

X-Ray Diffraction

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Using X-ray diffraction, crystal structure and lattice constants of NaCl and LiF, were experimentally determined. The experimentally determined lattice constant of NaCl, $a_0 = (521.17 \pm 67.11) \text{ pm}$, deviates from the accepted value of 564.02 pm by less than 1σ . The experimentally determined lattice constant of LiF was $a_0 = (428.44 \pm 117.10) \text{ pm}$. This deviates from the accepted value of 402.6 pm by less than 1σ .

INTRODUCTION

Using Bragg diffraction, the K_α and K_β peaks of two cubic crystals were analyzed. This was done to determine both crystal structure and respective lattice constant, a_0 , of NaCl and LiF. Such regular crystalline structures are classified by their unit cells - the smallest volumetric structure containing the necessary information for constructing the entire solid. Identifying the unit cell required using the Bragg condition:

$$n\lambda = 2d\sin\theta$$

where n is the order, λ is the wavelength, d is the lattice spacing, and θ is the diffraction angle. Maximums and minimums in the diffraction pattern give insight into the atomic structure. For cubic crystals, the lattice constant, a_0 , is twice the lattice spacing:

$$a_0 = 2d = \frac{n\lambda}{\sin\theta}.$$

William Lawrence Bragg discovered this in 1912 and pioneered the field of X-ray crystallography [1]. Analysis of structures at the atomic level aided our understanding of microscopic structures. In 1953, X-ray crystallography revealed the structure of DNA [1].

APPARATUS AND PROCEDURE

Plateauing the high-voltage supply (HV) showed the ideal operating voltage to be 0.384 V . Power from the HV was sent to the Geiger-Mueller counter (GM tube). The signal was then sent to a pre-amplifier and onto an amplifier (Amp). Finally, the signal was sent to the scalar and oscilloscope. A schematic for the experimental apparatus is shown in Figure 1.

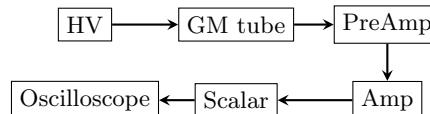


FIG. 1. The electronics used in this apparatus are labeled in this schematic.

Background detections were established by collecting data over the full angular range, with no crystal. To account for angular dependent background, detections recorded with no crystal were subtracted from data collected using NaCl and LiF crystals. Background from scattered X-rays were minimized by placing small pieces of lead around the apparatus. While collecting data, the Amp introduced significant noise, causing its removal from the final experimental apparatus.

DATA

In order to calculate the lattice constants of NaCl and LiF, the weighted average of angles at which these peaks occur was taken, on the $n = 1$ and $n = 2$ lines [3]. Lack of detector sensitivity made it impossible to distinguish between the K_{α_1} and K_{α_2} peaks, in our data. For comparison to theoretical literature, a weighted average of the angles these peaks occur at was also taken [2].

Nickel has a K-absorption edge at 148.8 pm , causing it to absorb radiation from Cu K_β much more strongly than it absorbs Cu K_α radiation [3]. By taking data with and without a Ni filter, the K_α peaks isolated.

NaCl		
Peak	Filter	Measured Angle
K_β	none	26.94 ± 0.002
K_α	none	30.15 ± 27.04
K_α	Ni	30.16 ± 0.07

LiF		
Peak	Filter	Measured Angle
K_β	none	39.51 ± 0.04
K_α	none	44.12 ± 0.35
K_α	Ni	44.09 ± 0.10

TABLE I. K_α and K_β peak values for NaCl and LiF, with $n=1$.

NaCl		
Peak	Filter	Measured Angle
K_β	none	60.96 ± 5.32
K_α	none	65.00 ± 0.12
K_α	Ni	64.99 ± 6.94

LiF		
Peak	Filter	Measured Angle
K_β	none	86.56 ± 5.54

TABLE II. K_α and K_β peak values for NaCl and LiF, with $n=2$.

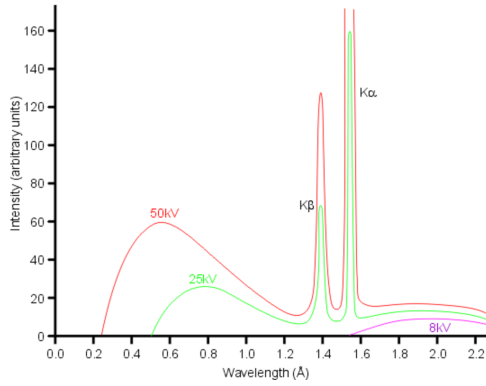


FIG. 2. Intensity as a function of wavelength.

Figure 2 [2] shows that K_β peaks occur at lower wavelengths with lower intensities than K_α peaks. For Copper the K_{α_1} , K_{α_2} , and K_β X-ray lines occur at 154.0 pm , 154.4 pm , and 139.2 pm , respectively [3].

NaCl

Tables I and II list the 2θ values corresponding to observed K_α and K_β peaks, for NaCl. Figures 3 and 4 show collected data with Gaussian fits, for NaCl at $n = 1$ and $n = 2$, respectively.

