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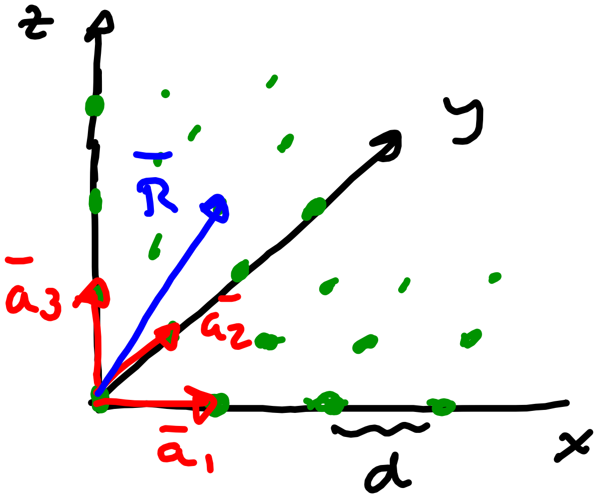
Dual and reciprocal space.

Consider a crystal:



$\bar{a}_1 = d\,\hat{x}$
$\bar{a}_2 = d\,\hat{y}$
$\bar{a}_3 = d\,\hat{z}$

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

Example: cubic lattice

d is the lattice constant.

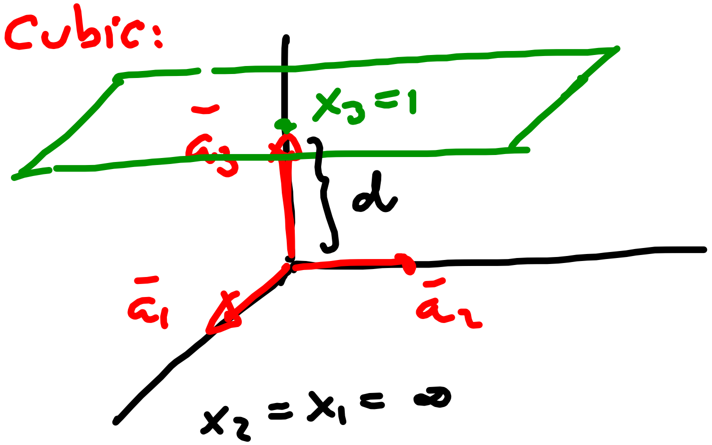
$\bar{a}_i$ connect an arbitrary ion chosen as the origin with nearest neighbors with $\{\bar{a}_i\}$ linearly independent.

- Any ion can be located by a vector $\bar{R}$ which is a linear combination of $\{\bar{a}_i\}$ with integer coefficients n_i.
- The $\{\bar{a}_i\}$ are the basis vectors in real space and they are covariant vectors
- The $\{\bar{a}_i\}$ have units of length.
- The crystal can also be described in terms of families of parallel planes defined by the ions.

- A lattice plane is defined by a set of 3 non-collinear points in the Bravais lattice.

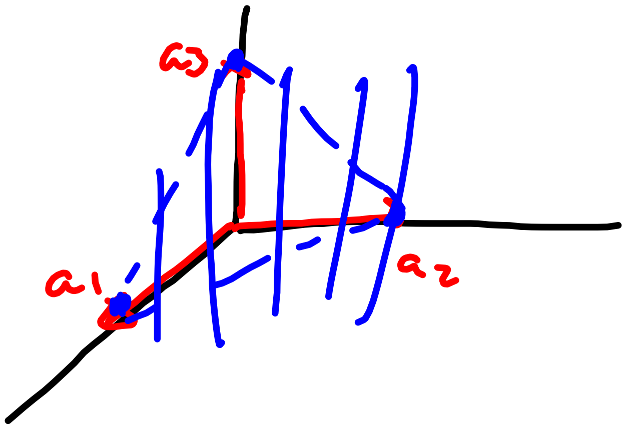
Miller's indices: are used to define families of planes.

