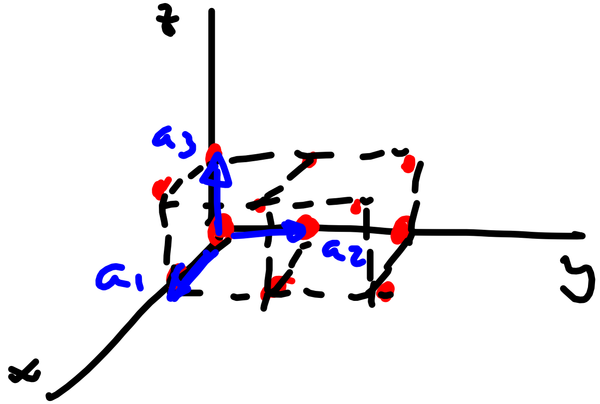
Real and Reciprocal space in crystals: 9/3

Last time:

$$\bar{R} = n_1 a_1 + n_2 a_2 + n_3 a_3$$

ion position



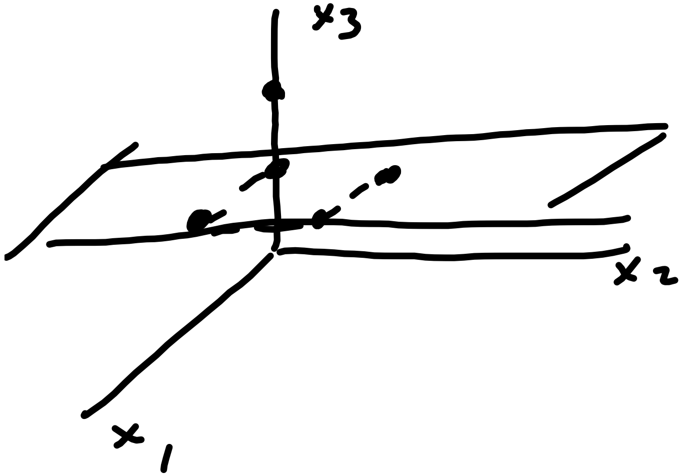
In addition we can use planes of ions to define the lattice:

Miller indeces:

How do we describe planes?

We need 3 points.

- Find the values x_1, x_2, x_3 where the plane cuts each axis.
- Find the plane in the family (of // planes) closest to the origin.
- Define $(h, k, \ell) = \left(\frac{1}{x_1}, \frac{1}{x_2}, \frac{1}{x_3}\right)$ Miller's indeces

