

Solid State Physics - IM2601

Laboration 1

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1 Introduction

The standard method for characterization of any material's crystalline structure is X-ray diffraction, also known as XRD. By studying how the X-rays reflects from the crystalline material, one can get an understanding of the material's properties and structure.

In this laboratory we are faced with two main tasks. Firstly, to compute the wavelength (λ) of the X-rays, by measuring the diffraction behavior of NaCl and comparing it to our theoretically calculated values. Secondly, for four samples, labeled A, B, C and D, determine either the material in question or the orientation of the crystal plane of said material.

2 Experiment procedure

2.1 $\beta - 2\beta$ scan

We can describe the reflection of an X-ray beam by treating it as specular (mirrorlike) and assuming elastic scattering. From these premises we can find Bragg's law

$$2 \cdot d(hkl) \cdot \sin(\theta) = \lambda \quad (1)$$

$d(hkl)$ is the distance between parallel lattice planes of the configuration (hkl) characterizing the reciprocal lattice vector $\mathbf{G} = \frac{2\pi}{a}(h, k, l)$, where a is the lattice constant. $d(hkl)$ can be shown to be equal to $\frac{2\pi}{|\mathbf{G}|} = \frac{2\pi}{a}\sqrt{h^2 + k^2 + l^2}$. In this laboratory we use a $\beta - 2\beta$ scan, also known as coupled mode. The incident beam hits the sample at an angle β ,

which is the same as the angle of the reflecting beam. This is done by rotating the sample to an angle β and subsequently moving the detector to an angle of 2β , as shown in figure 1.

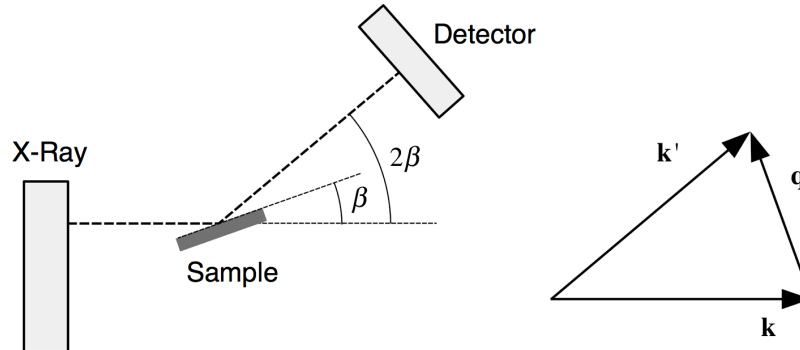


Figure 1: The $\beta - 2\beta$ scan setup and visualization of corresponding wave vector in reciprocal space

The scattering vector \mathbf{q} equals to the difference between the outgoing and incoming wavevectors, $\mathbf{k}' - \mathbf{k}$. By equation (20) in chapter 2 from [1] the scattering amplitude F is given by

$$F = \sum_{\mathbf{G}} \int dV n_{\mathbf{G}} e^{i(\mathbf{G} - \mathbf{q}) \cdot \mathbf{r}} \quad (2)$$

When the scattering vector equals a particular reciprocal lattice vector, $\mathbf{q} = \mathbf{G}$, the intensity of the reflection will peak in the diffractogram.

2.2 Structure factors

The second condition for a diffraction peak to appear is that the structure factor must be nonzero. The structure factor $S_{\mathbf{G}}$ of a crystal structure can be calculated as below. Here n is the number of atoms in the basic lattice, and atom j is at position \mathbf{r}_j with atomic form factor f_j . The atomic form factors are approximately equal to the atomic number.

$$S_{\mathbf{G}} = \sum_{j=1}^n f_j e^{-i(\mathbf{r}_j \cdot \mathbf{G})} \quad (3)$$

Say $\mathbf{G} = \frac{2\pi}{a} (h, k, l)$. The structure factor of an fcc lattice with lattice constant a is

$$S_{\mathbf{G}}^{fcc} = f \cdot \left[1 + (-1)^{h+k} + (-1)^{k+l} + (-1)^{l+h} \right] \quad (4)$$

The fcc structure factor is nonzero if and only if h , k and l are all even or all odd.

