2-Reciprocal Lattice

Primer in Materials

Spring 2021

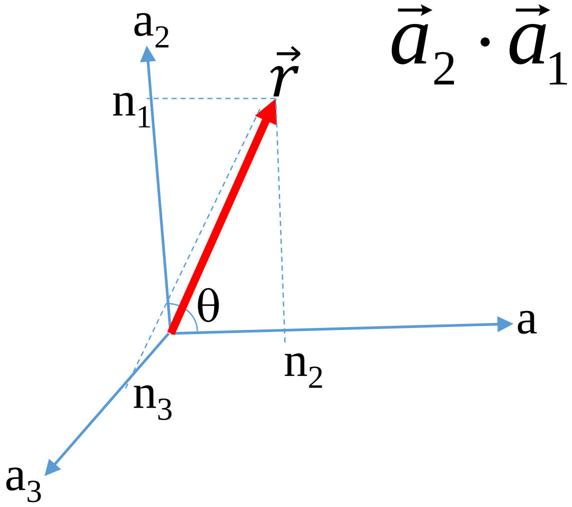
$$\vec{a}_2 \times \vec{a}_1 = a_1 a_2 \sin(\theta)\vec{N}$$

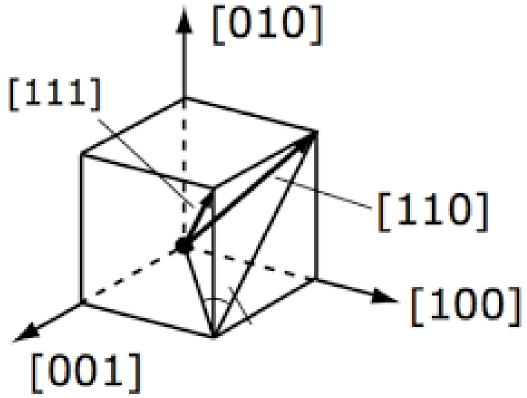
$$\vec{a}_2 \cdot \vec{a}_1 = a_1 a_2 \cos(\theta)$$

Lattice Vector:

$$\vec{r} = n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3$$

$$V = (\vec{a}_2 \times \vec{a}_1)\cdot\vec{a}_3$$





$[n_1n_2n_3]$ - a specific crystal direction

$\langle n_1n_2n_3 \rangle$ – a family of crystal directions

Reciprocal Lattice Vector:

$$\vec{H} = n_1'\vec{b}_1 + n_2'\vec{b}_2 + n_3'\vec{b}_3$$

$$\vec{b}_1 = \frac{\vec{a}_2 \times \vec{a}_3}{V} \qquad \vec{b}_2 = \frac{\vec{a}_1 \times \vec{a}_3}{V} \qquad \vec{b}_3 = \frac{\vec{a}_2 \times \vec{a}_1}{V} \qquad V_R = \frac{1}{V}$$

Example 2.1

Determine the basic reciprocal lattice vectors for orthorhombic and hexagonal lattice.

Orthorhombic:

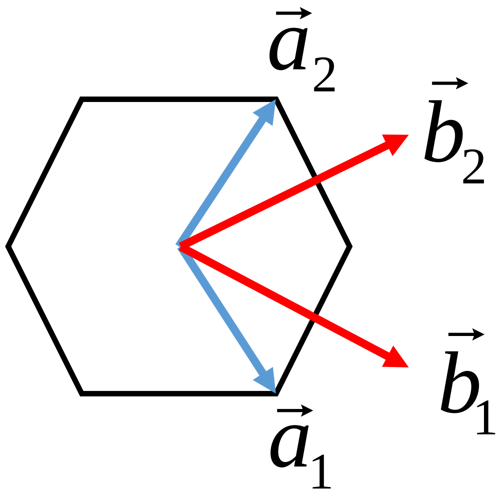
$$\vec{a}_2 \perp \vec{a}_1 \perp \vec{a}_3 \qquad V = a \times b \times c$$

$$\vec{b}_1 = \frac{\vec{a}_2 \times \vec{a}_3}{V} = \frac{1}{a}\vec{a}_1 \quad \vec{b}_2 = \frac{\vec{a}_1 \times \vec{a}_3}{V} = \frac{1}{b}\vec{a}_2 \qquad \vec{b}_3 = \frac{\vec{a}_2 \times \vec{a}_1}{V} = \frac{1}{c}\vec{a}_3$$

