**SSP Exercise 2**

To be handed in by 4pm, Thursday 26 January.

For a simple cubic lattice the reflections with the following Miller indices are possible: (100), (110),(111), (200), (210), (211), (220), (etc.). An x-ray diffraction experiment with the wavelength of $\lambda$ = 1Å reveals a set of peaks recorded at the following angles $\vartheta$ (deg.):

| |
|---|
| 5.74 |
| 8.13 |
| 9.98 |
| 11.54 |
| 12.93 |
| 14.19 |
| 16.44 |

a. Show that this x-ray diffraction picture corresponds to a simple cubic lattice. **Hint**, note that the sequence *n* formed by $n = h^2+k^2+l^2$ for a simple cubic lattice is 1,2,3,4,5,6,8. Rewrite the Bragg law in the form

$$sin^2\theta = \frac{\lambda^2}{4d^2} \quad Eq.\ 1$$

and express *d* via *a* and h,k,l. Can you obtain the sequence *n* above from the recorded peaks using *Eq.1*? **[10]**

b. Calculate the value of the lattice constant *a*. **[5]**

**Solution:**

a. From *Eq.1* the Brag law can be rewritten as

$$sin^2\theta = \frac{\lambda^2}{4a^2} * n = C * n, where\ we\ use\ a = \frac{d}{\sqrt{h^2+k^2+l^2}}$$

Now if we use the sequence of angles above in the form

$$sin^2\theta_1 = C * n_1$$
$$sin^2\theta_2 = C * n_2$$
$$sin^2\theta_3 = C * n_3$$
$$....$$
$$sin^2\theta_8 = C * n_8$$

and assuming that $n_1$=1 divide as follows

$$\frac{sin^2\theta_2}{sin^2\theta_1} = \frac{n_2}{n_1} \approx \frac{0.02}{0.01} = n_2 = 2$$
$$...$$
$$\frac{sin^2\theta_8}{sin^2\theta_1} \approx \frac{0.08}{0.01} = 8$$

To recover the sequence 1, 2,3,4,5,6,8.

b. Now use the Bragg law in the form:

$$sin^2\theta = \frac{\lambda^2}{4a^2}(h^2 + k^2 + l^2)$$

to obtain

$a = \frac{\lambda}{2*sin\theta}(\sqrt{h^2 + k^2 + l^2})$

and for (100) we have $a = \frac{\lambda}{2*sin\theta_1} = \frac{1}{2*0.1} = 5\acute{Å} = 5 * 10^{-10}m$