X-Ray Diffraction

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I. Abstract

This lab used x-ray diffraction to measure the lattice constants of NaCl and LiF. The number of x-rays as a function of angle was measured using a Geiger-Muller tube. The data was plotted and Bragg's Law was used for the maxima along with the Miller indices for the various planes within the crystal. This gave results for the lattice constants of NaCl and LiF that agreed with the known values of 0.563nm and 0.402nm[1], respectively.

II. Introduction

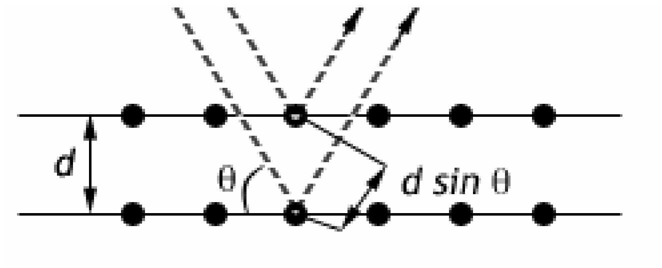

Figure 1: Bragg Diffraction[2]

When x-rays are incident on crystal surfaces as shown in Figure 1, the ray incident on the lower surface travels a distance of 2dsinθ farther. As a result, the reflected ray is out of phase. According to Bragg's Law constructive interference occurs when $2d\sin\theta=n\lambda$, where n is an integer and λ is the wavelength of the incoming rays. It is known that NaCl and LiF are face-centered cubic lattices and lattice constant, a_o, is related to d by the equation $a_o=2d$.

III. Apparatus

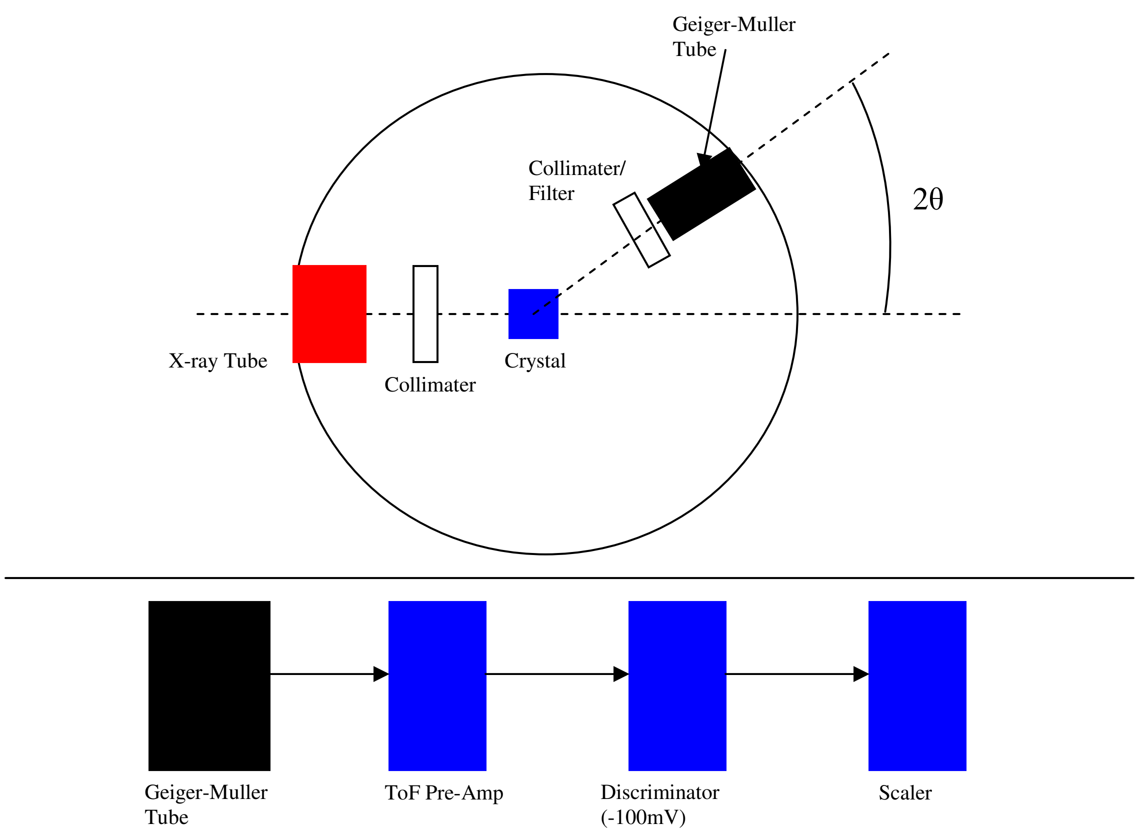

Figure 2: Experimental apparatus (top) and electronic setup (bottom)

The apparatus shown in Figure 3 was used to collect data. A copper target x-ray tube emitted x-rays of wavelength 0.154nm and 0.138nm. The x-rays diffracted off of a crystal (NaCl or LiF), passed through columnaters, and were detected by a Geiger-Muller tube run at 400 V. The tube was moveable and the angle at which it detected the x-rays was 2θ. The output from the tube was discriminated with a threshold of -100mV and discriminated signal was counted by a scaler.