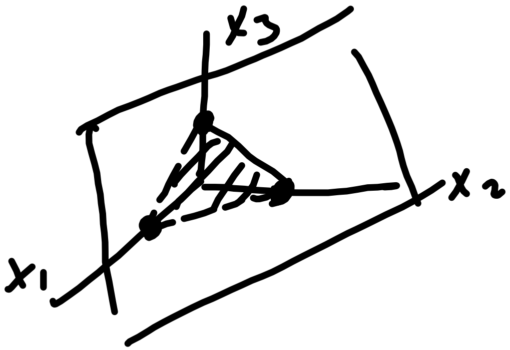


$(x_1, x_2, x_3) = (\infty, \infty, 1)$

then

$(h, k, l) = (0, 0, 1)$

Also

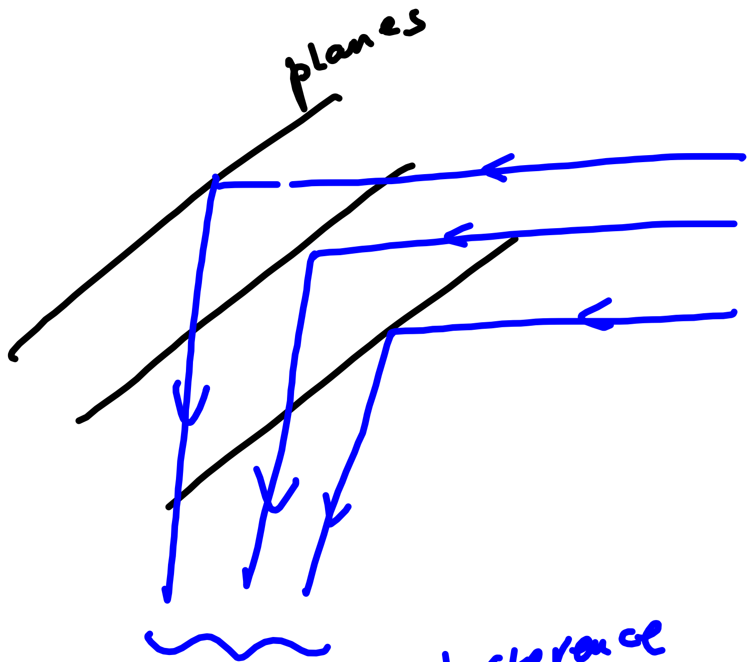


$(x_1, x_2, x_3) = (1, 1, 1)$

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

It is not $\perp$ to any of the basis vectors $\bar{a}_i$.

Why are the planes important?



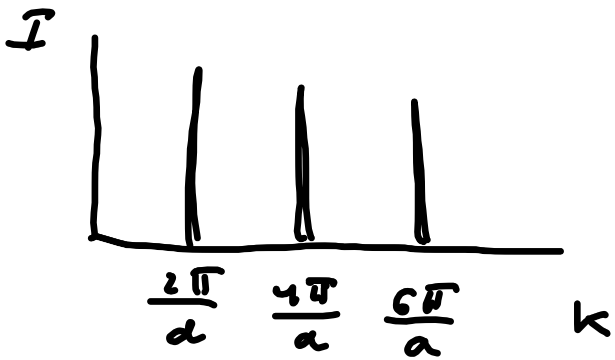
x-rays $\propto e^{-i \bar{k} \cdot \bar{x}}$

$\bar{k}$: wave number

$[\bar{k}]$: $\frac{1}{\text{length}}$

study interference

The pattern depends on $\bar{k}$ and the distance between the planes



In order to see interference peaks

$$e^{i\bar{k}\cdot\bar{R}} = 1 \quad (1)$$

n : integer for all vector $\bar{R}$ in the lattice.

then

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

$\bar{K}$ are the values of $\bar{k}$ that satisfy (1)

It can be proved that $\bar{K}$ are vectors that form a lattice in $\bar{k}$ space. This lattice is called the reciprocal lattice. We will find the vectors $\bar{b}_i$ that expand $\bar{K}$.

$\bar{k}$ is in reciprocal space

$\bar{k} \cdot \bar{r}$ has a physical meaning and in terms of tensors it is given by

$$k_i \, r^i$$

covariant

contravariant

Also we want to evaluate $r = r_i \, r^i$

contravariant

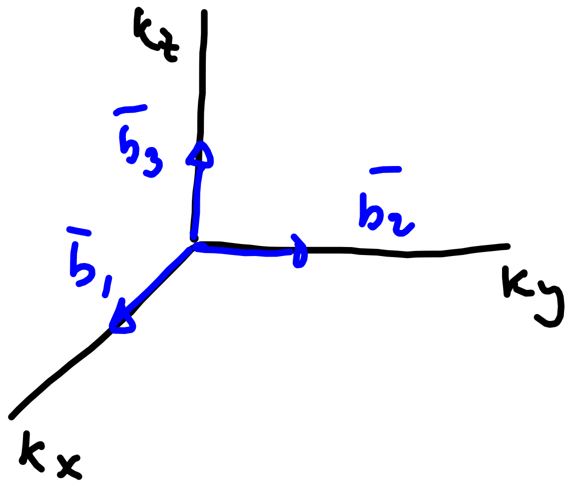
covariant form in dual space.

We will see that the basis of reciprocal space for $\bar{r}$ is parallel to the basis for dual space.

Reciprocal basis:

We will define a basis $\{b_i\}$ that expands $\bar{K}$. Since $\bar{K} \equiv k_i$ then $b_i \equiv b^i$

contra-variant



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

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

we know that $\bar{K} \cdot \bar{R} = 2\pi n$

$\bar{K} \cdot \bar{R} = K_i R^i = 2\pi m_i n_i$

if $a_i b^j = 2\pi \delta_i^j$ In reciprocal space.

