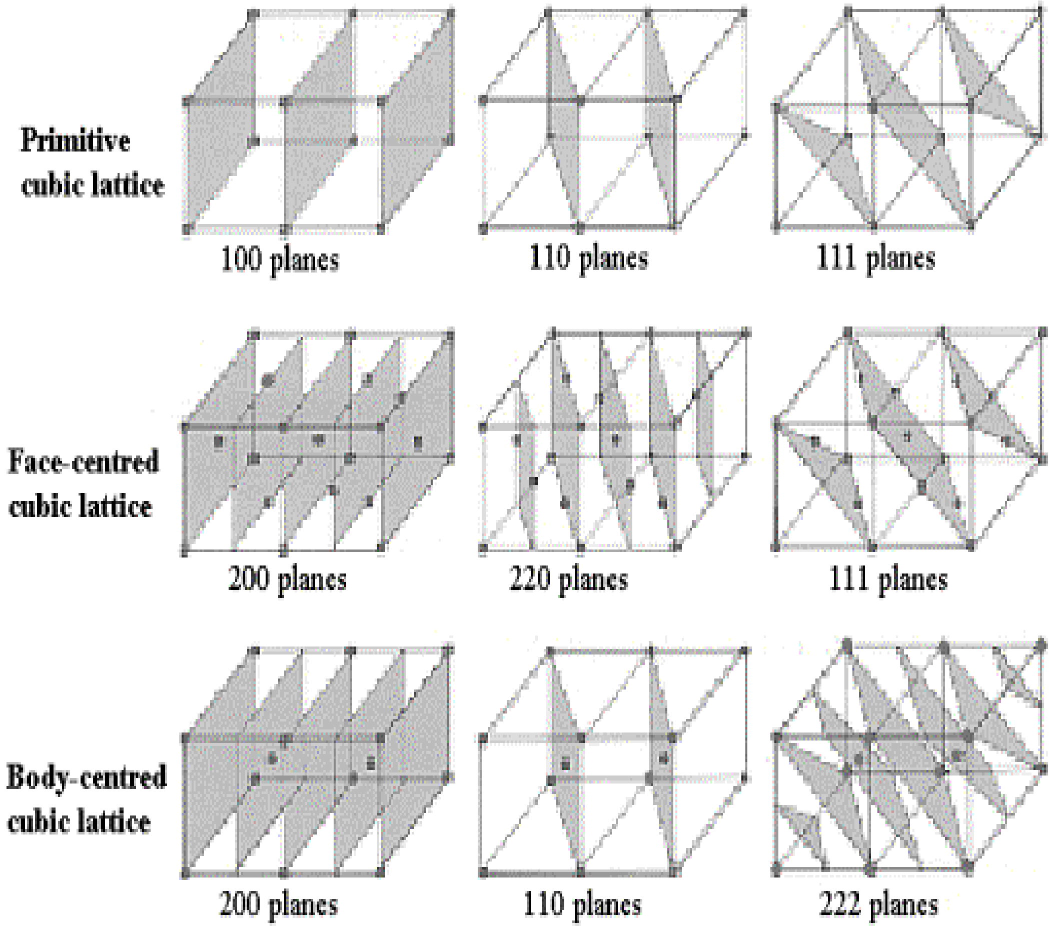

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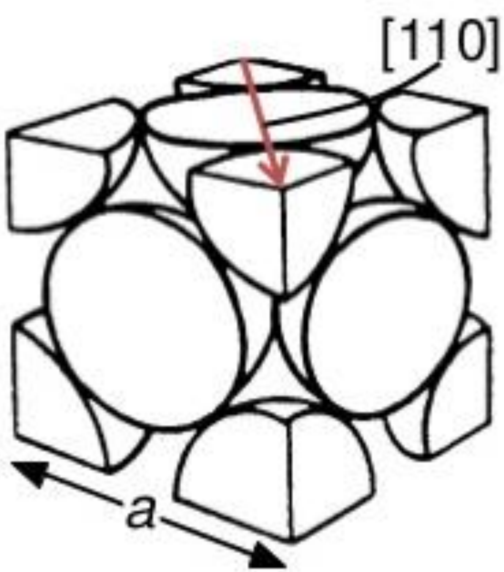
Linear Density and Planar Density

$$\text{Linear density (LD)} = \frac{\text{Number of atoms along a direction}}{\text{Length of the direction}}$$



ex: linear density of Al in [110] direction

$a = 0.405$ nm

$$\text{LD} = \frac{\overbrace{2}^{\#\text{ atoms}}}{\underbrace{\sqrt{2}a}_{\text{length}}}$$

