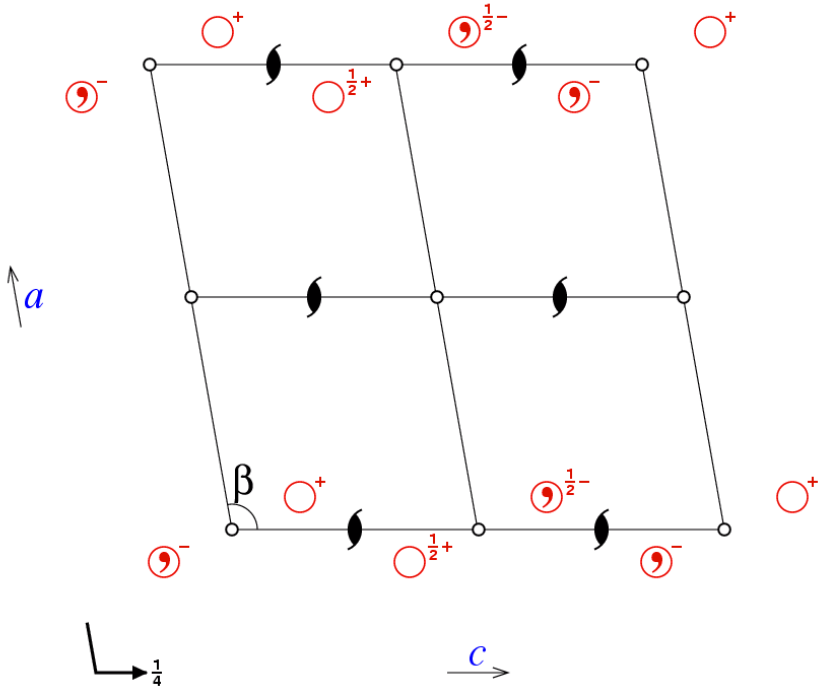
Li_2 Structure Factor Calculations

(No Computers allowed)

Monoclinic Space Group $P2_1/c$

$P2_1/c$ $P\ 1\ 2_1/c\ 1$ $2/m$ No. 14



1 x, y, z

2 $\bar{x}, \frac{1}{2}+y, \frac{1}{2}-z$

3 $\bar{x}, \bar{y}, \bar{z}$

4 $x, \frac{1}{2}-y, \frac{1}{2}+z$

Reflection Conditions

(general)

$h0l:\ l=2n$

$0k0:\ k=2n$

$00l:\ l=2n$

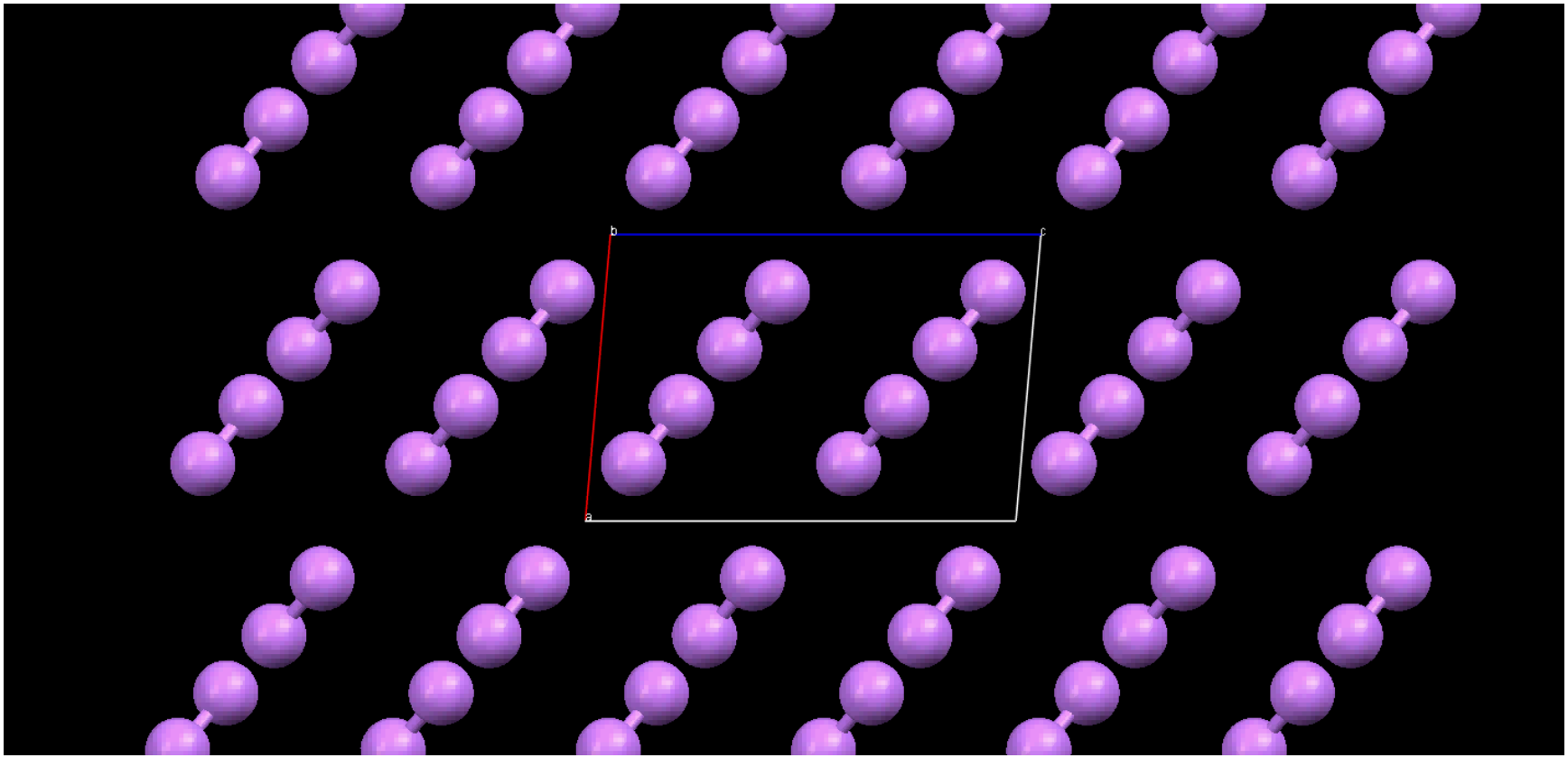
http://img.chem.ucl.ac.uk/sgp/mainmenu.htm