In dual space the condition is

$$\underbrace{\hat{e}_i \, \hat{e}^j}_{} = \delta_i^{\,j}$$

dual base

In 3D there is an expression to obtain $\bar{b}_i$:

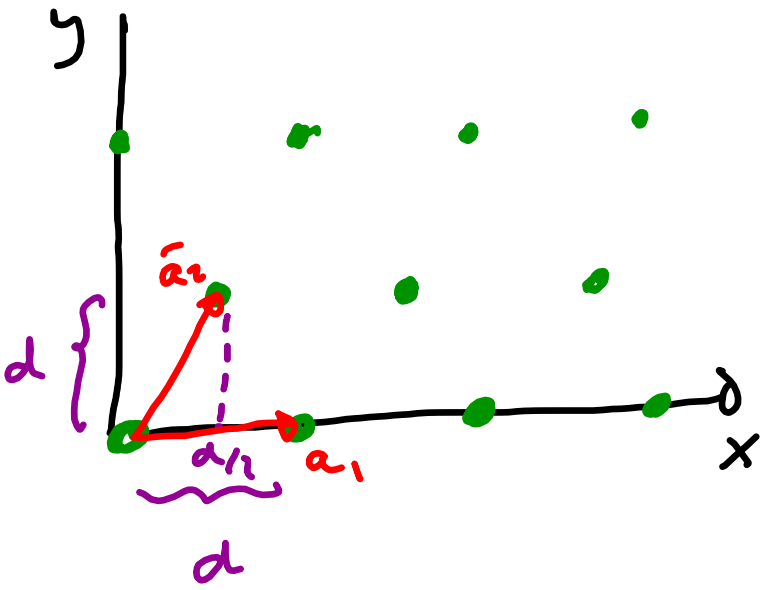
ensures $b_i \cdot a^j = 0$ if $i \neq j$.

$$\bar{b}_i = 2\pi \frac{\overbrace{\bar{a}_j \times \bar{a}_k}^{}}{\underbrace{\bar{a}_i \cdot (\bar{a}_j \times \bar{a}_k)}_{d^3 \text{ for cubic lattice}}}$$

i, j, k in cyclic order

$\bar{b}_i$ has units of $\frac{1}{\ell}$.

Example: 2D crystal. Oblique Bravais lattice.



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

$|\bar{a}_2| = \frac{\sqrt{5}}{2} d$

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

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

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

$\bar{a}_2 : \left(\frac{d}{2}, d\right)$

$\bar{b}_1 \perp$ to planes // $\bar{a}_1$

$\bar{b}_2 \perp$ to planes // $\bar{a}_2$

Let's find b^i (reciprocal vectors).

$$a_i \, b^j = 2\pi m$$

Define $b^1 = (b^1_x, b^1_y)$ $\qquad b^2 = (b^2_x, b^2_y)$

$\bar{a}_1 \cdot \bar{b}^1 = d\, b^1_x = 2\pi$ if $m = 1$

$\bar{a}_2 \cdot \bar{b}^2 = \frac{d}{2} b^2_x + d\, b^2_y = 2\pi$

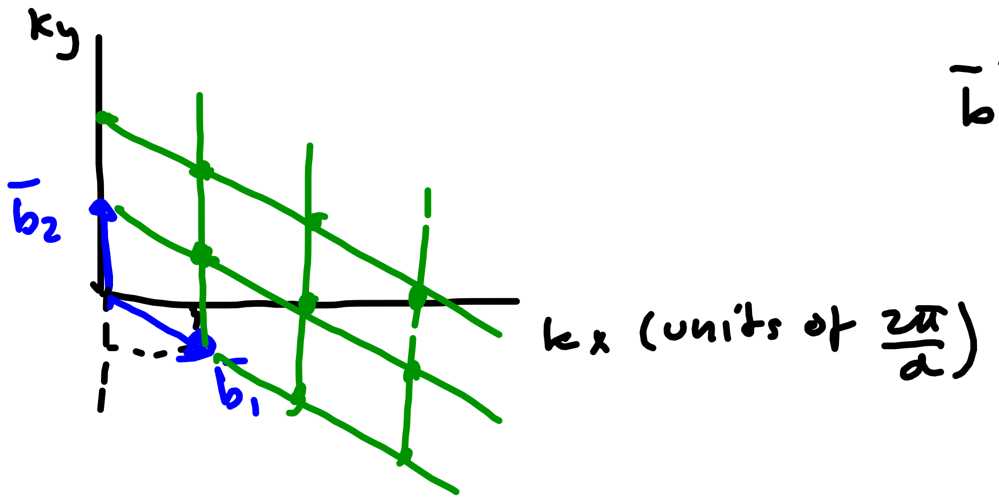
$\bar{a}_1 \cdot \bar{b}^2 = \bar{a}_2 \cdot \bar{b}^1 = 0$

