F. Directions in Crystals

Consider a lattice vector

$$\vec{R} = u_1\vec{a}_1 + u_2\vec{a}_2 + u_3\vec{a}_3$$

Rules: (i) $\vec{R}$, of course, specifies a direction.

$$\boxed{\text{We represent the direction of } \vec{R} \text{ as } [u_1 u_2 u_3] \text{ (note: use square brackets)}}$$

e.g. $\vec{R} = 3\vec{a}_1 + 2\vec{a}_2 + \vec{a}_3$

The direction of $\vec{R}$ is given by $[321]$ square brackets

Recall: $\vec{a}_1, \vec{a}_2, \vec{a}_3$ are, in general, not orthogonal.

Q: What does [111] mean?

(ii) A negative index is indicated by a bar above its magnitude.

e.g. $\vec{R} = 3\vec{a}_1 + 2\vec{a}_2 - \vec{a}_3$

Direction: $[32\bar{1}]$

(iii) Any common divisors of u_1, u_2, u_3 are omitted.

e.g. Since $(3\vec{a}_1 + 2\vec{a}_2 - \vec{a}_3)$ and $(6\vec{a}_1 + 4\vec{a}_2 - 2\vec{a}_3)$ are in the same direction, $[32\bar{1}] = [64\bar{2}]$.

$\therefore$ $[32\bar{1}]$ represents the direction of $6\vec{a}_1 + 4\vec{a}_2 - 2\vec{a}_3$

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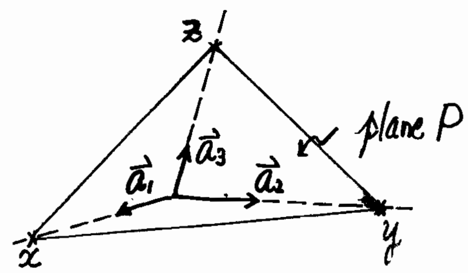
† Note: $\vec{a}_1, \vec{a}_2, \vec{a}_3$ are, in general, NOT mutually perpendicular.

G. Lattice Planes

- Aim: A lattice plane is a plane that passes through lattice points. A set of parallel lattice planes contain all the lattice points.
  - How can we label lattice plane?
  - What is the direction normal to a lattice plane?

- A lattice plane can be identified by giving 3 lattice points on the plane (recall: coordinate geometry)
- Consider a lattice plane P. Let x be the intercept of the plane in the direction along $\vec{a}_1$, y along $\vec{a}_2$, z along $\vec{a}_3$.



Note: There may or may not be lattice points at the intercepts, but this does not matter! (In most cases, the intercepts are lattice pts.)

- 3 points (or 2 vectors) on the plane characterize a plane

Let $\vec{R}_1 = l_1\vec{a}_1 + l_2\vec{a}_2 + l_3\vec{a}_3$

$\vec{R}_2 = m_1\vec{a}_1 + m_2\vec{a}_2 + m_3\vec{a}_3$

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

be <u>3 lattice points</u> on plane P

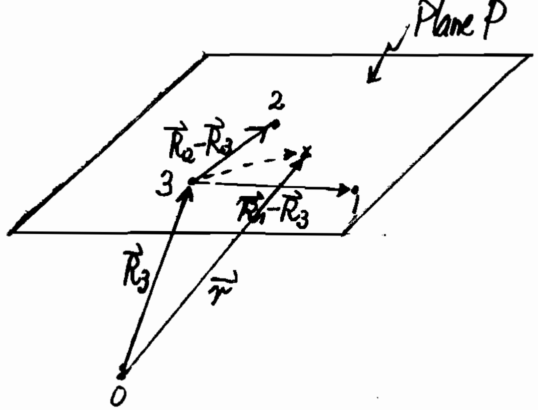
Q: Express the intercepts x, y, z in terms of $\underbrace{\{l_i\}, \{m_i\}, \{n_i\}}_{\text{9 integers}}$

$\vec{R}_1 - \vec{R}_3$ and $\vec{R}_2 - \vec{R}_3$ are 2 vectors on P (see figure)