2.2.1 NaCl

The two atoms in the conventional cell of NaCl, one Na and one Cl, are each in an fcc structure. Putting an Na at the origin, the Cl structure will be displaced by $\frac{a}{2}\mathbf{e}_x$. The structure factor sums can then be expressed using the fcc structure factor above as

$$\begin{aligned} S_{\mathbf{G}}^{NaCl} &= \left(f_{Na} + f_{Cl} e^{2\pi i \cdot \frac{h}{2}} \right) \cdot \left[1 + (-1)^{h+k} + (-1)^{k+l} + (-1)^{l+h} \right] \\ &= \left(f_{Na} + f_{Cl} (-1)^h \right) \cdot S_{\mathbf{G}}^{fcc} \end{aligned} \quad (5)$$

With $f_{Na} = 11$ and $f_{Cl} = 17$ the structure factor will only be 0 when the fcc part is 0.

2.2.2 Si

Silicon is monoatomic with two atoms in the conventional cell, at $(0, 0, 0)$ and at $a(\frac{1}{4}, \frac{1}{4}, \frac{1}{4})$. The structure factor becomes

$$S_{\mathbf{G}}^{Si} = f_{Si} \cdot \left(1 + e^{\pi i \frac{h+k+l}{2}} \right) \cdot S_{\mathbf{G}}^{fcc} \quad (6)$$

GaAs and InP

The other two crystals in this lab both have a zincblende structure with two different atomic factors, say f_{α}, f_{β} . The α -atoms are in an fcc structure starting at the origin and the β -atoms are displaced by $\frac{1}{4}\frac{1}{4}\frac{1}{4}$, again in a cubic fcc structure. The structure factor becomes

$$S_{\mathbf{G}}^{\alpha\beta} = \left(f_{\alpha} + f_{\beta} e^{\pi i \frac{h+k+l}{2}} \right) \cdot S_{\mathbf{G}}^{fcc} \quad (7)$$

The atomic form factors are $f_{Ga} = 31$, $f_{As} = 33$, $f_{In} = 49$ and $f_P = 15$. The structure factor for InP is only zero if and only if the fcc structure factor is zero. The same goes for GaAs, except when $h + k + l \equiv_4 2$ the structure factor becomes small which might affect the diffraction peaks.

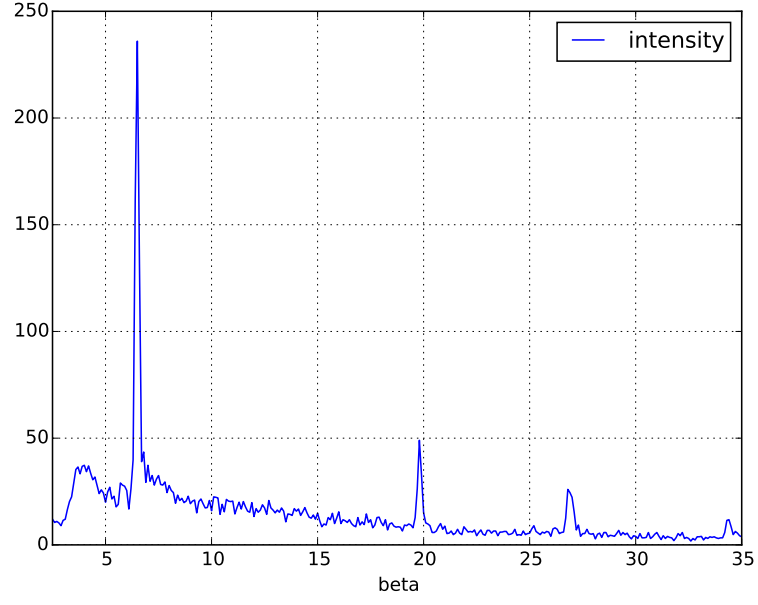


Figure 2: Description A

3 Measurements results

Sample A	
β_1	6.5°
β_2	19.8°
β_3	26.9°
(β_4)	(34.4°)