$(h,k,\ell) = (0,0,1)$



- Find the values x_1, x_2, x_3 where the plane cuts the axis.
- Find the plane in the family that is closest to the origin.
- Define $(h,k,\ell) = \left(\frac{1}{x_1}, \frac{1}{x_2}, \frac{1}{x_3}\right)$

Notice that a crystal has many families of planes - For example



$(h,k,l) = (1,1,1)$

This plane can characterize the cubic lattice but it is not perpendicular to any of the basis vectors.

It is perpendicular to

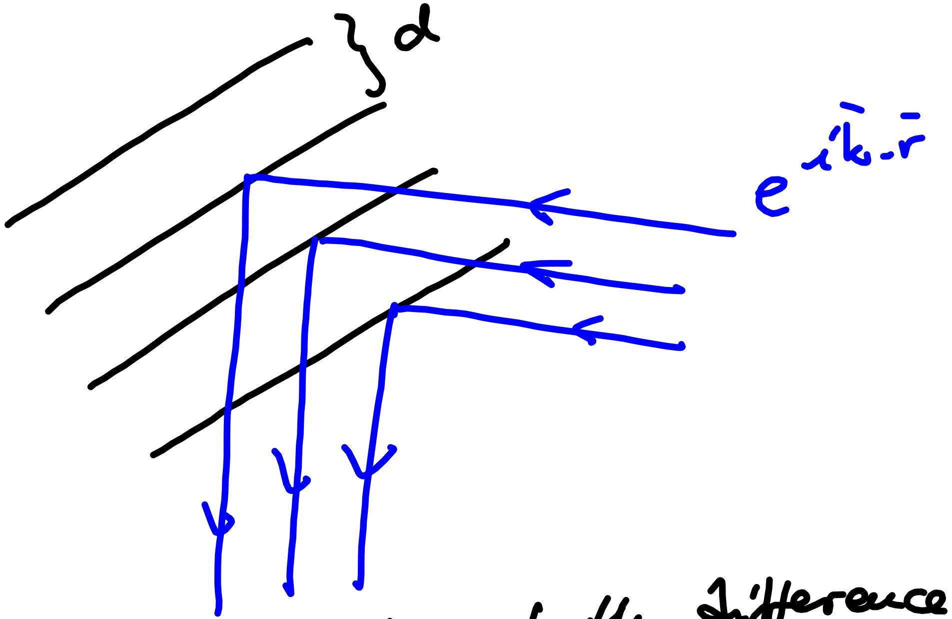
$\bar{R} = \bar{a}_1 + \bar{a}_2 + \bar{a}_3$

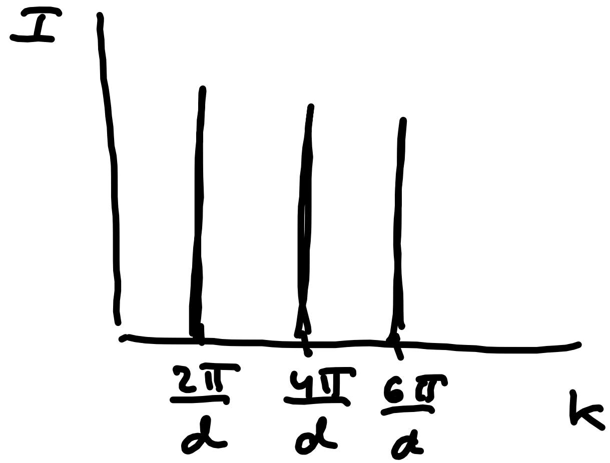
Why are planes important?

Lattice structure is studied by looking at the pattern obtained from interference of the light reflected on the lattice planes.

Light can be represented by a plane wave of the form $e^{i\bar{k}.\bar{r}}$.

$\bar{k}$: wave number $[\bar{k}] = \frac{1}{\text{length}}$ since $[\bar{r}]$ = length.





when the path difference is equal to an integer number of wavelengths we observe constructive interference

The reflected light has the form

$e^{i\bar{k}\cdot(\bar{r}+\bar{R})}$ where $\bar{R}$ is the position of an ion in real space.

The intensity of the reflected waves is maximum when

$$e^{i\bar{k}\cdot\bar{R}} = 1 \Rightarrow \bar{k}\cdot\bar{R} = 2\pi n \qquad (1)$$

n → integer.