Solving the 4 eq. with 4 unknowns you get:

$\bar{b}^1 = \frac{2\pi}{d}(1, -\frac{1}{2})$ $\qquad \bar{b}^2 = \frac{2\pi}{d}(0, 1)$

$$\bar{b}^1 = \frac{2\pi}{a}\left(1, -\frac{1}{2}\right)$$

$$\bar{b}^2 = \frac{2\pi}{a}(0, 1)$$



Covariant and contravariant vectors.

We know that r^i is the prototype contravariant vector and it transforms between S and S' as:

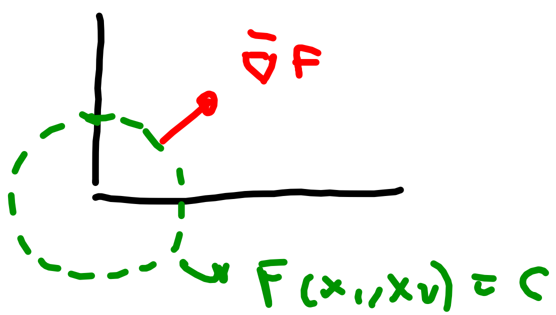
$$r'^i = \frac{\partial x'^i}{\partial x^j} r^j$$

Now we are going to see how the gradient of a scalar function transforms going from S to S'.

$F(x_1, x_2)$ is a scalar function.

$$\bar{\nabla} F(x_1, x_2) = \frac{\partial F}{\partial x_1} \hat{x}_1 + \frac{\partial F}{\partial x_2} \hat{x}_2 = \left(\frac{\partial F}{\partial x_1}, \frac{\partial F}{\partial x_2} \right)$$

If $F(x_1, x_2) = \text{constant}$ defines a surface then $\bar{\nabla} F$ is normal to that surface.



Let's change from S to S':

$$\bar{\nabla} F = \frac{\partial F}{\partial x^i} \equiv \partial_i F = B_i$$

Seems covariant from the notation.

Demonstration:

$$R'^i = \frac{\partial x'^i}{\partial x^j} R^j \quad \text{contravariant.}$$

(scalar function)

$$F(x'_1, x'_2) \equiv F(x_1, x_2)$$

Now

$$\bar{\nabla}' F' = \bar{\nabla}' F = \left(\frac{\partial F(x')}{\partial x'_1}, \frac{\partial F(x')}{\partial x'_2} \right) = \left(\frac{\partial F(x)}{\partial x'_1}, \frac{\partial F(x)}{\partial x'_2} \right)$$

$$= \left(\frac{\partial F(x_1,x_2)}{\partial x_1} \frac{\partial x_1}{\partial x'_1} + \frac{\partial F(x_1,x_2)}{\partial x_2} \frac{\partial x_2}{\partial x'_1}, \frac{\partial F(x)}{\partial x_1} \frac{\partial x_1}{\partial x'_2} + \frac{\partial F(x)}{\partial x_2} \frac{\partial x_2}{\partial x'_2} \right) =$$

$$= \left(B_1 \frac{\partial x^1}{\partial x'_1} + B_2 \frac{\partial x^2}{\partial x'_1},\ B_1 \frac{\partial x^1}{\partial x'_2} + B_2 \frac{\partial x^2}{\partial x'_2} \right) =$$

$$= (B'_1, B'_2)$$

In compact way:

$$\boxed{B'_i = B_j \frac{\partial x^j}{\partial x'^i}}$$

B_j transforms as the inverse of r^i

Then $B_j = \partial_j F$ is covariant.

Contravariant components always used in this expression.