Generation of Li_2 Cell contents

Cell: 4.000 5.000 6.000 90 95.00 90

#	Label	X	Y	Z	Symm. op.
1	**LI1**	**0.8**	**0.2**	**0.1**	**x,y,z**
2	**LI2**	**0.6**	**0.3**	**0.2**	**x,y,z**
3	LI1	0.2	0.7	0.4	1-x,1/2+y,1/2-z
4	LI2	0.4	0.8	0.3	1-x,1/2+y,1/2-z
5	LI1	0.2	0.8	0.9	1-x,1-y,1-z
6	LI2	0.4	0.7	0.8	1-x,1-y,1-z
7	LI1	0.8	0.3	0.6	x,1/2-y,1/2+z
8	LI2	0.6	0.2	0.7	x,1/2-y,1/2+z

The DiLithium Crystal



The Structure Factor (simplified)

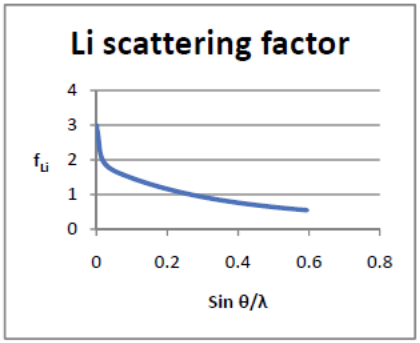
$$F(hkl) = \sum_{j=1}^{n} \left(f_j e^{(2\pi i(hx_j + ky_j + lz_j))}\right)$$