- <u>Any point (position)</u> $\vec{r}$ on plane P can be expressed as:

$\vec{r} = \vec{R}_3 + \text{- - - -}\rightarrow$

(see figure)



$\therefore$ We can write

$$\underbrace{\vec{r}}_{\substack{\text{any position}\\ \text{on plane P}}} = \vec{R}_3 + \alpha(\vec{R}_1 - \vec{R}_3) + \beta(\vec{R}_2 - \vec{R}_3)$$

where α, β are numbers

- In terms of $\{l_i\}, \{m_i\}, \{n_i\}$,

$$\vec{r} = [n_1 + (l_1 - n_1)\alpha + (m_1 - n_1)\beta]\vec{a}_1 + [n_2 + (l_2 - n_2)\alpha + (m_2 - n_2)\beta]\vec{a}_2 + [n_3 + (l_3 - n_3)\alpha + (m_3 - n_3)\beta]\vec{a}_3 \quad \text{---}(*)$$

- In particular, the intercept x along $\vec{a}_1$-axis is a point on P given by $\vec{r} = x\vec{a}_1 + 0\cdot\vec{a}_2 + 0\cdot\vec{a}_3$

$\therefore$ We have:

$$\left.\begin{aligned} n_2 + (l_2 - n_2)\alpha + (m_2 - n_2)\beta &= 0 \\ n_3 + (l_3 - n_3)\alpha + (m_3 - n_3)\beta &= 0 \end{aligned}\right\} \Rightarrow \alpha \text{ and } \beta$$

and

$$x = n_1 + (l_1 - n_1)\alpha + (m_1 - n_1)\beta$$

$$= \frac{l_1(m_2n_3 - m_3n_2) + l_2(m_3n_1 - m_1n_3) + l_3(m_1n_2 - m_2n_1)}{(l_2 - n_2)(m_3 - n_3) - (l_3 - n_3)(m_2 - n_2)}$$

(after substituting in α and β) (Ex.)

$$\Rightarrow \quad x = \frac{N}{\Delta_{23}}$$

where N is the numerator

and $\Delta_{23} = \begin{vmatrix} l_2 - n_2 & m_2 - n_2 \\ l_3 - n_3 & m_3 - n_3 \end{vmatrix}$

- We can also apply (*) to the intercept along $\vec{a}_2$ and get:

$$y = \frac{N}{\Delta_{31}} \quad \text{where} \quad \Delta_{31} = \begin{vmatrix} l_3 - n_3 & m_3 - n_3 \\ l_1 - n_1 & m_1 - n_1 \end{vmatrix}$$

- Applying (*) to the intercept along $\vec{a}_3$, we get

$$z = \frac{N}{\Delta_{12}} \quad \text{where} \quad \Delta_{12} = \begin{vmatrix} l_1 - n_1 & m_1 - n_1 \\ l_2 - n_2 & m_2 - n_2 \end{vmatrix}$$

We have succeeded in expressing x, y, z in terms of $\{l_j\}, \{m_j\}, \{n_j\}$.

- Consider the ratio of the inverse of the intercepts:

$$\frac{1}{x} : \frac{1}{y} : \frac{1}{z} = \Delta_{23} : \Delta_{31} : \Delta_{12}$$
$$= h : k : l$$

where h, k, l are the three smallest integers that satisfy these ratios, i.e., h, k, l do not have a common integer divisor other than 1.

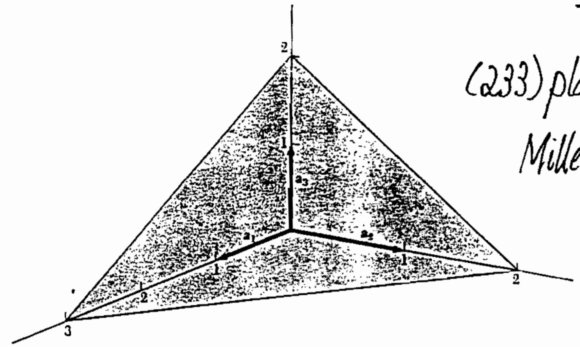
> These numbers h, k, l represent a plane or a set of parallel planes. They are called the Miller indices.
> The notation is (hkl).

