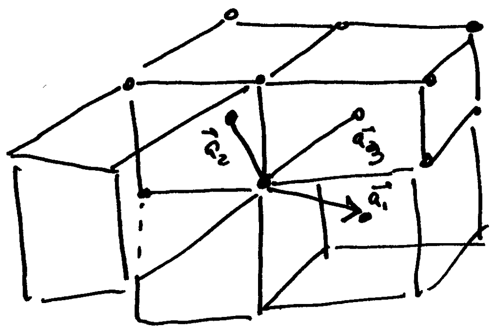
3. Rede recíproca de uma rede c.c.c.

Vectores primitivos:

i)



Com esta escolha:

$$\vec{a}_1 = \frac{1}{2} a (\hat{x} + \hat{y} - \hat{z})$$

$$\vec{a}_2 = \frac{1}{2} a (-\hat{x} + \hat{y} + \hat{z})$$

$$\vec{a}_3 = \frac{1}{2} a (\hat{x} - \hat{y} + \hat{z})$$

Reciprocal lattice

$$\frac{1}{4} a^2 \begin{vmatrix} \hat{x} & \hat{y} & \hat{z} \\ -1 & 1 & 1 \\ 1 & -1 & 1 \end{vmatrix} = \frac{1}{4} a^2 (2\hat{x} + 2\hat{y})$$

$$\frac{1}{2} a (\hat{x} + \hat{y} - \hat{z}) \cdot \frac{1}{4} a^2 (2\hat{x} + 2\hat{y}) =$$

$$= \frac{1}{8} a^3 (2 + 2) = \frac{1}{2} a^3$$

$$a_1^* = \frac{2\pi}{\frac{1}{2} a^3} \frac{1}{2} a^2 (1, 1, 0)$$

$$a_2^* = \frac{2\pi}{\frac{1}{2} a^3} (\bar{a}_3 \wedge \bar{a}_1) = \frac{2\pi}{\frac{1}{2} a^3} \frac{1}{2} a^2 (0, 1, 1) \qquad \frac{1}{4} a^2 \begin{vmatrix} \hat{x} & \hat{y} & \hat{z} \\ +1 & -1 & 1 \\ 1 & 1 & -1 \end{vmatrix} =$$

$$\frac{1}{4} a^2 (0, 2, 2)$$

$$a_3^* = \frac{2\pi}{\frac{1}{2} a^3} (\bar{a}_1 \wedge \bar{a}_2) =$$

$$\frac{1}{4} a^2 \begin{vmatrix} \hat{x} & \hat{y} & \hat{z} \\ 1 & 1 & -1 \\ -1 & 1 & 1 \end{vmatrix} = \frac{1}{4} a^2 (2, 0, 2)$$

$$a_1^* = \frac{2\pi}{a}(1,1,0) \qquad a_2^* = \frac{2\pi}{a}(0,1,1) \qquad a_3^* = \frac{2\pi}{a}(1,0,1)$$

$$a_1 = \frac{1}{2}a(1,1,-1) \qquad a_2 = \frac{1}{2}a(-1,1,1) \qquad a_3 = \frac{1}{2}a(1,-1,1)$$

$$\cancel{\begin{bmatrix} 1 & 1 & -1 \\ -1 & 1 & 1 \\ 1 & -1 & 1 \end{bmatrix} \begin{bmatrix} 1 & 1 & 0 \\ 0 & 1 & 1 \\ 1 & 0 & 1 \end{bmatrix}} = \Bigg[$$

Transpost

$$\frac{1}{2}a \begin{bmatrix} 1 & -1 & 1 \\ 1 & 1 & -1 \\ -1 & 1 & 1 \end{bmatrix} \begin{bmatrix} 1 & 1 & 0 \\ 0 & 1 & 1 \\ 1 & 0 & 1 \end{bmatrix} = \begin{bmatrix} 2 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 2 \end{bmatrix} = a \begin{bmatrix} 1 & & \\ & 1 & \\ & & 1 \end{bmatrix}$$

(...)

$\vec{b}_1 = \dfrac{\vec{a}_2 \wedge \vec{a}_3}{\Omega}$; $\vec{b}_2 = \dfrac{\vec{a}_3 \wedge \vec{a}_1}{\Omega}$; $\vec{b}_3 = \dfrac{\vec{a}_1 \wedge \vec{a}_2}{\Omega}$ $\qquad \Omega = \dfrac{\vec{a}_1 \cdot (\vec{a}_2 \wedge \vec{a}_3)}{2\pi}$

$a_1^* = \dfrac{\vec{b}_2 \wedge \vec{b}_3}{\Omega'}$, $\qquad \Omega' = \dfrac{\vec{b}_1 \cdot (\vec{b}_2 \wedge \vec{b}_3)}{2\pi}$

$$a_1^* = \frac{1}{\Omega^2} (\vec{a}_3 \wedge \vec{a}_1) \wedge (\vec{a}_1 \wedge \vec{a}_2) \frac{1}{\Omega'} =$$

$$= \frac{1}{\Omega^2 \Omega'} (\vec{a}_3 \wedge \vec{a}_1) \wedge (\vec{a}_1 \wedge \vec{a}_2) =$$

$$= \cancel{\frac{1}{\Omega^2\Omega'} \left[\vec{a}_3 \wedge \vec{a}_1 \wedge a \right.}$$