F – Amplitude of diffracted intensity: Structure Factor

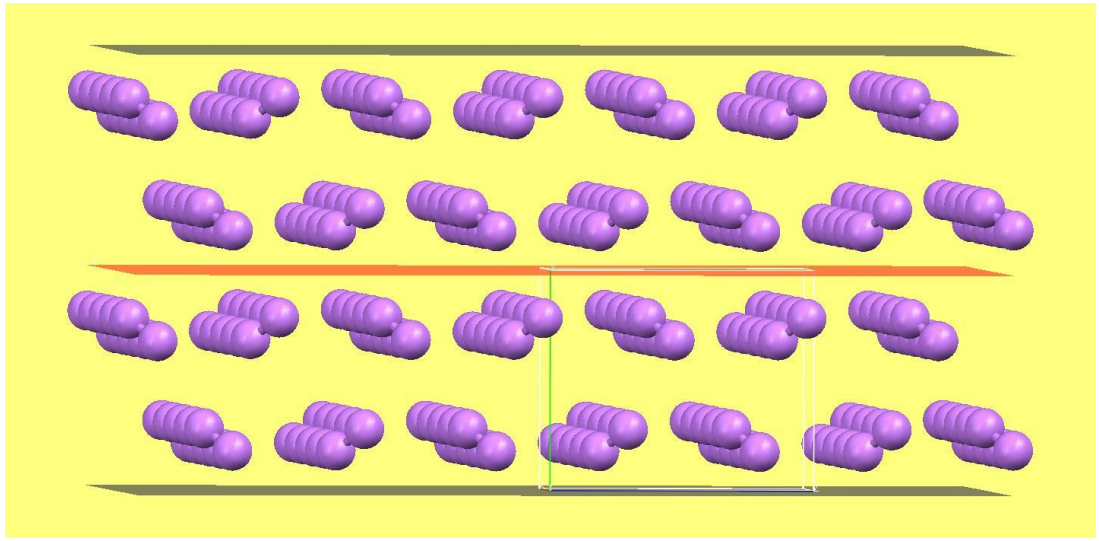
hkl – integer indices: Refers to diffraction planes in Direct Space, or spot position in Reciprocal Space

n - atoms in the unit cell, at positions (x_j, y_j, z_j)

f_j - atomic scattering factor. For X-rays, scales with number of electrons in atom ***n*** and drops off with scattering angle



F_{010} = ±?.??? for Li_2



d = 5.000 Å

f_j is the atomic scattering factor

$$\mathbf{F}_{hkl} = \sum \mathbf{f}_j \, e^{2\pi i(hxj+kyj+lzj)}$$

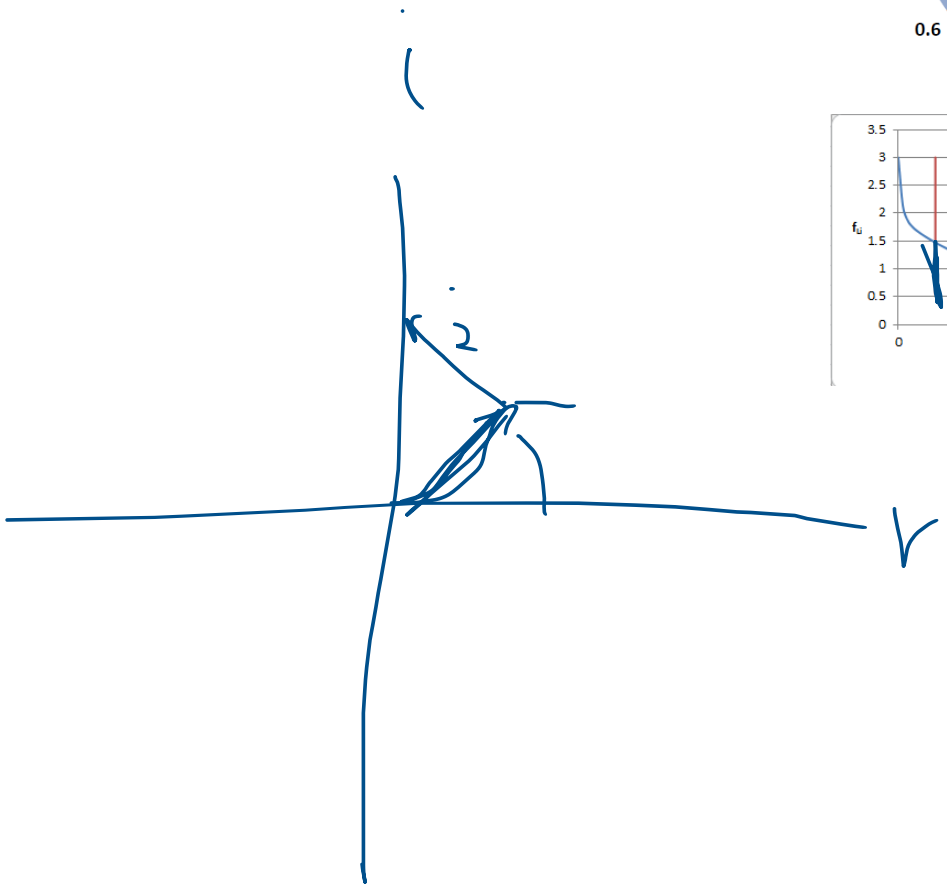
$$F(hkl) = \sum_{j=1}^{n} \left(f_j e^{(2\pi i (hx_j + ky_j + lz_j))} \right)$$