Intercepts: 3, 2, 2

$$\frac{1}{x} : \frac{1}{y} : \frac{1}{z} = \frac{1}{3} : \frac{1}{2} : \frac{1}{2}$$
$$= 2 : 3 : 3$$

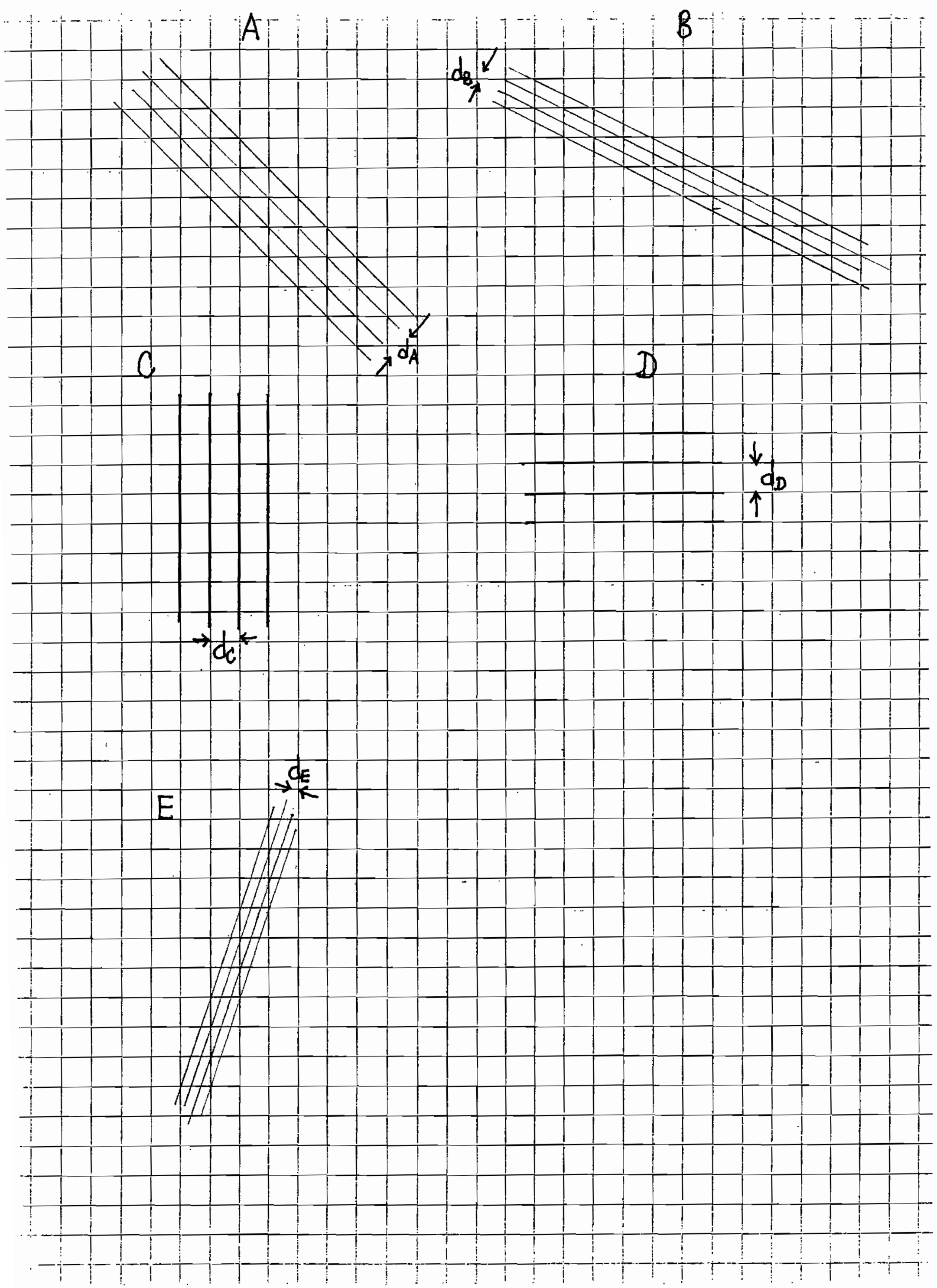
(233) plane

Miller indices (233)