Hexagonal:

$$V = (\vec{a}_2 \times \vec{a}_1) \cdot \vec{a}_3 = a^2 c \sin 60 = \frac{a^2 c\sqrt{3}}{2}$$

$$\vec{b}_1 = \frac{\vec{a}_2 \times \vec{a}_3}{V} = \frac{2}{a\sqrt{3}} \vec{N}_{3,2} \qquad \vec{b}_2 = \frac{\vec{a}_1 \times \vec{a}_3}{V} = \frac{2}{a\sqrt{3}} \vec{N}_{3,1} \qquad \vec{b}_3 = \frac{\vec{a}_2 \times \vec{a}_1}{V} = \frac{1}{c} \vec{a}_3$$



Miller Indices

h, k, l are three integers that determine the reciprocal lattice vector, which is orthogonal to a specific crystal plane.

$$\vec{H}_{(hkl)} = h\vec{b}_1 + k\vec{b}_2 + l\vec{b}_3$$

$$-h \equiv \overline{h}$$

(hkl) - a specific crystal plane

{hkl} – a family of crystal planes

To determine Miller indices (hkl) of a plane, take the following steps:

1.Find the intercepts on the three axes in multiples or fractions of the edge lengths along each axis.

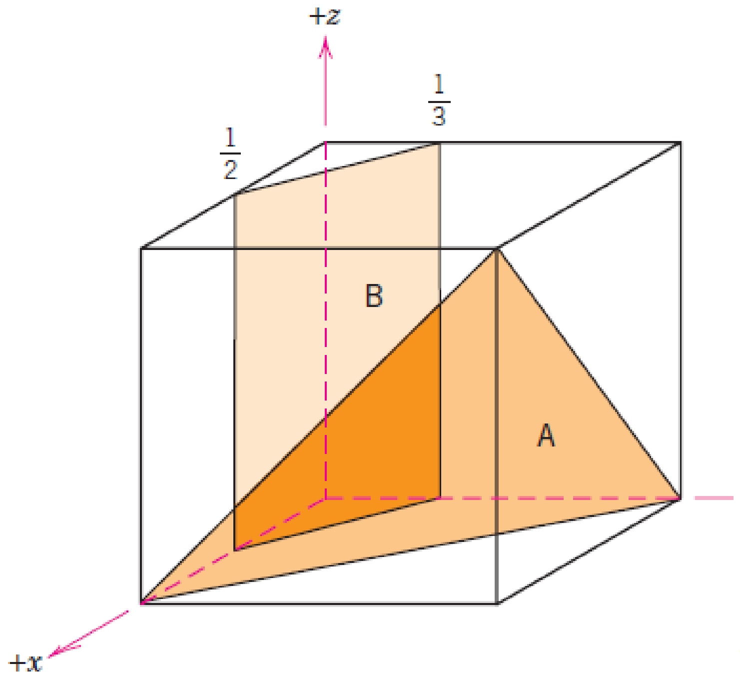
2.Determine the reciprocals of these numbers.

3.Reduce the reciprocals to the three smallest integers having the same ratio as the reciprocals.