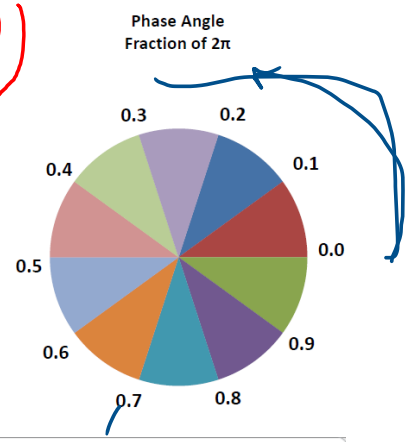
Li_2 in $P2_1/c$

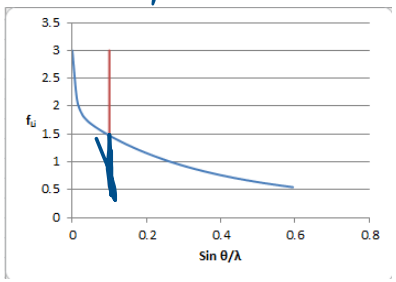
a = 4.000Å
b = 5.000Å
c = 6.000Å
α = 90 °
β = 95.00 °
γ = 90 °

j

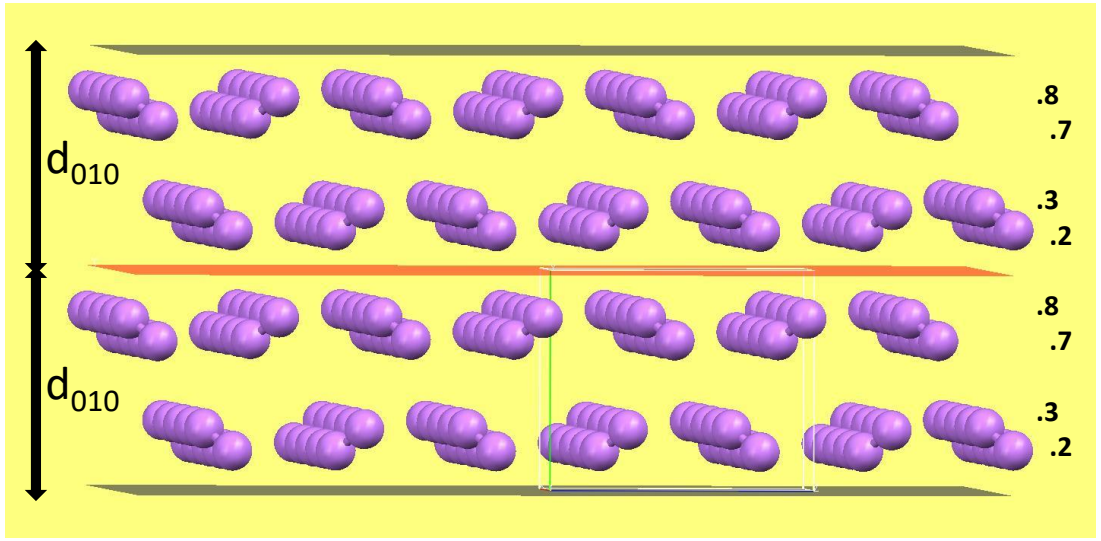
1 Li1 0.8, 0.2, 0.1
2 Li2 0.6, 0.3, 0.2
3 Li1 0.2, 0.7, 0.4
4 Li2 0.4, 0.8, 0.3
5 Li1 0.2, 0.8, 0.9
6 Li2 0.4, 0.7, 0.8
7 Li1 0.8, 0.3, 0.6
8 Li2 0.6, 0.2, 0.7



