- Solution to Ex 1 - homework 1.

	d_1	d_2	Z_1	Z_2	PF.
SC	a	$a\sqrt{2}$	6	12	0.52
FCC	$a/\sqrt{2}$	a	12	6	0.74
BCC	$a\sqrt{3}/2$	a	8	6	0.68
HCP	a	$a\sqrt{8/3}$	12	2	0.74
Diamond	$a\sqrt{3}/4$	$a/\sqrt{2}$	4	12	0.34

- Ex2 (Kittel, Chap 2 , pb 1)

a) $\vec{G} = h\,\vec{b}_1 + k\,\vec{b}_2 + \ell\,\vec{b}_3 \perp (hk\ell)$ plane? By construction,

3 points of $(hk\ell)$ plane are $\frac{1}{h}\vec{R}_1$, $\frac{1}{k}\vec{R}_2$, $\frac{1}{\ell}\vec{R}_3$

A vector perpendicular to this plane is $\vec{V} = \left(\frac{1}{h}\vec{R}_1 - \frac{1}{k}\vec{R}_2\right) \times \left(\frac{1}{h}\vec{R}_1 - \frac{1}{\ell}\vec{R}_3\right)$

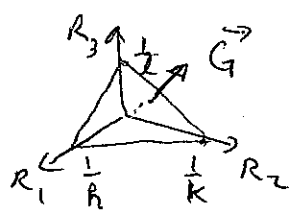
$$\vec{V} = \frac{1}{h\ell}\left(\vec{R}_3 \times \vec{R}_1\right) + \frac{1}{hk}\left(\vec{R}_1 \times \vec{R}_2\right) + \frac{1}{k\ell}\left(\vec{R}_2 \times \vec{R}_3\right)$$

$$= \frac{1}{h\ell}\,\vec{b}_2\,\frac{\Omega}{2\pi} + \frac{1}{hk}\,\vec{b}_3\,\frac{\Omega}{2\pi} + \frac{1}{k\ell}\,\vec{b}_1\,\frac{\Omega}{2\pi}$$

$$= \frac{\Omega}{2\pi\, hk\ell}\left[h\,\vec{b}_1 + k\,\vec{b}_2 + \ell\,\vec{b}_3\right] \propto \vec{G}$$

QED.

b) $d_{(hk\ell)} = \frac{2\pi}{|G|}$?



$$d = \frac{1}{h}\vec{R}_1 \cdot \hat{G} = \frac{1}{k}\vec{R}_2 \cdot \hat{G} = \frac{1}{\ell}\vec{R}_3 \cdot \hat{G}$$

$$= \frac{1}{h}(\vec{R}_1)\cdot(h\,\vec{b}_1 + k\,\vec{b}_2 + \ell\,\vec{b}_3)/G = \frac{2\pi}{|G|}$$

c) In Simple cubic $|\vec{b}_i| = \frac{2\pi}{a} \Rightarrow |G| = (h^2+k^2+\ell^2) \times \frac{2\pi}{a} \Rightarrow d = \frac{a}{h^2+k^2+\ell^2}$

- Ex 3 (Kittel, chap 2, pb 5)

a) Structure factor of diamond (8 atoms / cube basis)

atomic coordinates of the 8 atoms are. (in units of $(a\hat{x}, a\hat{y}, a\hat{z})$)

$(0,0,0)$ $(0\ \tfrac{1}{2}\ \tfrac{1}{2})$ $(\tfrac{1}{2}\ 0\ \tfrac{1}{2})$ $(\tfrac{1}{2}\ \tfrac{1}{2}\ 0)$

$(\tfrac{1}{4}, \tfrac{1}{4}, \tfrac{1}{4})$ $(\tfrac{1}{4}\ \tfrac{3}{4}\ \tfrac{3}{4})$ $(\tfrac{3}{4}\ \tfrac{1}{4}\ \tfrac{3}{4})$ $(\tfrac{3}{4}\ \tfrac{3}{4}\ \tfrac{1}{4})$

$$S(\vec{q}) = \sum_{R_i} e^{i\vec{q}.\vec{R}_i} \quad \text{if} \quad \vec{q} = (h\,\vec{G}_1 + k\,\vec{G}_2 + l\,\vec{G}_3),$$

then
$$S(\vec{q}) = \underbrace{\left[1 + e^{i2\pi(h+k+l)/4}\right]}_{1}\underbrace{\left[1 + e^{i2\pi(k+l)/2} + e^{i2\pi(h+k)/2} + e^{i2\pi(k+l)/2}\right]}_{2}$$

(b) Zeros of S : $S(\vec{q}) = 0$ if $\frac{h+k+l}{4} = n + \frac{1}{2}$ $(1 = 0)$

or $(2 = 0)$

$1 = 0$: $h+k+l = 4n+2 = -2, 2, 6, 10, \ldots$ $\Leftrightarrow$ all 3 need to be even, or 1 even 2 odd)

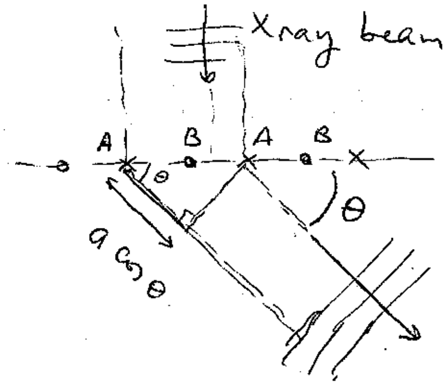
$2 = 0$: $(h, k, l) \to$ 2 even one odd like $(0\ 0\ 1)$ $(0\ 2\ 1)$ $(2\ 2\ 1)\ldots$
1 even two odd like $(0\ 1\ 1)$ $(2\ 1\ 1)$ $(0\ 1\ 3)\ldots$
this is 6 out of 8 possibilities

So if $(h+k+l)$ is even but not of the form $4n+2$, but $4n$

or all 3 odd then $S(q) \neq 0$

$\Rightarrow S(q)_{hkl} \neq 0$ for $(1,1,1)$ $(1,1,3)\ldots$ and (004) $(022)\ldots$

• Ex 4 (Kittel, chap 2, pb 7)



(a) AB AB AB ... $d_{AB} = \frac{a}{2}$

f_A, f_B : form factors

phase difference $\Delta\phi = ka\cos\theta$

must be a multiple of 2π for constructive interference.

$$ka\cos\theta = 2\pi n$$

or $\frac{2\pi}{\lambda} a\cos\theta = 2\pi n \iff \boxed{a\cos\theta = n\lambda}$

(b) $I \propto \left| f_A + f_B \, e^{ik\frac{a\cos\theta}{2}} \right|^2$

Since the phase difference between the wave coming from A and that coming from its nearest neighbor B is $k.\left(\frac{a}{2}\cos\theta\right)$

But if $ka\cos\theta = 2\pi n$ then $\frac{ka\cos\theta}{2} = \pi n$

$$I \propto \left| f_A + f_B \, e^{in\pi} \right|^2 = |f_A + f_B|^2 \text{ or } |f_A - f_B|^2$$

(c) So if A = B, or B has similar electronic environment as A (so that $f_A \approx f_B$) then one out of every 2 peaks becomes extinct (for n odd)