Sample B	
β_1	14.7°
(β_2)	(30.2°)

Sample C	
β_1	15.1°
β_2	27.6°
β_3	31.4°

Sample D	
β_1	6.0°
β_2	12.1°
β_3	18.3°
β_4	24.8°

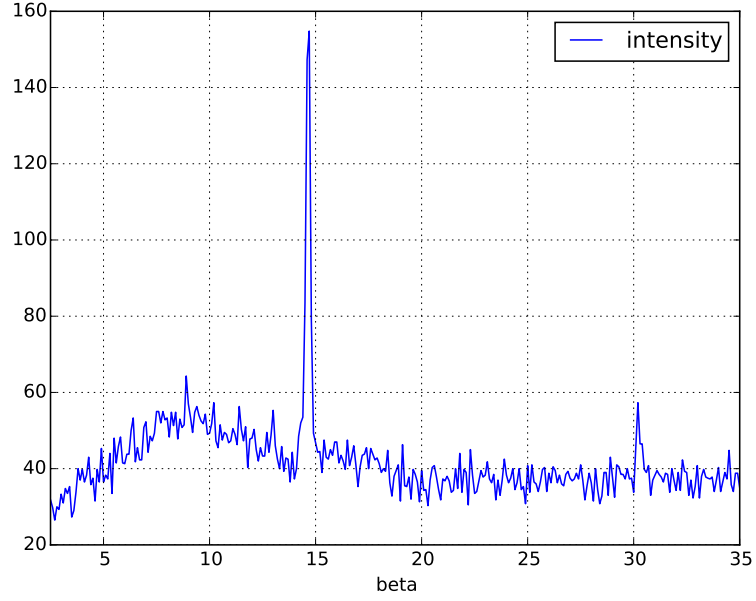


Figure 3: Description B

Sample NaCl	
β_1	7.2°
β_2	14.5°
β_3	22.1°

4 Discussion of the results

4.1 Finding the X-ray wavelength from the NaCl diffraction pattern

The crystal surface is cut parallel to the (1,0,0) lattice plane. In coupled mode the hkl -vectors will be integer multiples of this Miller index. $\mathbf{G} = \frac{2\pi}{a}(n, 0, 0)$ where n is an integer. The structure factor for NaCl is nonzero when h, k, l are all even or all odd. This happens when n is even. From (??) our diffraction maxima occurs when

$$\frac{2a}{n} \sin\theta = \lambda$$

Inputting the measured peak angles gives the following values for λ :

By Bragg's beard!