Now: $\quad \vec{A} \wedge (\vec{B} \wedge \vec{C}) = (\vec{A} \cdot \vec{C}) \vec{B} - \vec{C} (\vec{A} \cdot \vec{B})$

$$(\vec{a}_3 \wedge \vec{a}_1) \wedge (\vec{a}_1 \wedge \vec{a}_2) = \left[(\vec{a}_3 \wedge \vec{a}_1) \cdot \vec{a}_2 \right] \vec{a}_1 - \vec{a}_2 \left(\vec{a}_3 \wedge \vec{a}_1 \right) \cdot \vec{a}_1 =$$

$$= \underbrace{\left[(\vec{a}_3 \wedge \vec{a}_1) \cdot \vec{a}_2 \right]}_{\Omega \cdot 2\pi} \vec{a}_1$$

$$a_1^* = \frac{1}{\Omega^2} \frac{1}{\Omega'} \cdot 2\pi \, \Omega \, \vec{a} = \frac{2\pi}{\Omega \Omega'} \vec{a}_1$$

Hm $\quad \Omega \Omega'$

Problema 7

7. Índices de Miller:

(1) $m\vec{a}_1$, $n\vec{a}_2$, $r\vec{a}_3$ definem 3 pontos não colineares:

consideremos os seus inversos:

$$\left(\frac{1}{m}, \frac{1}{n}, \frac{1}{r}\right)$$

Seja p o menor múltiplo comum de m, n, r)

então $p\left(\frac{1}{m}, \frac{1}{n}, \frac{1}{r}\right) = (h, k, \ell)$ definem os índices de Miller do plano.

(2) (h, k, ℓ) definem as coordenadas de um vector da RR perpendicular ao plano considerado. Prova:

$$(m\vec{a}_1 - n\vec{a}_2) \qquad (r\vec{a}_3 - n\vec{a}_2)$$

$$mr(\bar{a}_1 \wedge \bar{a}_3) - mn(\bar{a}_1 \wedge \bar{a}_2) - nr(\bar{a}_2 \wedge \bar{a}_3)$$

Multiplicamos este vector (perpendicular ao plano) por

$$-\frac{2\pi}{mnr \cdot \vec{a}_1 \cdot (\vec{a}_2 \wedge \vec{a}_3)}$$; obtemos:

$$-\frac{2\pi}{mnr\, \bar{a}_1 \cdot (\bar{a}_2 \wedge \bar{a}_3)} \left[mr(\bar{a}_1 \wedge \bar{a}_3) - mn(\bar{a}_1 \wedge \bar{a}_2) - nr(\bar{a}_2 \wedge \bar{a}_3) \right] =$$

$$= -\frac{2\pi}{\bar{a}_1 \cdot (\bar{a}_2 \wedge \bar{a}_3)} \left[-\frac{1}{n}(\bar{a}_3 \wedge \bar{a}_1) - \frac{1}{r}(\bar{a}_1 \wedge \bar{a}_2) - \frac{1}{m}(\bar{a}_2 \wedge \bar{a}_3) \right] =$$

$$2\pi \left[\frac{1}{m} \vec{b}_2 + \frac{1}{n} \vec{b}_3 + \frac{1}{m} \vec{b}_1 \right] = \frac{2\pi}{p} \left[k \cdot \vec{b}_2 + l \vec{b}_3 + h \vec{b}_1 \right]$$

$$\frac{2\pi \, \vec{G}_{hkl}}{p} \equiv \perp \text{ as plane dodo.}$$

6. $\vec{r}_1 = (\bar{a} - \bar{b})$, $\vec{r}_2 = 2\hat{a} + \vec{c}$ $\quad \vec{r}_3 = 3\bar{b} + \vec{c}$

$$\vec{A} = \vec{r}_1 - \vec{r}_2 = -\vec{a} - \vec{b} + \vec{c}$$

$$\vec{B} = \vec{r}_1 - \vec{r}_3 = \vec{a} - 4\vec{b} - \vec{c}$$

$$(\vec{A} \wedge \vec{B}) = (-\vec{a} - \vec{b} + \vec{c}) \wedge (\vec{a} - 4\vec{b} - \vec{c}) = 4(\vec{a} \wedge \vec{b}) + (\vec{a} \wedge \vec{c}) -$$

$$-(\vec{b} \wedge \vec{a}) + (\vec{b} \wedge \vec{c}) +$$

$$+(\vec{c} \wedge \vec{a}) - 4(\vec{c} \wedge \vec{b}) =$$

$$= 5(\vec{a} \wedge \vec{b}) + 0\,(\vec{c} \wedge \vec{a}) + 5(\vec{b} \wedge \vec{c})$$

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