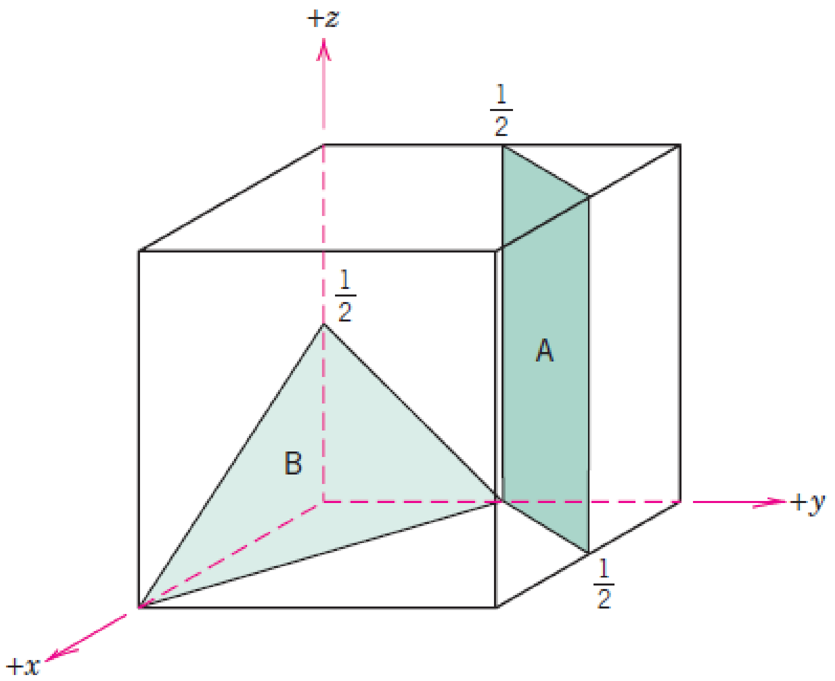
4.Enclose these three integral numbers in parentheses,e.g.,(hkl).

Example 2.2

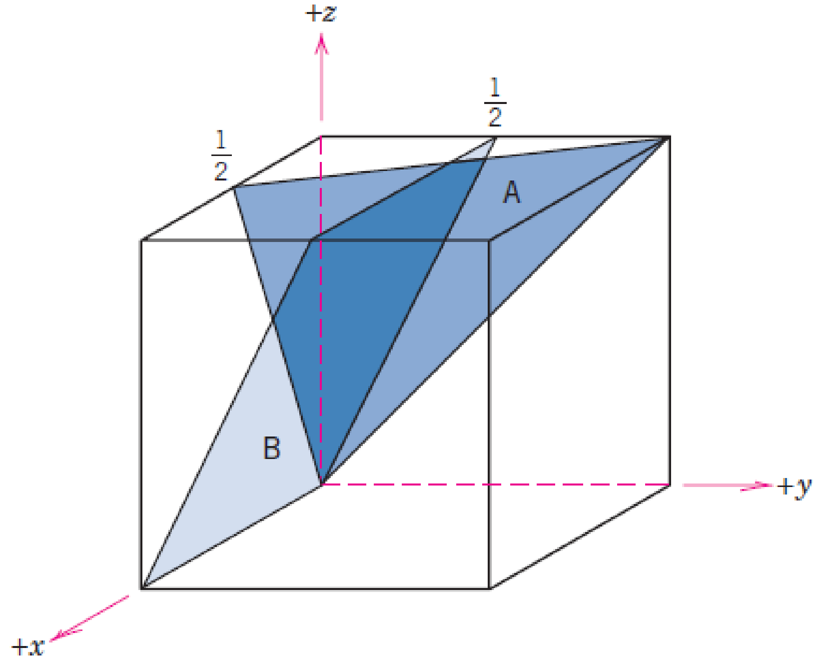
Determine the Miller indices for the planes shown in the following unit cells:



B – (230); A – $(11\bar{1})$



A – $(\bar{2}20)$; B – (122)