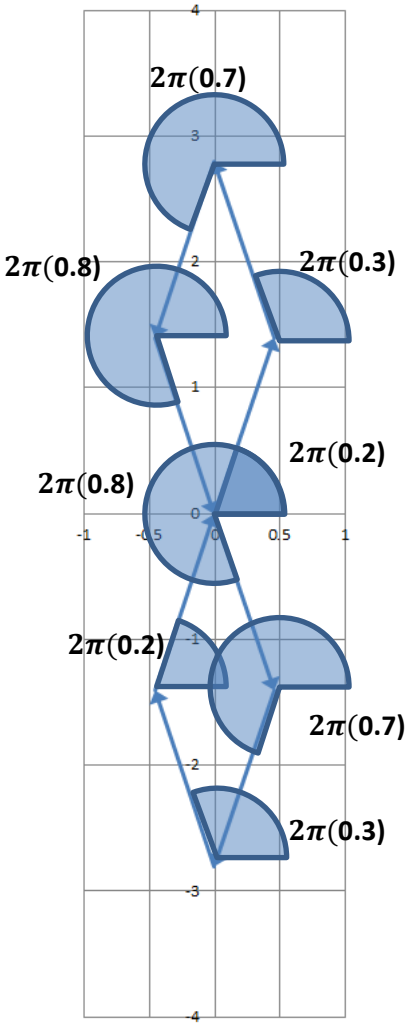




F_{010} = 0.000 for Li_2



2π

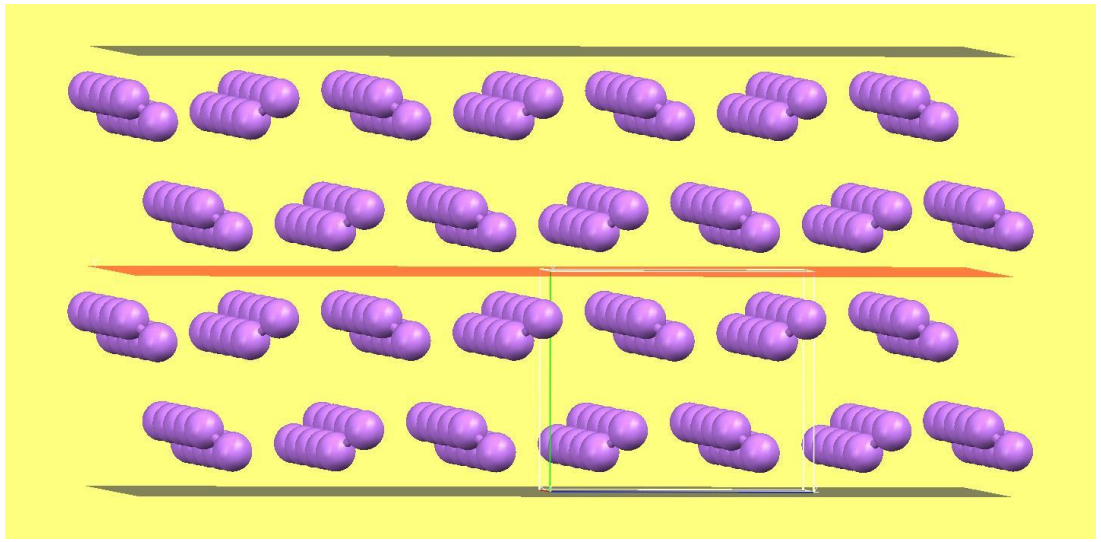


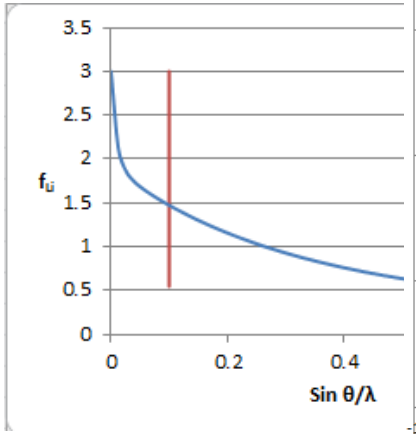
d = 5.000 Å

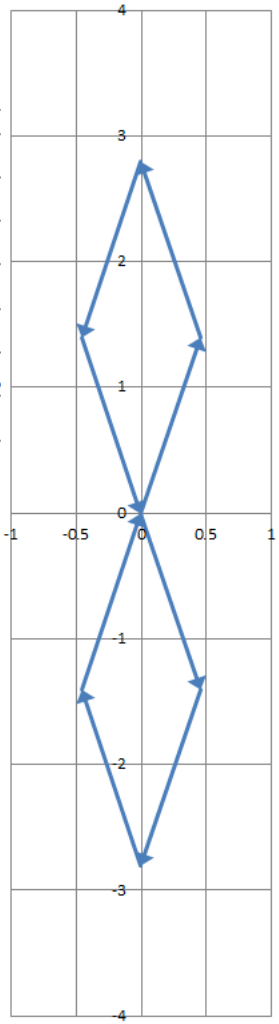
$2\pi(hxj + kyj + lzj) = 2\pi(0x_j + 1y_j + 0z_j)$ **is the phase angle for each atom in the cell**