The $\bar{k}$'s that satisfy (1) are called $\bar{K}$.

$\bar{K}$ are vectors that expand a crystal-like structure in reciprocal space.

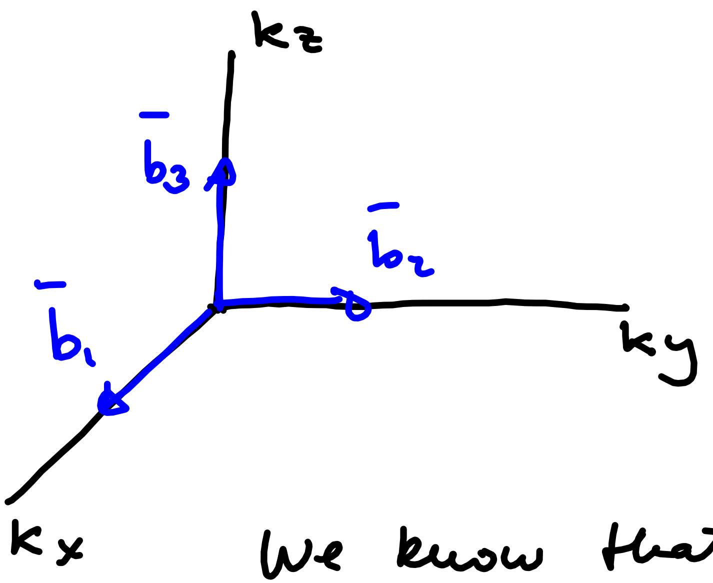
$$\bar{K} \cdot \bar{R} = 2\pi m$$

Reciprocal basis:

We want to obtain a set of vectors $\{\bar{b}_i\}$ that expand all the vectors $\bar{K}$ in the reciprocal lattice.

Warning: in tensor notation $\bar{b}_i = b^i$ contravariant.

Example: Cubic lattice. Reciprocal space



$$\bar{K} = m_1 \bar{b}_1 + m_2 \bar{b}_2 + m_3 \bar{b}_3$$

m_i : integers.

$\bar{K}$: points in the reciprocal lattice.

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

We know that $\bar{K} \cdot \bar{R} = K_i R^i = 2\pi n$

$$\begin{aligned} \bar{K} \cdot \bar{R} = {} & m_1 n_1 \bar{b}_1 \cdot \bar{a}_1 + m_1 n_2 \bar{b}_1 \cdot \bar{a}_2 + m_1 n_3 \bar{b}_1 \cdot \bar{a}_3 + \\ & + m_2 n_1 \bar{b}_2 \cdot \bar{a}_1 + m_2 n_2 \bar{b}_2 \cdot \bar{a}_2 + m_2 n_3 \bar{b}_2 \cdot \bar{a}_3 + \\ & + m_3 n_1 \bar{b}_3 \cdot \bar{a}_1 + m_3 n_2 \bar{b}_3 \cdot \bar{a}_2 + m_3 n_3 \bar{b}_3 \cdot \bar{a}_3 = 2\pi n \end{aligned}$$

(2)

To ensure that (2) is satisfied I request that

$$\bar{a}_i \cdot \bar{b}_i = 2\pi \quad \text{and} \quad \bar{a}_i \cdot \bar{b}_j = 0 \text{ if } i \neq j$$

Then

$$\boxed{a_i b^j = \delta_i^{\ j} \, 2\pi}$$

For dual basis which is the space generated by the contravariant basis vectors mathematicians use:

$$e_i e^j = \delta_i^{\ j} \quad \text{(without the } 2\pi \text{ factor).}$$

In 3D there is a "recipe" to find $\bar{b}_i$ if you know $\bar{a}_i$:

ensures $\bar{b}_i \cdot \bar{a}_j = \bar{b}_i \cdot \bar{a}_k = 0$

$$\bar{b}_i = 2\pi \frac{\bar{a}_j \times \bar{a}_k}{\underbrace{\bar{a}_i \cdot (\bar{a}_j \times \bar{a}_k)}_{\text{volume of the unit cell in real space.}}}$$

i, j, k are in cyclic order

For cubic lattice:

really k_x.