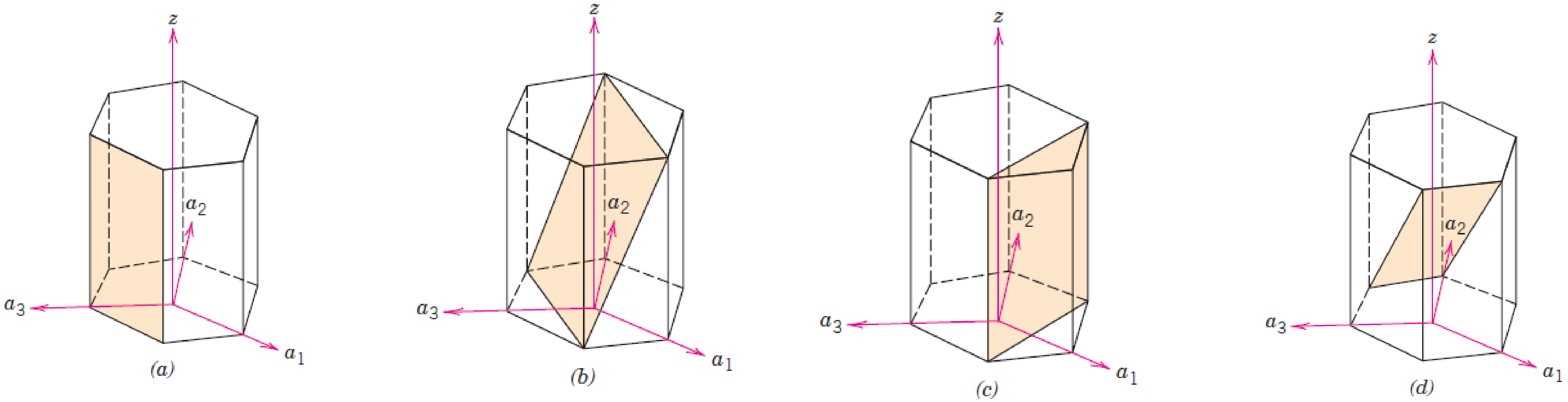
A – $(21\bar{1})$; B – $(02\bar{1})$

Miller Indices for Hexagonal

$(hkl) \rightarrow (hkil),\ i = -(h+k)$

Example 2.3

Determine the Miller indices for the planes shown in the following unit cells:



$(0\bar{1}10)$ $(\bar{1}\bar{1}22)$ $(2\bar{1}\bar{1}0)$ $(\bar{1}102)$

Angle Between Two Planes

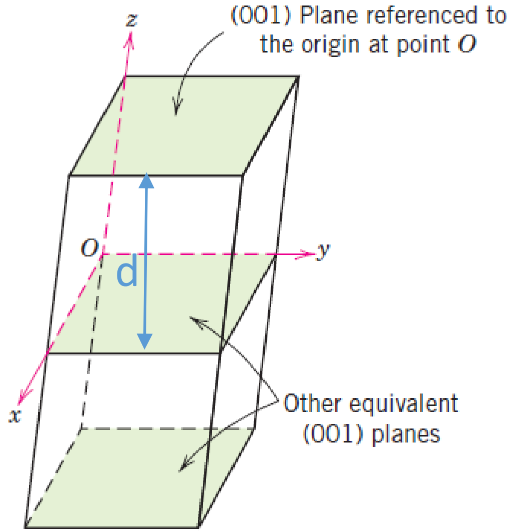
$$\cos\varphi = \frac{\vec{H}_1 \cdot \vec{H}_2}{\left|\vec{H}_1\right|\left|\vec{H}_2\right|}$$

Example 2.4

Calculate the angle between hexagonal (100) plane and (010) plane :

$$\cos\varphi = \frac{\vec{H}_1 \cdot \vec{H}_2}{\left|\vec{H}_1\right|\left|\vec{H}_2\right|} = \frac{\frac{4}{3a^2}\cos 60}{\frac{4}{3a^2}} = \frac{(10\bar{1}0)(01\bar{1}0)}{\sqrt{2}\times\sqrt{2}} = \frac{1}{2};\varphi = 60^\circ$$

d - Spacing



d – spacing is the shortest distance between to equivalent planes

$$d_{hkl} = \frac{1}{\left|\vec{H}_{hkl}\right|} = \frac{1}{\sqrt{(h\vec{b}_1 + k\vec{b}_2 + l\vec{b}_3)\cdot(h\vec{b}_1 + k\vec{b}_2 + l\vec{b}_3)}}$$

Example 2.5

Develop the expression for d –spacing of hexagonal crystal.

$$d_{hkl}^{Hex} = \frac{1}{\left|\vec{H}_{hkl}\right|} = \frac{1}{\sqrt{(h\vec{b}_1 + k\vec{b}_2 + l\vec{b}_3)\cdot(h\vec{b}_1 + k\vec{b}_2 + l\vec{b}_3)}} =$$

$$\frac{1}{\sqrt{h^2\frac{4}{3a^2} + k^2\frac{4}{3a^2} + \frac{l^2}{c^2} + 2hk\frac{4}{3a^2}\cos 60}} = \frac{1}{\sqrt{\frac{4}{3a^2}(h^2 + k^2 + hk) + \frac{l^2}{c^2}}}$$