$$\mathbf{F}_{hkl} = \sum \mathbf{f}_j \, e^{2\pi i(hxj+kyj+lzj)}$$

$F_{010} = 0.000$ for Li_2

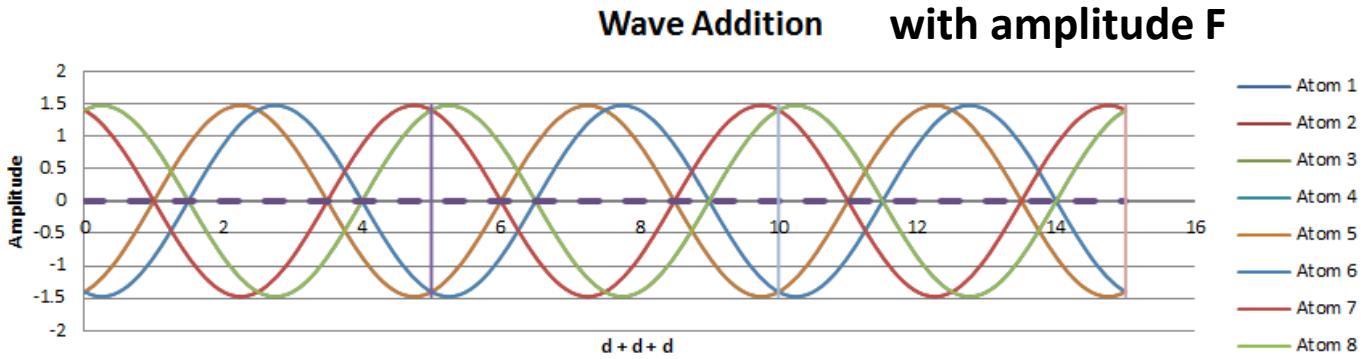






d = 5.000 Å

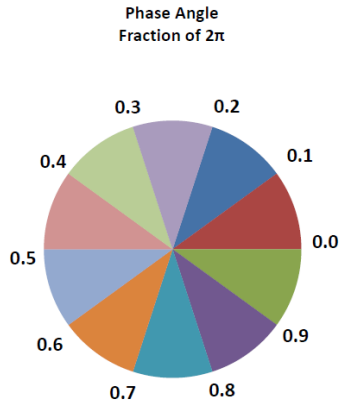
Dashed curve is total wave with amplitude F

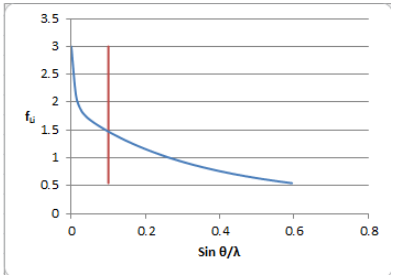


$$F(hkl) = \sum_{j=1}^{n} (f_j e^{(2\pi i(hx_j + ky_j + lz_j)})$$

020

Li_2 in $P2_1/c$



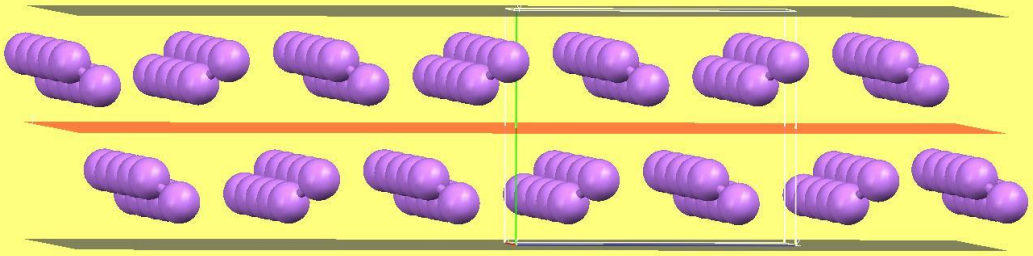


a = 4.000Å
b = 5.000Å
c = 6.000Å
α = 90 °
β = 95.00 °
γ = 90 °

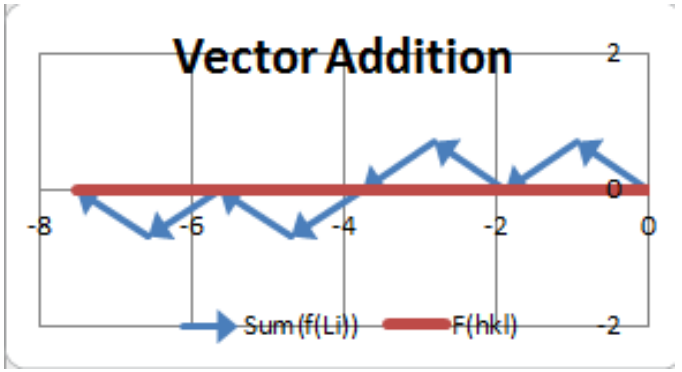
j

1 Li1 0.8, 0.2, 0.1
2 Li2 0.6, 0.3, 0.2
3 Li1 0.2, 0.7, 0.4
4 Li2 0.4, 0.8, 0.3
5 Li1 0.2, 0.8, 0.9
6 Li2 0.4, 0.7, 0.8
7 Li1 0.8, 0.3, 0.6
8 Li2 0.6, 0.2, 0.7