$$\bar{b}_1 = 2\pi \frac{\bar{a}_2 \times \bar{a}_3}{\bar{a}_1 \cdot (\bar{a}_2 \times \bar{a}_3)} = \frac{2\pi\, d^2 \hat{x}}{d^3} = \underbrace{\frac{2\pi}{d}}_{\frac{1}{\text{length}}} \hat{x}.$$

$$\bar{b}_2 = \frac{2\pi}{a}\hat{y}, \quad \bar{b}_3 = \frac{2\pi}{a}\hat{z}$$

Then the reciprocal lattice of the cubic lattice is also cubic but with a lattice constant equal to $\frac{2\pi}{a}$.

In tensor notation:

$$b^i = \frac{2\pi\, \varepsilon^{ijk} a_j a_k}{a_\ell\, \varepsilon^{\ell mn} a_m a_n}$$

i, j, k are cyclic.

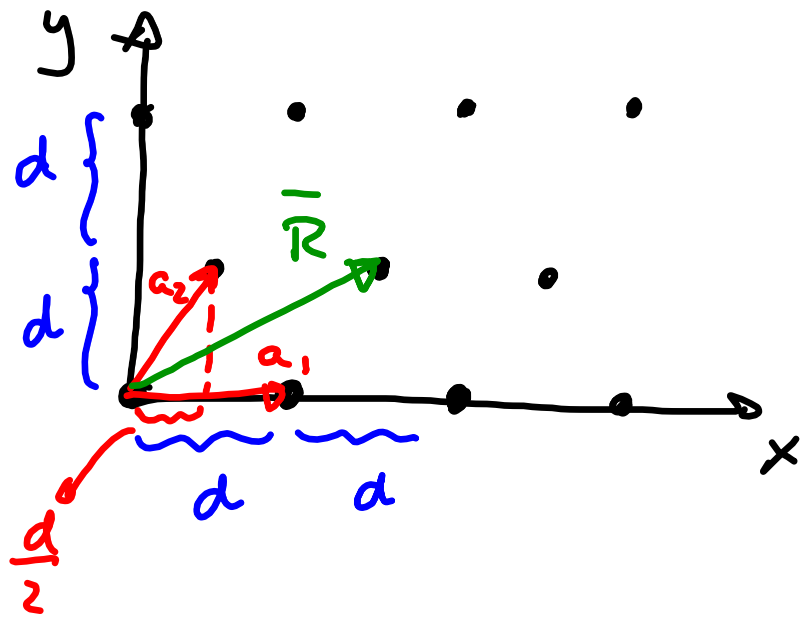
with $m, n \neq i$.

Contravariant or dual basis:

For each system defined in real space by a covariant bases, there is a contravariant basis that is orthogonal to the covariant one. $e_i \cdot e^j = \delta_i^{\ j}$.

The contravariant basis is defined in the dual or reciprocal space.

Example: Bravais lattice in 2 D. (oblique)



$$\bar{a}_1 = d\,\hat{x}$$

$$\bar{a}_2 = \frac{d}{2}\,\hat{x} + d\,\hat{y}$$

$$|\bar{a}_1| = d$$

$$|\bar{a}_2| = (\bar{a}_2 \cdot \bar{a}_2)^{1/2} =$$

$$= \left(\frac{d^2}{4} + d^2\right)^{1/2} = \frac{\sqrt{5}}{2}\,d$$

$$\bar{R} = n_1\,\bar{a}_1 + n_2\,\bar{a}_2$$

We will find the $\bar{b}_i$ vectors (b^i really) that expand the reciprocal lattice.

Since $\bar{K} = m_1 \bar{b}_1 + m_2 \bar{b}_2$

and I want that $\bar{K} \cdot \bar{R} = 2\pi m$

I need that

$$a_i b^j = 2\pi \delta_i^j \quad ①$$

Let's $\bar{b}_1 = (b_{1x}, b_{1y})$ and $\bar{b}_2 = (b_{2x}, b_{2y})$ ②

① Are 4 sets of equations that will allow us to solve ②.