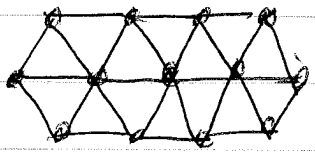
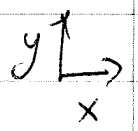
Hexagonal close packed

simple hexagonal B-lattice - obtained by stacking 2D triangular lattices directly above each other.

2D triangular lattice

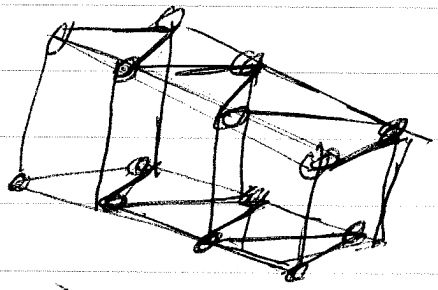




$\vec{a}_1 = a\hat{x}$

$\vec{a}_2 = \frac{a}{2}\hat{x} + \frac{\sqrt{3}}{2}a\hat{y}$

all angles 60°



stacked triangular lattices

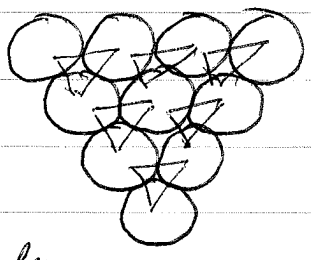
$\vec{a}_3 = c\hat{z}$

Hexagonal close packed -

two interpenetrating simple hexagonal Bravais lattices displaced by $\vec{d}_2 = \frac{\vec{a}_1}{3} + \frac{\vec{a}_2}{3} + \frac{\vec{a}_3}{2}$

with $c = \sqrt{\frac{8}{3}}\,a = 1.63299\,a$

obtained by close packing of hard spheres

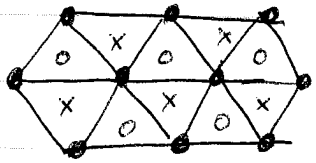


1st layer

put 2nd layer on top of "holes" in 1st layer - there are two choices how to do this - one choice is given by the triangles in picture on the left.

For the 3rd layer, put the sphere on the "holes" in the 2nd layer, so that they lie directly above the spheres in the 1st layer. This gives the hexagonal close-packed structure.

For each layer, there are always two choices



Let • be sites of 1st layer. Then can always put next layer down on top of the O's or the X's.

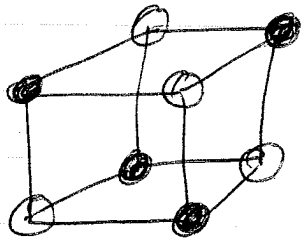
If put 2nd layer on the O's, then the 3rd layer can go on either the X's or the •'s. We can call these three sets of sites, A, B, C (for •, O, X).

Then the close packing corresponding to the stacking sequence ABABAB.... is the hexagonal closed packed. The stacking sequence ABCABCABC... turns out to give the fcc Bravais lattice!

Certain rare earth crystals have stacking ABACABAC...

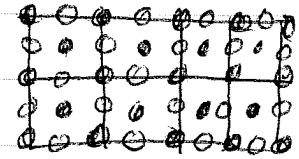
Could in principle ~~do~~ make the choice between the two possibilities at each layer randomly. This would give a random close packed structure.

NaCl structure



Space points where atoms sit is a single cubic Bravais lattice BUT sites are not equivalent since they are alternately occupied by different atoms (Na and Cl for salt)

Need to describe this as a fcc Bravais lattice with two point basis $\vec{d}_1 = 0$, $\vec{d}_2 = \frac{a}{2}(\hat{x}+\hat{y}+\hat{z})$



- Na at sites of fcc
- Cl at center of cube

(See A+M Fig 4.24)

Cesium Chloride Structure

equal numbers of cesium and chlorine at points of a bcc lattice so that each has 8 neighbors of the other kind.

described by single cubic Bravais lattice of Cs with Cl at center of unit cube

$\vec{d}_1 = 0$ Cs

$\vec{d}_2 = \frac{a}{2}(\hat{x}+\hat{y}+\hat{z})$ Cl

Zincblend Structure equal nubers of zinc and sulfur on a deamond lattice so that each has 4 nearest neighbors of the other type.

the Reciprocal Lattice of a Bravais lattice.