IV. Procedure

An NaCl crystal was examined first. The number of x-rays detected by the tube in 50 seconds was measured as a function of angle (2θ) from 20° to 75°. A LiF crystal was then examined and the number of x-rays detected by the tube in 95 seconds was measured as a function of angle from 20° to 70°. A Ni filter was then inserted in front of the Geiger-Muller tube and the number of x-rays detected by the tube in 95 seconds was measured as a function of angle from 20° to 70°.

V. Results

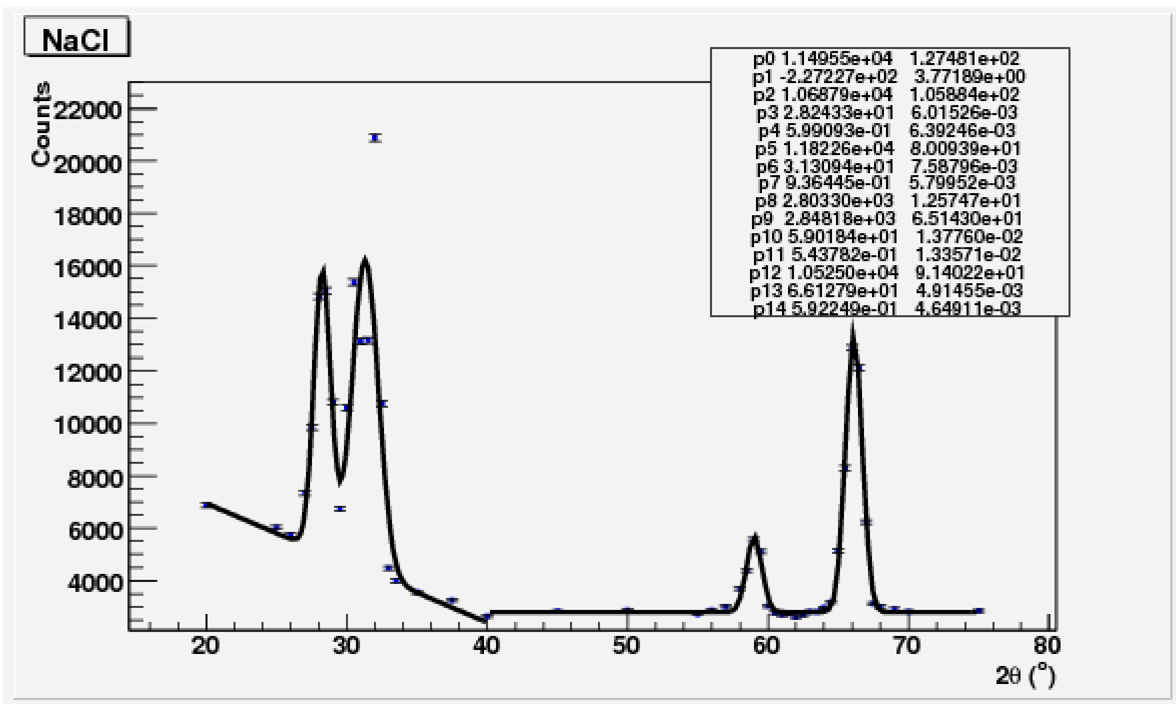

Figure 3: Data for NaCl plotted as number of counts vs 2θ.

Equation for range 20° to 40°: $1.15(10^4) - 2.27(10^2)x + 1.07(10^4)e^{\left(\frac{x-28.2}{.6}\right)^2} + 1.18(10^4)e^{\left(\frac{x-31.3}{.9}\right)^2}$,

Equation for range 40° to 75°: $2.80(10^3) + 2.84(10^3)e^{\left(\frac{x-59.0}{.5}\right)^2} + 1.05(10^4)e^{\left(\frac{x-66.1}{.6}\right)^2}$

The data for NaCl, shown in Figure 3, was plotted and each peak was fitted to a Gaussian plus a background. Data in the range 20° to 40° was fit with a linear background and data in the range 40° to 75° was fit with a constant background. From the graph, maxima were found at 2θ=28.2°±0.6°, 31.3°±0.9°, 59.0°±0.5°, and

66.1°±0.6°. These peaks correspond to the n=1 and n=2 diffraction maxima shown in Table 1. The pairs of peaks correspond to the K_α and K_β x-rays emitted by the Geiger-Muller tube. The values for d and a_o were also calculated.