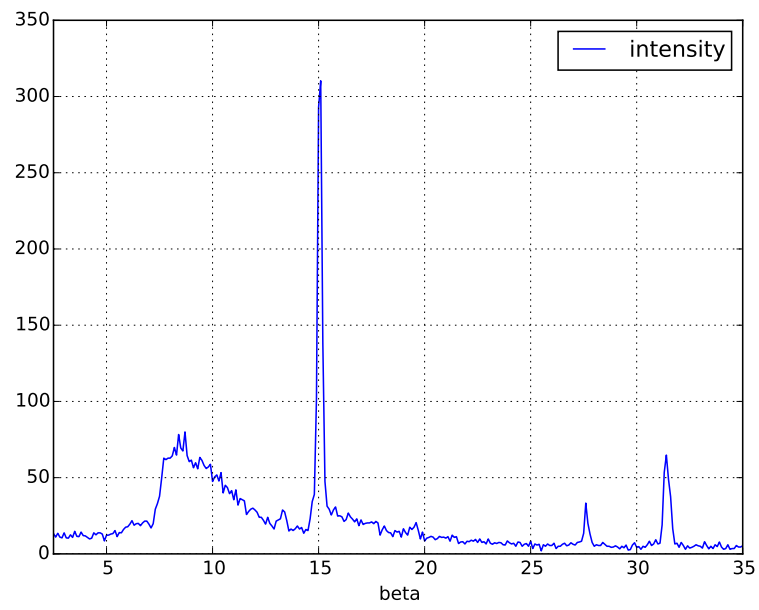


Figure 4: Description C

5 Conclusion

References

- [1] Charles Kittel, *Introduction to Solid State Physics 8th Edition*, 2005.

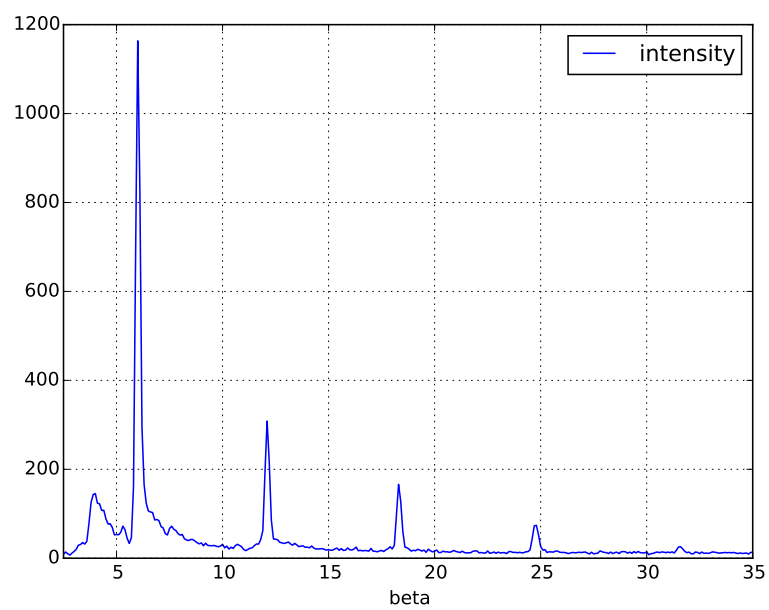


Figure 5: Description D

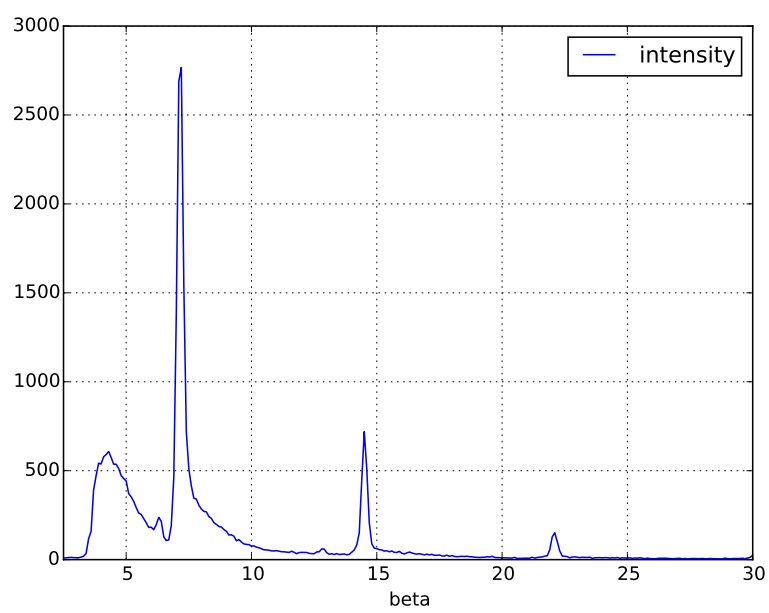


Figure 6: Description NaCl