Solid State Physics, WS 04/05

Reciprocal space

The base vectors of reciprocal space are defined as:

$$\vec{a}_1^* = \frac{2\pi}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)}(\vec{a}_2 \times \vec{a}_3) \tag{1}$$

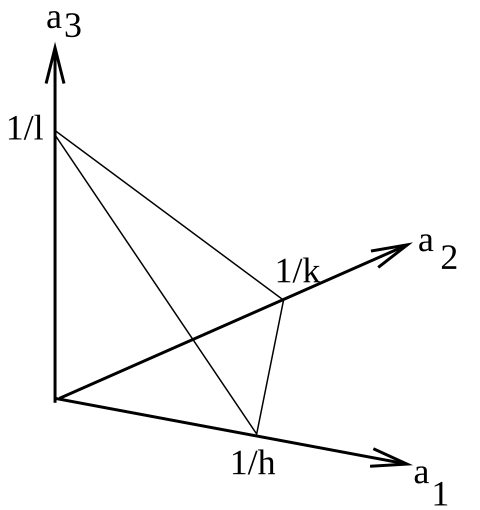
$$\vec{a}_2^* = \frac{2\pi}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)}(\vec{a}_3 \times \vec{a}_1) \tag{2}$$

$$\vec{a}_3^* = \frac{2\pi}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)}(\vec{a}_1 \times \vec{a}_2) \tag{3}$$

A vector of the reciprocal lattice is given by:

$$\vec{G} = h\vec{a}_1^* + k\vec{a}_2^* + l\vec{a}_2^* \tag{4}$$

A (set of) lattice plane is given by its Miller indices (hkl), defined as the reciprocal of the intersection distance of the plane with the base vector directions.



The distance $d_{(hkl)}$ between parallel planes is given as the distance to the origin of plane (hkl). The plane normal $\vec{n}$ is

$$\vec{n} = (-\frac{1}{h}\vec{a}_1 + \frac{1}{k}\vec{a}_2) \times (-\frac{1}{h}\vec{a}_1 + \frac{1}{l}\vec{a}_l) \tag{5}$$

$$= \frac{1}{hkl}\frac{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)}{2\pi}(h\vec{a}_1^* + k\vec{a}_2^* + l\vec{a}_3^*) \quad (6)$$

$$= \frac{1}{hkl}\frac{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)}{2\pi}\vec{G} \quad (7)$$

and the distance $d_{(hkl)}$

$$d_{(hkl)} = \frac{1}{h}\vec{a}_1 \cdot \frac{\vec{n}}{|\vec{n}|} \quad (8)$$

$$= \frac{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)}{hkl}\frac{1}{|\vec{n}|} \quad (9)$$

The absolute value of $\vec{G}$ is

$$|\vec{G}| = hkl\frac{2\pi}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)}|\vec{n}| \quad (10)$$

So the final expression for the lattice spacing in terms of reciprocal vectors is

$$d_{(hkl)} = \frac{2\pi}{|\vec{G}|}\,. \quad (11)$$

The Bragg condition:
The classical derivation of the Bragg condition gives

$$n\,\lambda = 2d_{(hkl)}\,\sin\Theta \quad (12)$$

For an incoming wave, the wave vector $\vec{k}$has an absolute value

$$|\vec{k}| = \frac{2\pi}{\lambda} \quad (13)$$

For elastic scattering, incoming and outgoing waves have same wave length, i.e.

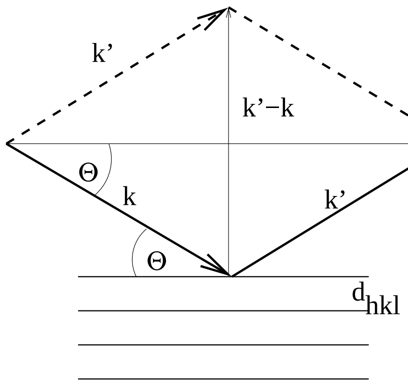
$$|\vec{k}| = |\vec{k}'| \quad (14)$$

Using the Bragg condition and eq. (11),

$$\frac{2\pi}{|\vec{k}|} = 2\frac{2\pi}{|\vec{G}|}\sin\Theta \quad (15)$$

or

$$|\vec{G}| = 2|\vec{k}|\sin\Theta \quad (16)$$



The direction of the vectors follows from figure (2): the direction of $\vec{k}' - \vec{k}$ is parallel to $\vec{G}$

$$\vec{k}' - \vec{k} = \alpha \vec{G} \tag{17}$$

and on the other hand

$$|\vec{k}' - \vec{k}| = 2|\vec{k}| \sin \Theta \tag{18}$$

what using eq. (16) is equal to

$$|\vec{k}' - \vec{k}| = |\vec{G}| \tag{19}$$

so $\alpha = 0$, and finally the Bragg condition is equivalent to

$$\vec{k}' - \vec{k} = \vec{G} \tag{20}$$