Physics 307 Experiment 7:
X-Ray production and diffraction

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1 Purpose

To study how voltage and current affect K_α, K_β, and bremsstrahlung radiation and to measure the lattice spacing of four different crystals through X-ray diffraction.

2 Theory

In this experiment, the source of our X-rays is electron deceleration. A hot filament inside a vacuum tube produces the electrons due to thermionic emission. The electrons are then accelerated from the cathode to the anode under a very high (15-35 kV) voltage. The electrons hit a molybdenum barrier and they rapidly decelerate, causing X-rays to be produced and radiate perpendicular to the electron velocity. Since the energy of the X-rays depends on how quickly the electrons are decelerated, the energies are a continuous spectrum. This radiation is called bremsstrahlung radiation.

In this experiment we also wanted to study the discrete X-ray emission lines caused by excited states of the Molybdenum. When electrons of a specific energy collide with the molybdenum, they have the chance of exciting valence electrons of the molybdenum to a higher energy state. When those electrons return to their ground state, discrete energy x-rays are produced. The radiation associated with the n=2 to n=1 transition is known as K_α and the energy associated with the n=3 to n=1 transition is known as K_β. Since these energy levels are quantized and fixed, the K_α and K_β energies are discrete.

Bragg's law determines how much light of a particular wavelength λ will scatter when it collides with a crystal lattice.

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

where d is the distance between atomic layers and n is the order of diffraction. Diffraction order depends on how many crystalline layers the incident radiation penetrates before scattering. The light that penetrates deeper will appear to be deflected more by the detector, so we should expect to see multiple peaks corresponding to different diffraction orders of K_α and K_β.

3 Procedure

In order to conduct our experiments, we used an X-ray diffractometer, which consisted of an X-ray source, Sodium Chloride (NaCl) crystal target, and a detector. First, we varied the tube voltage from 15 to 35 kV while holding the tube current at a constant 1mA. We swept the target angle from 2.5 to 10 degrees (0.1 degree increments) and measured how the K_α, K_β, and bremsstrahlung radiation were affected.

Next, we held the tube voltage constant and varied the tube current from 0.2 to 0.8 mA. We did the same scans as the voltage trial to compare how different amounts of current affected the radiation.

Lastly, we wanted to compare the atomic lattice spacing for different crystals. In order to calculate this, we had to capture multiple Bragg peaks, so this time we scanned the target from 2.5 to 25 degrees. We ran the vacuum tube at 1mA @ 35kV, and repeated the experiment for the Lithium Fluoride (LiF), Sodium Chloride (NaCl), Potassium Chloride (KCl) and Mica crystals.

4 Results

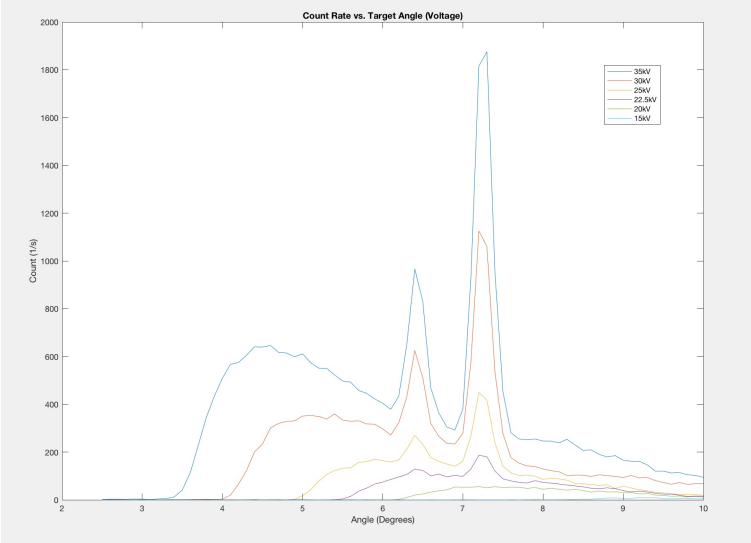

Figure 1: Count rate vs. target angle for our voltage-varying trials

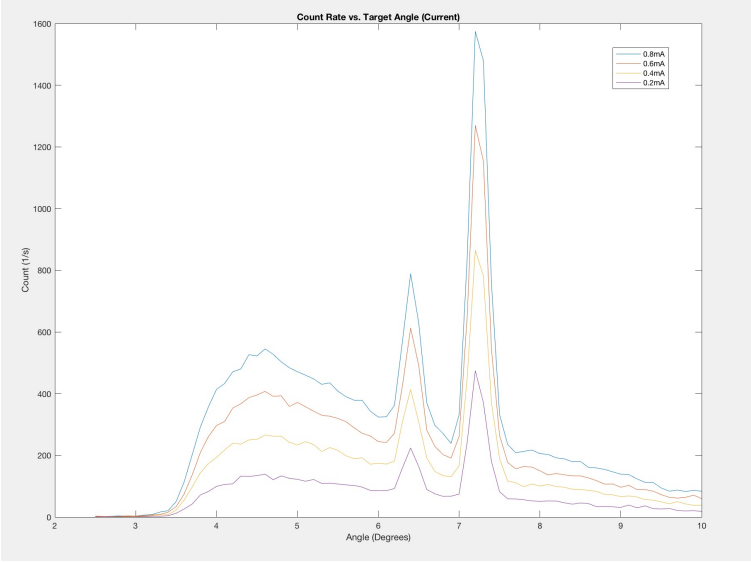

Figure 2: Count rate vs. target angle for our current-varying trials

Figures 1 and 2 show our results from the voltage-varying and current-varying trials for NaCl. The Molybdenum K_α and K_β peaks are clearly apparent in our count rate graphs. One interesting observation is that

the bremsstrahlung radiation threshold varied for our voltage trials, but not for our current trials (more discussion on this in post-question 1).