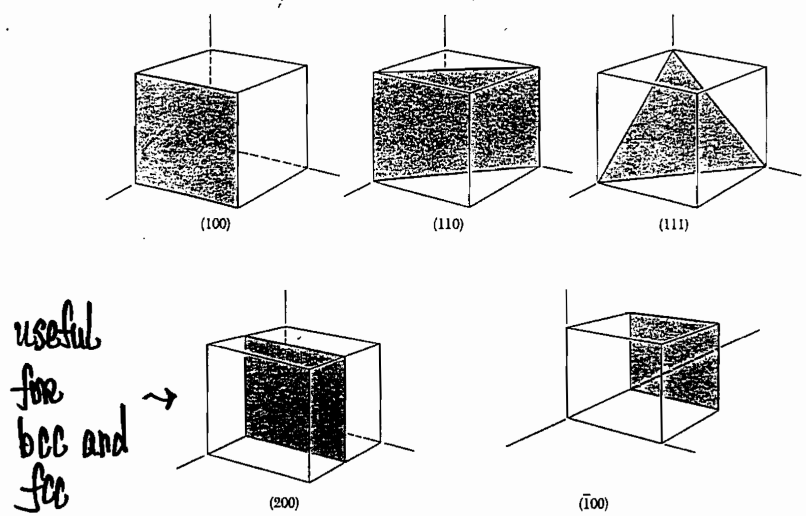


This plane intercepts the a_1, a_2, a_3 axes at $3a_1$, $2a_2$, $2a_3$. The reciprocals of these numbers are $\frac{1}{3}$, $\frac{1}{2}$, $\frac{1}{2}$. The smallest three integers having the same ratio are 2, 3, 3, and thus the indices of the plane are (233).

> **Summary:** The procedure to specify the orientation of a lattice plane by Miller indices is:
>
> (i) Find the intercepts on the axes $\vec{a}_1, \vec{a}_2, \vec{a}_3$. (Note: for convenience, the axes are sometimes taken as those of a non-primitive cell. Thus for bcc and fcc, the conventional cube is usually used.)
>
> (ii) If x, y, z are the intercepts, find the smallest integers such that $\frac{1}{x} : \frac{1}{y} : \frac{1}{z} = h : k : l$.
> If the intercept is at ∞, the corresponding index is zero.
>
> (iii) (hkl) gives the Miller indices of the plane.
>
> (iv) The lattice plane is normal to the vector
> $$\vec{q} = h(\vec{a}_2 \times \vec{a}_3) + k(\vec{a}_3 \times \vec{a}_1) + l(\vec{a}_1 \times \vec{a}_2).$$



Cubic lattices[+]

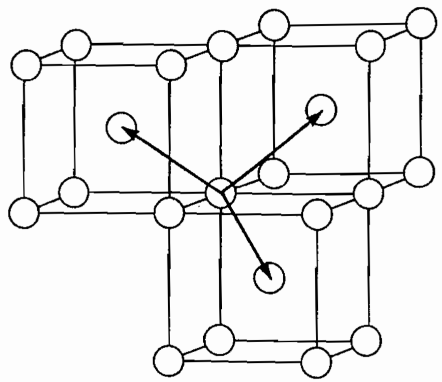


Indices of important planes in a cubic crystal. The plane (200) is parallel to (100) and to ($\bar{1}$00).

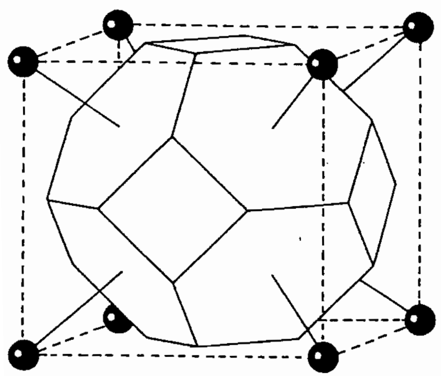
- Here, the (200) plane means a plane parallel to (100) but cutting the x-axis at $a/2$. (Useful in bcc and fcc) In doing so, the conventional unit cell description is used.

