# Physics 210 Lab 4B: Bragg Diffraction

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In this report, we describe the attempt to measure the crystalline lattice spacing of NaCL and LiF using the Bragg diffraction of X-rays through these crystals. We found lattice spacings of LiF to be 0.201 nm and for NaCl, 0.284 nm. Both measured values are in close agreement with the accepted values for LiF, 0.201 nm and NaCl, 0.282 nm. Error was not calculated for these measurements, since data was used from an existing set without uncertainties specified for some experimental parameters.

## I. INTRODUCTION

This experiment was carried out using a Tel-X-Ometer 580M X-ray Diffraction System Device. This device works by accelerating electrons through a high voltage into a copper target, producing Bremsstrahlung (breaking) radiation that is then directed towards the crystals to be Bragg-diffracted. The diffracted rays are then be measured at several  $2\theta$  angles on a basis of counts per 10 seconds. From this data, the crystalline lattice spacing, d, will be determined via Bragg's Law. The apparatus as used in these tests is shown in the figures below.

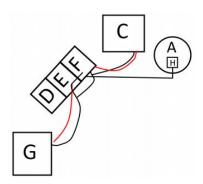


FIG. 1. A diagram of the setup. A: Tel-X-Ometer 580M, C: Keithley Model 178 Digiral Multimeter, D: Pasco + CDL 8000 Power Supply, E: PASO-CDL 8019 HV Power Supply, G: Hewlett Packard 1220A Oscilloscope, H: Geiger Mueller Tube

## II. THEORETICAL MODEL

The atomic crystalline structures of LiF and NaCl can both be modeled as a regularly repeating pattern of cubes. The mass of one molecule of either can be found using:

$$m_{\text{molecule}} = \frac{M_{\text{mol}}}{N_{A}}$$
 (1)

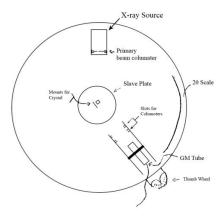


FIG. 2. A Diagram of the Tel-X-Ometer 580M, (A in Fig. 1

where  $M_{\rm mol}$  is the molar mass of the respective crystal, and  $N_A$  is avagadro's number,  $6.022 \times 10^{23}$ . Next, using the density equation:

$$\rho = \frac{m}{V} = \frac{m_{\text{molecule}} \cdot n}{V} \tag{2}$$

where n is the number of molecules, in conjunction with Eq. 1, we find the number of molecules per unit volume to be:

$$\frac{n}{V} = \frac{\rho}{m_{\text{molecule}}} = \frac{\rho}{M_{\text{mol}}/N_A} = \frac{\rho \cdot N_A}{M_{\text{mol}}}$$
(3)

To find the unit volume for a crystal, we use Eq. 2 and set n=1, and with the assumption the lattice is a regular cubic, giving us:

$$\frac{1}{d^3} = \frac{2\rho \cdot N_A}{M_{\text{mol}}} \tag{4}$$

where the 2 is added since both crystals are diatomic. Thus, the lattice spacing is:

$$d = \sqrt[3]{\frac{M_{\text{mol}}}{2\rho \cdot N_A}} \tag{5}$$

This gives us an expected value for the spacing. Experimentally, the lattice spacing will be found via Bragg's

Law:

$$n\lambda = 2d\sin(\theta) \tag{6}$$

rewriting to solve for d, we have:

$$d = \frac{n\lambda}{2\sin(\theta)} \tag{7}$$

Given the following experimental values:

For Copper, we have the characteristic wavelengths to be:

$$\lambda_a = 0.15425 \text{ nm}$$
$$\lambda_b = 0.13923 \text{ nm}$$

Densities of LiF and NaCl

$$\rho_{\text{LiF}} = 2.64 \times 10^3 \text{kg/}m^3$$

$$\rho_{\text{NaCl}} = 8.96 \times 10^3 \text{kg/}m^3$$

Molar Masses of LiF and NaCl:

$$M_{\text{mol, LiF}} = 0.025939 \text{kg/mol}$$
  
 $M_{\text{mol, NaCl}} = 0.063546 \text{kg/mol}$ 

The lattice spacings LiF and NaCl can then be calculated using the above values and Eq. 5, to then be compared to the experimentally measured spacings using Eq. 7.