The set of wave vectors $\{\vec{K}\}$ that specify the periodicity of a Bravais lattice of sites $\{\vec{R}\}$.

Will be useful in discussing X-ray scattering off ions and electron eigenstates in ionic potential.

Suppose we have a function $U(\vec{r})$ that is periodic on the Bravais lattice, i.e. we have

$$U(\vec{r}+\vec{R}) = U(\vec{r})$$

for all $\vec{R}$ in the Bravais lattice. You may think of the ionic potential the electron sees as a physical example. Taking the Fourier transform

$$U(\vec{r}) = \int \frac{d^3k}{(2\pi)^3} e^{i\vec{k}\cdot\vec{r}} U(\vec{k})$$

the above condition becomes

$$U(\vec{r}+\vec{R}) = \int \frac{d^3k}{(2\pi)^3} e^{i\vec{k}\cdot(\vec{r}+\vec{R})} U(\vec{k})$$

$$= \int \frac{d^3k}{(2\pi)^3} e^{i\vec{k}\cdot\vec{r}} U(\vec{k}) = U(\vec{r})$$

If this is to be true, then the only values of $\vec{k}$ for which $U(\vec{k}) \neq 0$ must be the set of $\{\vec{K}\}$ such that $e^{i\vec{K}\cdot\vec{R}} = 1$ for all

$\vec{R}$ in the Bravais lattice. This defines the reciprocal lattice $\{\vec{K}\}$.

Alternatively, the set of wave vectors $\{\vec{K}\}$ that yield plane waves with the periodicity of the Bravais lattice is called the reciprocal lattice

$$e^{i\vec{K}\cdot(\vec{r}+\vec{R})} = e^{i\vec{K}\cdot\vec{r}} \quad \text{for all } \vec{R} \text{ in B.L.}$$

↑ plane wave is invariant under translation by $\{\vec{R}\}$.

$$\Rightarrow \boxed{e^{i\vec{K}\cdot\vec{R}} = 1 \quad \text{for all } \{\vec{R}\} \text{ in B.L.}}$$

The reciprocal lattice is itself a Bravais lattice

If $\vec{a}_1, \vec{a}_2, \vec{a}_3$ are the primitive vectors of a B.L. then

$$\vec{b}_1 \equiv 2\pi \frac{\vec{a}_2 \times \vec{a}_3}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)}$$

$$\vec{b}_2 \equiv 2\pi \frac{\vec{a}_3 \times \vec{a}_1}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)}$$

$$\vec{b}_3 \equiv 2\pi \frac{\vec{a}_1 \times \vec{a}_2}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)}$$

} are primitive vectors for the reciprocal lattice

~~Proof~~

Note that $\vec{b}_i \cdot \vec{a}_j = 2\pi \delta_{ij}$ and that $\vec{b}_i$'s are not all in the same plane since the $\vec{a}_i$'s are not.

$\Rightarrow \{\vec{b}_i\}$ can be taken as a set of basis vectors for $\vec{k}$-space, ie we can write any wave vector $\vec{k}$ as a linear combination

$$\vec{k} = k_1 \vec{b}_1 + k_2 \vec{b}_2 + k_3 \vec{b}_3 \qquad (k_i \text{ not necessarily integers})$$

then for any $\vec{R}$ in the B.L.

$$\vec{k} \cdot \vec{R} = (k_1 \vec{b}_1 + k_2 \vec{b}_2 + k_3 \vec{b}_3)(n_1 \vec{a}_1 + n_2 \vec{a}_2 + n_3 \vec{a}_3)$$

$$= 2\pi (n_1 k_1 + n_2 k_2 + n_3 k_3)$$

If $\vec{k}$ is in the reciprocal lattice, we must have

$$e^{i\vec{k}\cdot\vec{R}} = 1 \quad \text{for all } \vec{R}$$

$\Rightarrow$ $n_1 k_1 + n_2 k_2 + n_3 k_3 =$ integer for all integers n_1, n_2, n_3

$\Rightarrow$ k_1, k_2, k_3 must be integer

$\Rightarrow$ reciprocal lattice vectors $\vec{K}$ must be of the form

$$\vec{K} = k_1 \vec{b}_1 + k_2 \vec{b}_2 + k_3 \vec{b}_3 \quad \text{with } k_1, k_2, k_3 \text{ integer}$$

The reciprocal of the reciprocal lattice is the original Bravais lattice - in this context the original B-L is called the "direct" lattice.

proof

If $\{\vec{G}\}$ are vectors of the reciprocal to the reciprocal lattice, then $e^{i\vec{G}\cdot\vec{K}} = 1$ for all $\vec{K}$ in R.L.