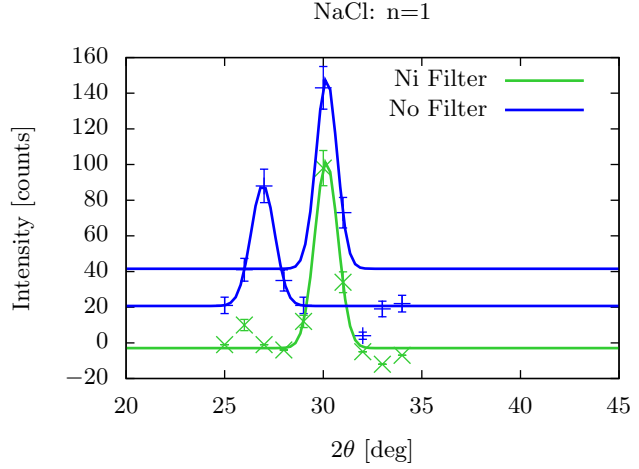


FIG. 3. NaCl with various filters, at $n=1$.

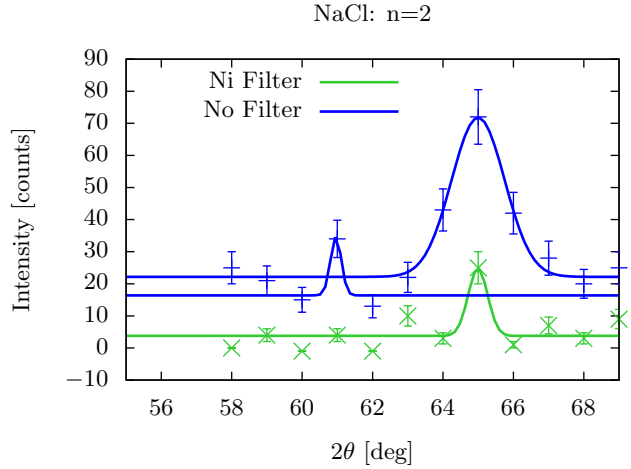


FIG. 4. NaCl with various filters, at $n=2$.

LiF

K_β peaks occur at lower angles than K_α peaks. Due to the detector's limited angle range, no K_α was observed for LiF with $n = 2$, shown by Figure 6. The K_α peak is expected to occur at $2\theta = 100^\circ$, but the apparatus could only achieve a maximum of $2\theta = 95^\circ$.

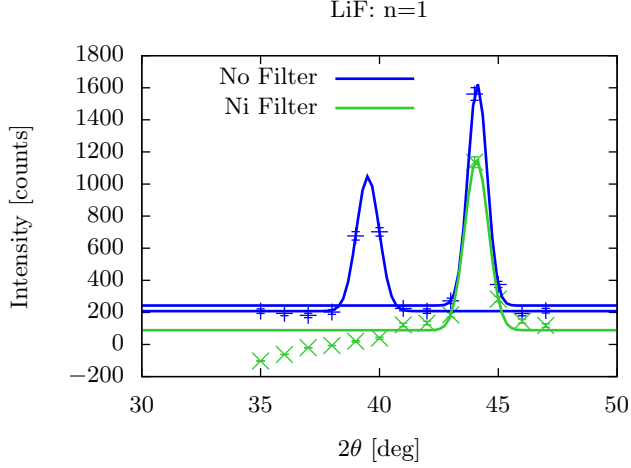


FIG. 5. LiF with various filters, at $n=1$.

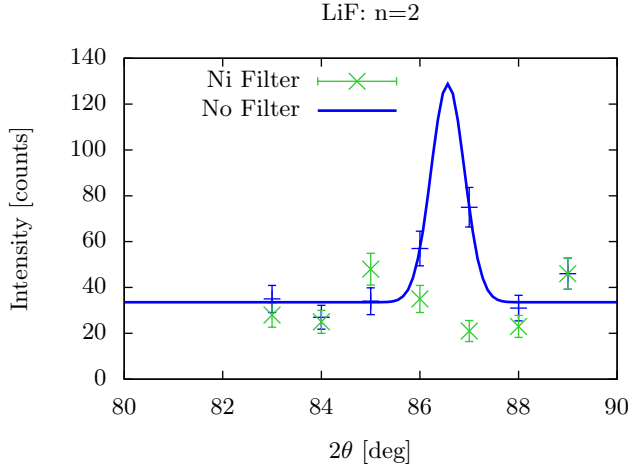


FIG. 6. LiF with various filters, at $n=2$.

Tables I and II list the 2θ values corresponding to observed K_α and K_β peaks, for LiF. Figures 5 and 6 show collected data with Gaussian fits, for LiF at $n = 1$ and $n = 2$, respectively.

RESULTS AND ANALYSIS

The lattice constant of NaCl was experimentally determined to be (521.17 ± 67.11) pm. This deviates by 0.64σ , from the accepted value of 564.02 pm [6]. The lattice constant of LiF was experimentally determined to be (428.44 ± 177.10) pm with a deviation of 0.15σ , from the accepted value of 402.6 pm [4]. Minor variation between experimental and theoretical values are likely due to crystal orientation. If not seated perfectly, the diffraction patterns will occur at angles offset from theoretical values.

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