[+] Very often, the cube is also used for bcc and fcc as it has better geometry. But then it should be noted that it is used as a conventional (non-primitive cell).

BCC

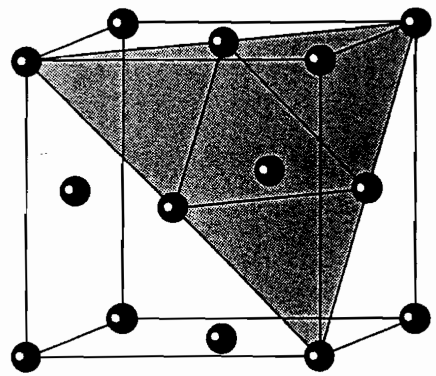


- Three neighboring conventional unit cells
- primitive vectors shown

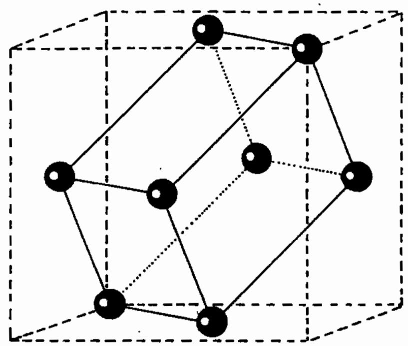


The shape outlined by the solid lines is the Wigner-Seitz cell of a bcc lattice.

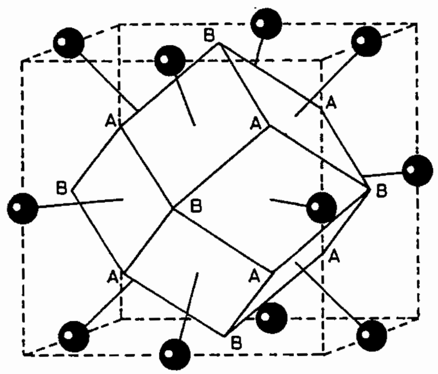
FCC



- a conventional unit cell is shown
- Conventionally, for cubic lattices, we use the conventional unit cell to determine the Miller indices.
- The shaded plane is then the (111) plane.



← shows the primitive unit cell of fcc.



The shape outlined by the solid lines is the Wigner-Seitz cell of a fcc lattice.

Q: Construct a vector that is perpendicular (normal) to a lattice plane P having Miller indices $(hk\ell)$.

Idea: If $\vec{r}_1$ and $\vec{r}_2$ are vectors on P, then $\vec{r}_1 \times \vec{r}_2 \perp$ plane P

We note that:
$$\left.\begin{aligned}\vec{r}_1 &= y\vec{a}_2 - x\vec{a}_1\\ \vec{r}_2 &= z\vec{a}_3 - x\vec{a}_1\end{aligned}\right\}\text{ are vectors on P}$$
(see fig. on p.II-(28))

$$\vec{r}_1 \times \vec{r}_2 = xyz\left[\frac{\vec{a}_2\times\vec{a}_3}{x} + \frac{\vec{a}_3\times\vec{a}_1}{y} + \frac{\vec{a}_1\times\vec{a}_2}{z}\right]$$
$$= \mathcal{A}\left[h(\vec{a}_2\times\vec{a}_3) + k(\vec{a}_3\times\vec{a}_1) + \ell(\vec{a}_1\times\vec{a}_2)\right]$$
$$= \underset{\text{some number}}{\mathcal{A}}\ \vec{g}$$
$\vec{g}$: a vector normal to plane P characterized by $(hk\ell)$

$$\boxed{\therefore \text{ The vector } \vec{g} = h(\vec{a}_2\times\vec{a}_3) + k(\vec{a}_3\times\vec{a}_1) + \ell(\vec{a}_1\times\vec{a}_2) \text{ is normal to the set of planes } (hk\ell).}$$