## III. EXPERIMENT

## A. Procedure

- 1. Locate the Primary Beam Collimator 582.001 in front of the emitter. Place Collimator 562.016 in the 13 slot and Collimator 562.015 in the 18 slot.
- Pay special attention to check that the collimators are aligned.
- 3. Set the X-ray tube's accelerating voltage to  $30~\rm kV$ , the counter's high voltage to  $475~\rm V$ , and the counting time to  $10~\rm s$ .
- 4. Conduct a test count at  $0^{\circ}$  to ensure that X-rays are traversing through both collimators.
- 5. Mount each crystal such that the colored end is on top, and the matte finish is facing the X-ray source (so that the X-rays will reflect off of this face). Turn the measuring arm clockwise.
- 6. Starting with as small of an angle as allowed, begin collecting counts/ 10s for each degree location.

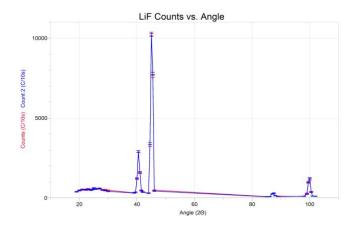


FIG. 3. A plot of the two trials siplaying the number of counts / 10 seconds at each measureable double angle,  $2\theta$  for X-rays refractied by the LiF crystal lattice. Error bars are 68 % CI Poissan statistics error.

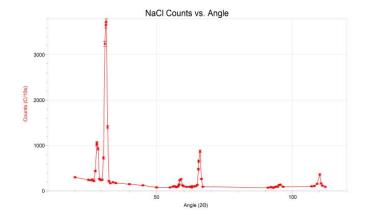


FIG. 4. A plot of the number of counts / 10 seconds at each measureable double angle,  $2\theta$ , for X-rays diffracted by the NaCl crystal. Error bars are 68 % CI Poissan statistics error.

#### B. Data

Data was collected twice for the LiF crystal and once for the NaCl crystal using the above procedure. The plots below summarize the data collected.

Observing the graphs, it can be seen that LiF has peaks at  $\theta=20.25^{\circ}, 22.5^{\circ}, 43.75^{\circ}$ , and 50°. In a similar manner, it can be seen that NaCl has peaks at  $\theta=14.05^{\circ}, 15.75^{\circ}, 29.75^{\circ}$ , and 33°.

## IV. ANALYSIS

Using Eq. 7, with the correct copper characteristic wavelengths, we can find the crystalline lattice spacings d.

Due to the lack of instrument uncertainties for several

TABLE I. LiF

Peak $\#$	Order (n)	$\theta$ (Deg)	$\theta$ (Rad)	$\lambda_{ m Char}$	d (nm)
1	1	20.25	0.353	0.13923	0.201
2	1	22.5	0.393	0.15425	0.202
3	2	43.75	0.763	0.13923	0.201
4	2	50	0.872	0.15425	0.201

Avg. Spacing: 0.201 Exp. Spacing: 0.201

## TABLE II. NaCl

Peak #	Order (n)	$\theta$ (Deg)	$\theta$ (Rad)	$\lambda_{ m Char}$	d (nm)
1	1	14.0535	0.245	0.13923	0.287
2	1	15.75	0.275	0.15425	0.284
3	2	29.5	0.515	0.13923	0.283
4	2	33	0.576	0.15425	0.283

Avg. Spacing: 0.284 Exp. Spacing: 0.282 parameters of the data set, uncertainties were not calculated.

## V. CONCLUSION

For the LiF crystal, the measured spacing of 0.201 nm was in agreement with the expected spacing of 0.201 nm. For the NaCl crystal, the measured spacing of 0.284 nm was close to the expected spacing 0.282 nm. Both measured values were reasonably close to their respective expected values. Potential improvements could be including experimental error with the measured values, and running more trials for each crystal.

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