But $\{\vec{R}\}$ satisfies this ~~definition~~ condition by the definition of $\{\vec{K}\}$. So clearly $\{\vec{R}\}$ is a subset of $\{\vec{G}\}$. Now suppose there was some $\vec{G} \in \{\vec{G}\}$ but $\vec{G} \notin \{\vec{R}\}$. Then $\vec{G} = x_1\vec{a}_1 + x_2\vec{a}_2 + x_3\vec{a}_3$ where at least one of the x_i is not integer. But then we would have $e^{i\vec{G}\cdot\vec{R}} = \prod e^{i2\pi x_i k_i} \neq 1$, so there can't be any such $\vec{G}$. $\therefore \Rightarrow \{\vec{G}\} = \{\vec{R}\}$.

Examples

1) single cubic $\begin{cases} \vec{a}_1 = a\hat{x} \\ \vec{a}_2 = a\hat{y} \\ \vec{a}_3 = a\hat{z} \end{cases}$

$$\Rightarrow \begin{cases} \vec{b}_1 = \frac{2\pi}{a}\hat{x} \\ \vec{b}_2 = \frac{2\pi}{a}\hat{y} \\ \vec{b}_3 = \frac{2\pi}{a}\hat{z} \end{cases}$$

so R.L. is also single cubic with side of length $\frac{2\pi}{a}$

2) fcc $\begin{cases} \vec{a}_1 = \frac{a}{2}(\hat{y}+\hat{z}) \\ \vec{a}_2 = \frac{a}{2}(\hat{z}+\hat{x}) \\ \vec{a}_3 = \frac{a}{2}(\hat{x}+\hat{y}) \end{cases}$

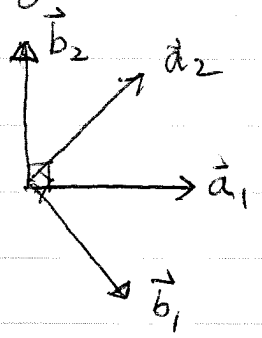
construct the $\vec{b}_i$ to get $\begin{cases} \vec{b}_1 = \frac{2\pi}{a}(\hat{y}-\hat{x}+\hat{z}) \\ \vec{b}_2 = \frac{2\pi}{a}(\hat{z}-\hat{y}+\hat{x}) \\ \vec{b}_3 = \frac{2\pi}{a}(\hat{x}-\hat{z}+\hat{y}) \end{cases}$

these $\vec{b}_i$ are just the primitive vectors of a bcc lattice with side of the cubic unit cell equal to $\frac{4\pi}{a}$

3) bcc since the reciprocal of the reciprocal lattice is the direct lattice, we conclude from (2) that the reciprocal of the bcc lattice is an fcc lattice. If the bcc direct lattice has a unit cubic cell of length a, then the reciprocal fcc lattice has unit cubic cell of length $\frac{4\pi}{a}$

4) The reciprocal of the <u>simple hexagonal</u> Bravais lattice with lattice constants a and c is also a simple hexagonal lattice with lattice constants $|\vec{b}_1| = |\vec{b}_2| = \frac{4\pi}{\sqrt{3}a}$ and $|\vec{b}_3| = \frac{2\pi}{c}$

The directions of $\vec{b}_1$ and $\vec{b}_2$ are rotated with respect to $\vec{a}_1$ and $\vec{a}_2$



angle between $\vec{a}_1$ and $\vec{a}_2$ is 60°

angle between $\vec{b}_1$ and $\vec{b}_2$ is 120°

If v is the volume of the primitive cell of the direct lattice, then $(2\pi)^3/v$ is the volume of the primitive cell of the reciprocal lattice.

The Wigner-Seitz primitive cell for the reciprocal lattice is known as the <u>First Brillouin Zone</u> (later we will see the 2nd and higher Brillouin Zones)

The 1st Brillouin Zone of an fcc direct lattice is the Wigner-Seitz cell of a bcc reciprocal lattice and vice versa.