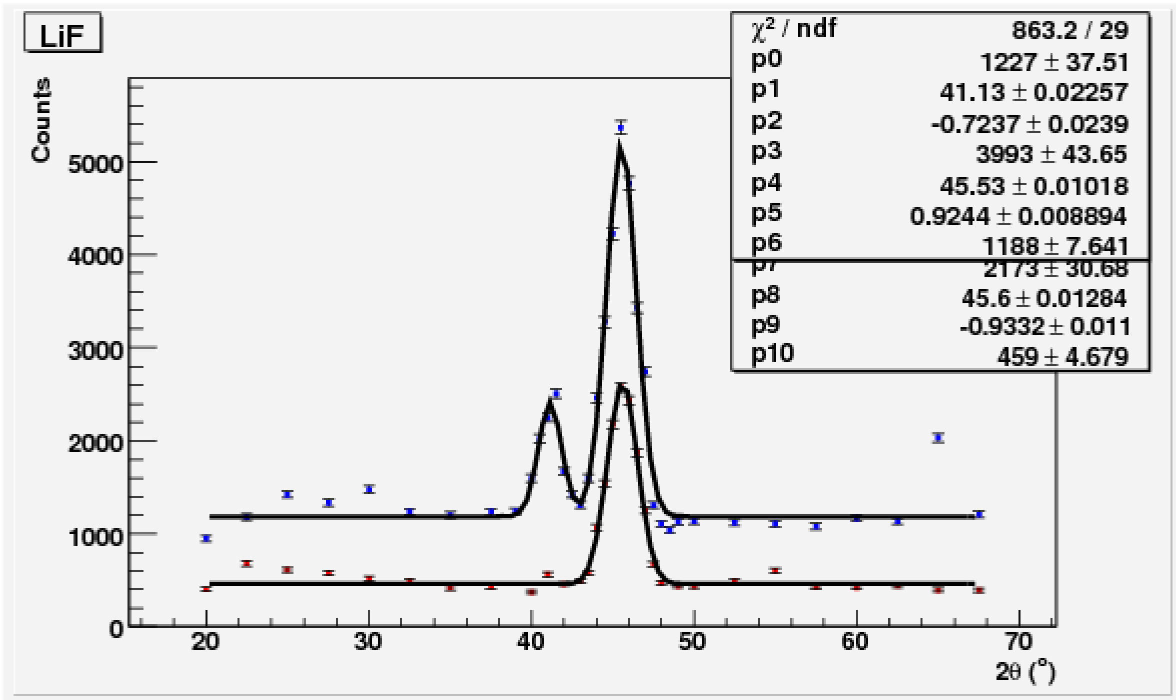

Figure 4: Data for LiF with the Ni filter (red) and without the Ni filter (blue) plotted as counts vs 2θ.

Fit equation for data without filter: $1.19(10^3)+1.23(10^3)e^{\left(\frac{x-41.1}{.7}\right)^2}+3.99(10^3)e^{\left(\frac{x-45.5}{.9}\right)^2}$.

Fit equation for data with filter: $4.59(10^2)+2.17(10^3)e^{\left(\frac{x-45.6}{.9}\right)^2}$.

The data for LiF taken with and without the Ni filter is plotted in Figure 4. The measurements without the filter gave two peaks: 41.1°±0.7°, and 45.5°±0.9°. The measurements with the filter gave one peak at 45.6°±0.9°. These peaks correspond to the n=1 diffraction maxima shown in Table 1. The data taken with the filter shows only one peak because the Ni filter blocks the x-rays of wavelength 0.138nm much more efficiently than x-rays of wavelength 0.154nm. This filtering also results in lower background.

Using Bragg's Law, d was found by the equation $d=\frac{n\lambda}{2\sin\theta}$. The error in d was given by $\Delta d=\frac{n\lambda\cos\theta}{2\sin^2\theta}\Delta\theta$. The lattice constant was then found by using a_o=2d.

Crystal	2θ (º)	λ of x-ray (nm)	n	D (nm)	a_o (nm)
NaCl	28.2 ±0.6	.138	1	0.283±0.006	0.566±0.013
NaCl	31.3±0.9	.154	1	0.285±0.008	0.571±0.016
NaCl	59.0±0.5	.138	2	0.280±0.002	0.560±0.004
NaCl	66.1±0.6	.154	2	0.282±0.002	0.565±0.005
LiF (no filter)	41.1±0.7	.138	1	0.197±0.003	0.395±0.007
LiF (no filter)	45.5±0.9	.154	1	0.199±0.004	0.398±0.008
LiF (filter)	45.6±0.9	.154	1	0.199±0.004	0.399±0.008

Table 1 Calculated values for NaCl and LiF data

Using the values for a_o in Table 1, the weighted average for the NaCl lattice constant was found to be 0.566±0.008nm. A weighted average for the LiF lattice constant was also calculated and found to be 0.397±0.008nm.

VI. Conclusion

The known value for a_o in NaCl is 0.563nm. This agrees with the experimentally calculated weighted average of 0.566±0.008nm. The known value for a_o in LiF is 0.402nm. This also agrees with the calculated value of 0.397±0.008nm.

VII. References

1. *Optics Land*. http://www.sciner.com/Opticsland.

2. "Image: DiffractionPlanes.Png." *Wikipedia.* http://en.wikipedia.org/wiki/Image:DiffractionPlanes.png.