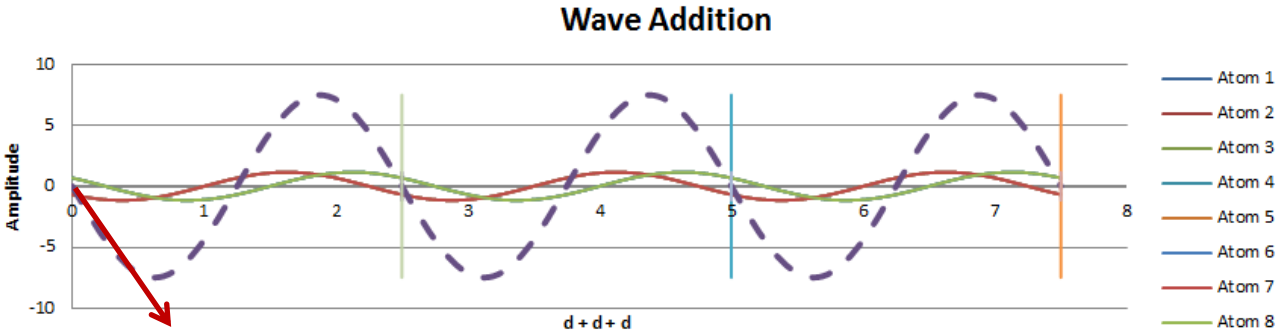
F_{020} = -7.492 for Li_2

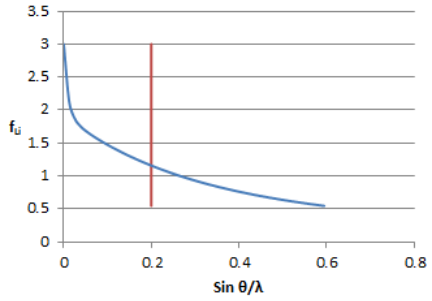


d = 2.500 Å



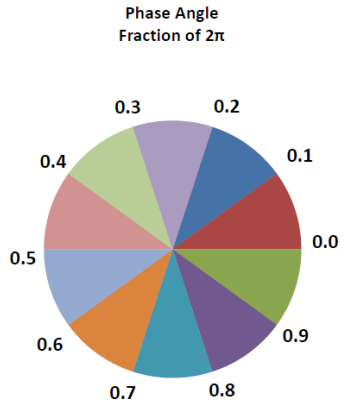
When the average electron density is *between* the planes, the structure factor has a *negative* phase angle.