Remark: The vectors $\vec{a}_2\times\vec{a}_3$, $\vec{a}_3\times\vec{a}_1$, $\vec{a}_1\times\vec{a}_2$ play a special role in SSP. They are so important that we will define three vectors: (see Ch. IV)

$$\vec{b}_1 = \frac{2\pi\,\vec{a}_2\times\vec{a}_3}{\Omega_c}\ ;\quad \vec{b}_2 = \frac{2\pi\,\vec{a}_3\times\vec{a}_1}{\Omega_c}\ ;\quad \vec{b}_3 = \frac{2\pi\,\vec{a}_1\times\vec{a}_2}{\Omega_c}\ ;\quad \Omega_c = |\vec{a}_1\cdot(\vec{a}_2\times\vec{a}_3)|$$

and go into reciprocal lattice generated by $\vec{b}_1, \vec{b}_2, \vec{b}_3$.

Distance between adjacent parallel planes

$(hk\ell)$ describes a set of parallel planes (including all lattice points)

d = distance between adjacent planes

$$\boxed{\text{Key result: } d = \frac{\Omega_c}{|\vec{g}|}\quad \Omega_c = \text{Volume of primitive cell} = |\vec{a}_1\cdot(\vec{a}_2\times\vec{a}_3)|,\quad \vec{g} = h\,\vec{a}_2\times\vec{a}_3 + k\,\vec{a}_3\times\vec{a}_1 + \ell\,\vec{a}_1\times\vec{a}_2}$$

Proof: Take a lattice point as origin. There must be a plane $(hk\ell)$ that passes through the origin. An adjacent plane has intercepts $x = \frac{1}{h}$, $y = \frac{1}{k}$, $z = \frac{1}{\ell}$.

$x\vec{a}_1$ = vector from origin to intercept on $\vec{a}_1$-axis

$\frac{\vec{g}}{|\vec{g}|}$ = unit vector normal to planes

d = separation between plane through origin and adjacent plane
$$= \left|x\vec{a}_1\cdot\frac{\vec{g}}{|\vec{g}|}\right| = \frac{|x\,h\,\vec{a}_1\cdot(\vec{a}_2\times\vec{a}_3)|}{|\vec{g}|} = \frac{\Omega_c}{|\vec{g}|}$$
◻

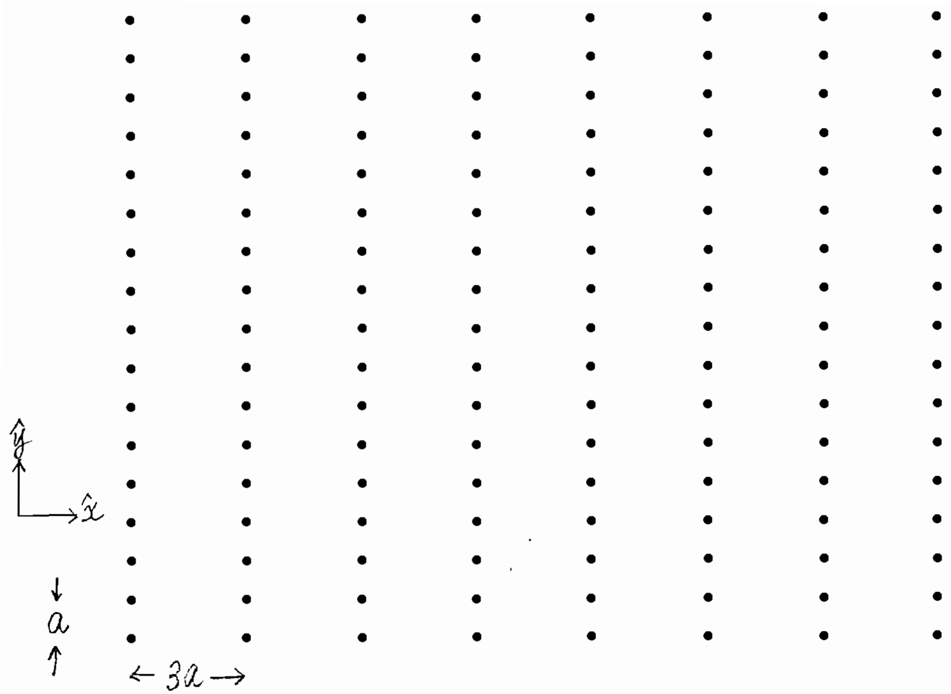
E.g. SC: $(hk\ell)$ planes
$$d = \frac{a^3}{|\vec{g}|} = \frac{a}{\sqrt{h^2+k^2+\ell^2}}\ ,\quad \text{since } \vec{g} = h a^2\hat{x} + k a^2\hat{y} + \ell a^2\hat{z}$$