$$\text{Planar density } (\delta) = \frac{\text{nd}}{\text{V}}$$

$\text{n} = \text{Number of atoms in the unit cell}$

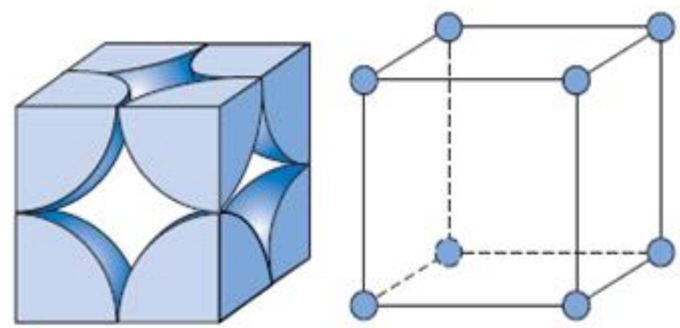
$\text{d} = \text{Interplanar spacing between two (hkl)planes}$

$\text{V} = \text{Volume of the unit cell}$

$$\delta_{100} = \frac{1 \times d_{100}}{a^3} = \frac{1 \times a}{a^3} = \frac{1}{a^2}$$

$$\delta_{110} = \frac{1 \times d_{110}}{a^3} = \frac{1 \times a}{\sqrt{2}a^3} = \frac{1}{\sqrt{2}a^2}$$

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



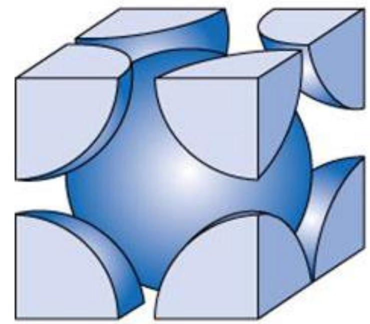
(a) (b)

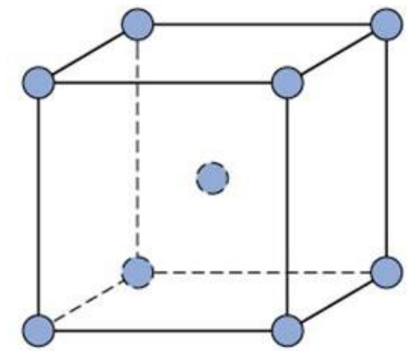
SC

$$\delta_{100} = \frac{2 \times d_{100}}{a^3} = \frac{2 \times a}{2 \times a^3} = \frac{1}{a^2}$$

$$\delta_{110} = \frac{2 \times d_{110}}{a^3} = \frac{2 \times a}{\sqrt{2}a^3} = \frac{\sqrt{2}}{a^2}$$

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



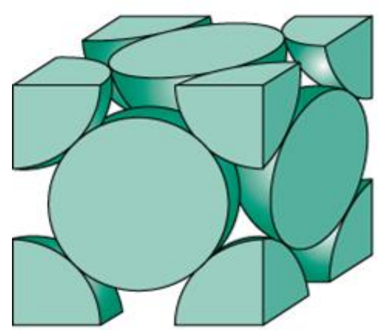


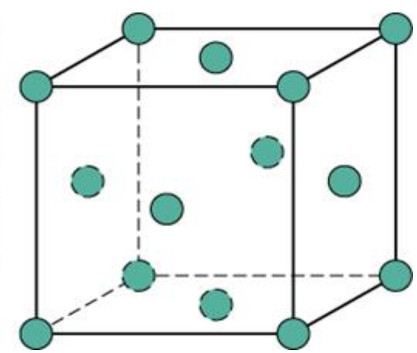
BCC

$$\delta_{100} = \frac{4 \times d_{100}}{a^3} = \frac{4 \times a}{2 \times a^3} = \frac{2}{a^2}$$

$$\delta_{110} = \frac{4 \times d_{110}}{a^3} = \frac{4 \times a}{2\sqrt{2}a^3} = \frac{\sqrt{2}}{a^2}$$

$$\delta_{111} = \frac{4 \times d_{111}}{a^3} = \frac{4 \times a}{\sqrt{3}a^3} = \frac{4}{\sqrt{3}a^2}$$





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Sample Problems

- The distance between consecutive (111) planes in a cubic crystal is 2 *Å*. Determine the lattice parameter. [Ans: 3.46 Å]
- In a tetragonal crystal, the lattice parameters $a=b=2.42$ *Å* and $c=1.74$ *Å*. Deduce the interplanar spacing between consecutive (101) planes. [Ans: 1.41 Å]
- Calculate the interplanar spacing for (321) plane in simple cubic lattice with the interatomic spacing $a= 4.21$ *Å*. [Ans: 1.01 Å]
- Worked out problems in the book “Solid State Physics” by M. A. Wahab, 2nd ed, Page no. 33,36. Practice the problems in the exercise of the mentioned chapter.