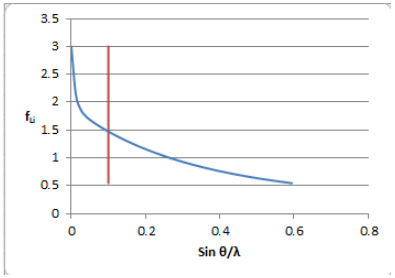




$$F(hkl) = \sum_{j=1}^{n} (f_j e^{(2\pi i(hx_j + ky_j + lz_j)})$$

Li_2 in $P2_1/c$ 102



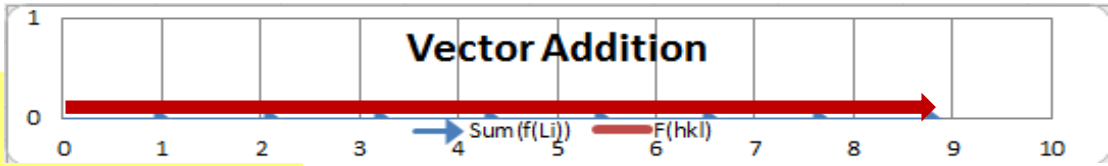


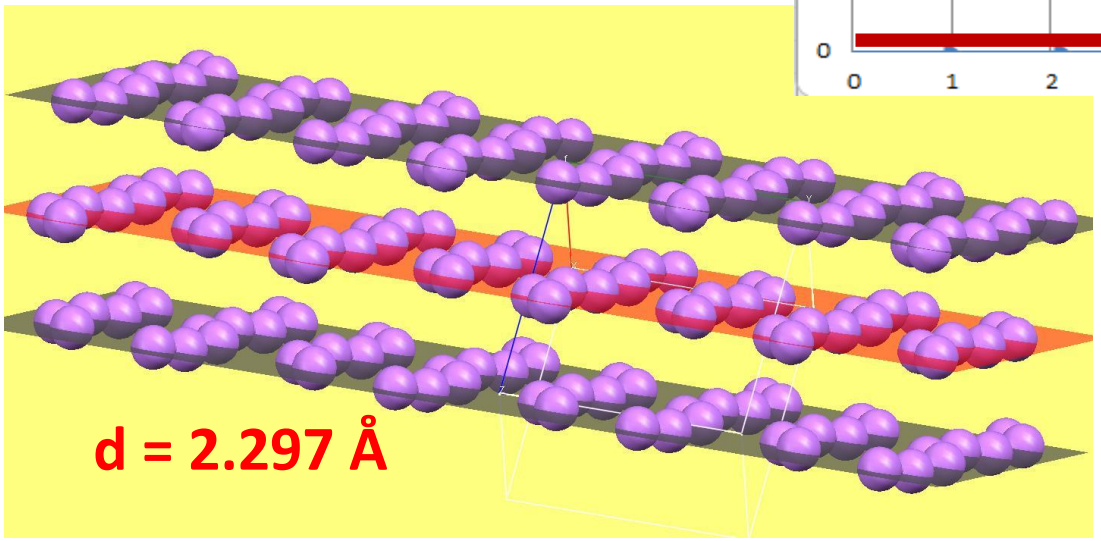
a = 4.000Å
b = 5.000Å
c = 6.000Å
α = 90 °
β = 95.00 °
γ = 90 °

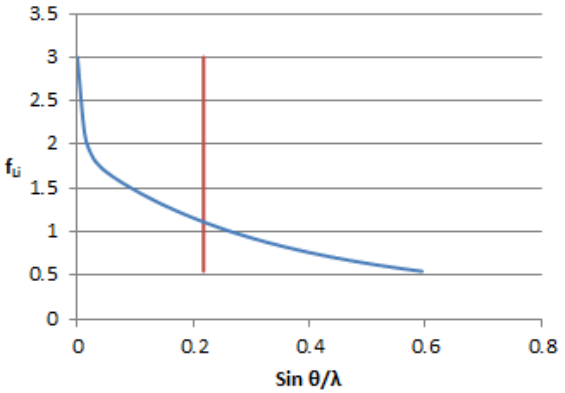
j

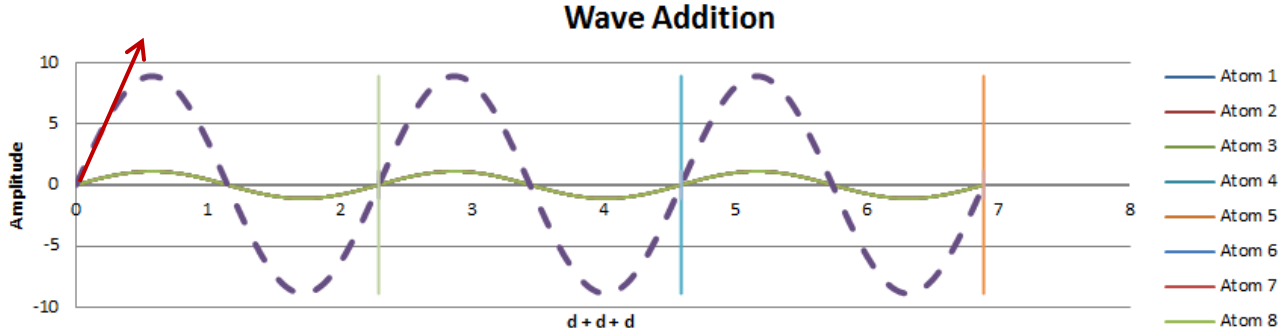
1 Li1 0.8, 0.2, 0.1
2 Li2 0.6, 0.3, 0.2
3 Li1 0.2, 0.7, 0.4
4 Li2 0.4, 0.8, 0.3
5 Li1 0.2, 0.8, 0.9
6 Li2 0.4, 0.7, 0.8
7 Li1 0.8, 0.3, 0.6
8 Li2 0.6, 0.2, 0.7

$F_{102} = 8.894$ for Li_2









When the average electron density is *on* the planes, the structure factor has a *positive* phase angle.

$F_{-1-2-2} = -6.072$ for Li_2