Summary

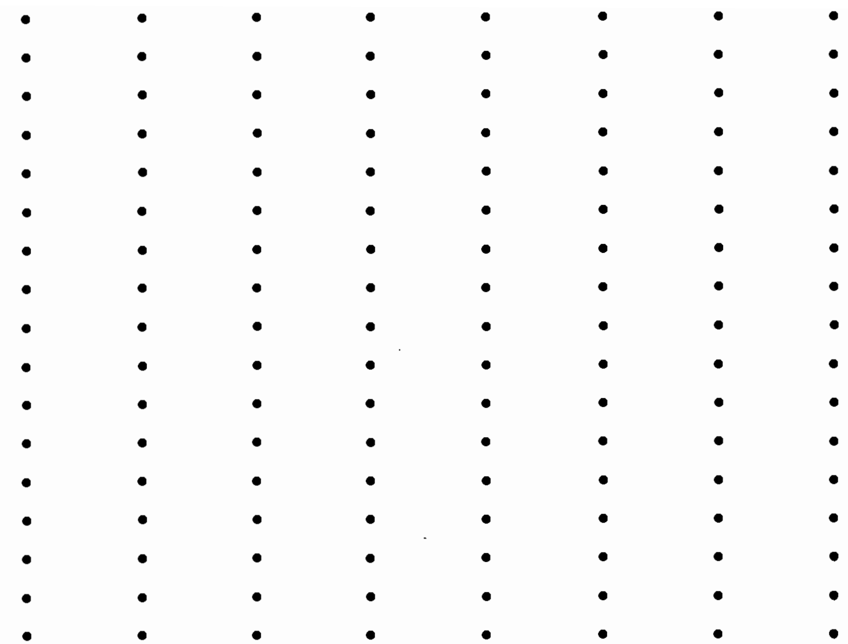
- Students should be able to:
  - state the definition of primitive vectors, primitive cell, lattice vectors, Wigner-Seitz cells, Miller indices
  - identify $\vec{a}_1, \vec{a}_2, \vec{a}_3$ and calculate Ω_c
  - realize that only finite types of lattices exist
  - specify directions in a lattice using $[u_1 u_2 u_3]$
  - specify crystal planes by Miller indices (hkl)
  - show that $\vec{g} = h(\vec{a}_2 \times \vec{a}_3) + k(\vec{a}_3 \times \vec{a}_1) + l(\vec{a}_1 \times \vec{a}_2)$ is a vector normal to the set of planes (hkl)
  - calculate separation between adjacent planes
  - work out various properties in SC, BCC, and FCC lattices
  - realize that the description of the structure of a crystal amounts to: $\underbrace{\text{Lattice}}_{\substack{\text{mathematical}\\ \text{(symmetry)}}} + \underbrace{\text{basis}}_{\substack{\text{atoms decorating}\\ \text{each lattice point}}}$

References:

- Kittel: Chapter 1
- Christman: Chapters 1, 2
- Hook and Hall: Sec. 1.1 – 1.3
- 黄昆: Sec. 1.1 – 1.3, 1.5, 1.7



- Write down 4 possible sets of primitive vectors $\vec{a}_1, \vec{a}_2$ and illustrate them in the figure
- For each set of $\vec{a}_1, \vec{a}_2$, illustrate the primitive cell and find the area of the primitive cell.
- Does the area depend on the choice of primitive vectors?



- Draw a few lattice planes corresponding to (350)