Crystal	K_α Lattice spacing (Å)	K_β Lattice spacing (Å)	Average Lattice spacing (Å)	Error (Å)
LiF	2.02	2.01	2.02	2.25
NaCl	2.85	2.79	2.82	4.28
KCl	3.18	3.22	3.20	5.29
Mica	3.68	4.94	4.31	7.79

Table 1: Our calculated lattice spacing for each K_α and K_β peak.

By plotting $n\lambda/2$ vs. $\sin(\theta)$, we can use a linear fit in order to find the lattice spacing from the Bragg relationship. See the appendix for images of our graphs and linear fit models. Table 1 shows our calculated values for each crystal. The values do not match the accepted values, which are 4.63Å, 5.63Å, 6.29Å for LiF, NaCl, and KCl respectively. However, they are correct to within an order of magnetide and the trend of increasing lattice spacing can be clearly seen in our data.

For most of the calculated lattice spacings, we only had 2-3 data points, so d is simply the slope between the endpoints. But $\Delta n\lambda/2 = 0$, so the formula we used to calculate the error in our lattice spacing was

$$\Delta d = 2d\frac{\Delta f}{f}$$

where $f = \sin(\theta)$. But $\frac{df}{d\theta} = \cos(\theta)$ so $\Delta f = \cos(\theta)\Delta\theta$ and

$$\Delta d = 2d\frac{\cos(\theta)\Delta\theta}{\sin(\theta)}$$

Crystal	FWHM (Degrees)
NaCl (n=1)	0.9 ± 0.1
NaCl (n=2)	0.7 ± 0.1
Mica (n=1)	1.3 ± 0.1
Mica (n=2)	1.1 ± 0.1

Table 2: Rocking curve full width at half-maximum for NaCl and Mica crystals.

Lastly, we measured the rocking curves for both the LiF and Mica crystals. The rocking curves measure the quality of the crystal by holding the detector still (centered at one of our K_α peaks) and varying the angle of the crystal to determine how "sharp" the peak is. A sharper peak corresponds to a higher quality crystal since more of the lattice is aligned. The full width at half-maximum values are given in table 2. The angle step for our trial was 0.1 degrees, so our error is 2*0.05, or 0.1 degrees.

From the rocking curves, we can tell that the NaCl is a slightly higher-quality crystal than the Mica we used. Also, I found it interesting that the higher order Bragg peaks had a narrower rocking curve. I would have expected that when the incident angle is steeper, crystal irregularities would have a larger impact, but this does not seem to be the case.

5 Post-Questions

1. Question: Does the threshold for X-ray emission vary with tube voltage? tube current? What is the functional relationship between the threshold wavelength (or energy) and tube voltage? Does you data

support this assertion?

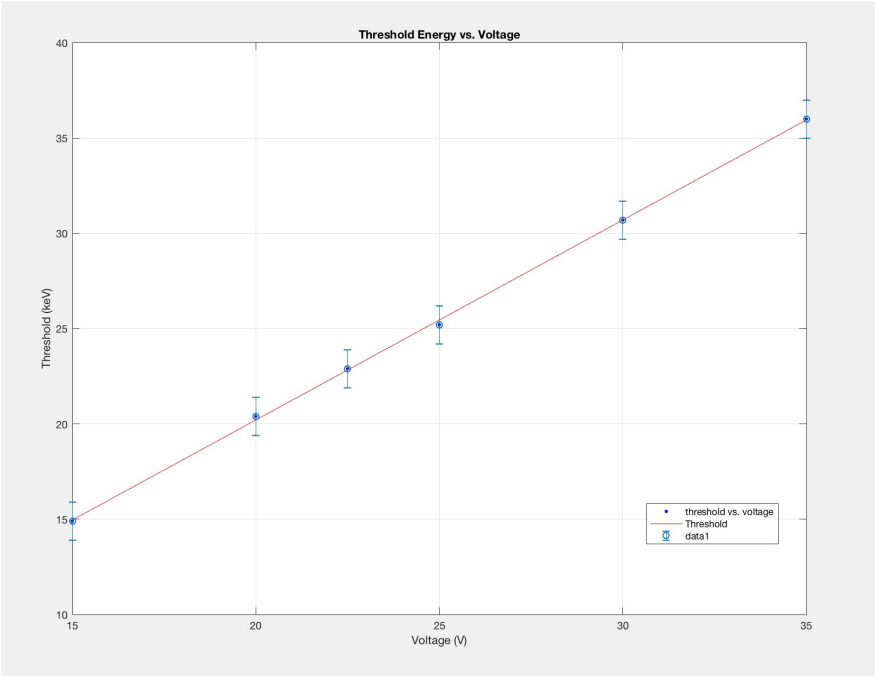

Figure 3: Threshold Energy vs. Voltage

Voltage (V)	Threshold (keV)
35	36 ± 1
30	30.7 ± 1
25	25.2 ± 1
22.5	22.9 ± 1
20	20.4 ± 1
15	14.9 ± 1

Table 3: The threshold energies for our different voltage trials

The threshold energy is nearly identical to the tube voltage. This makes sense because the radiation cutoff energy should be the same as the energy carried by the electrons. Our data shows that the threshold energy varies linearly with voltage, and can be approximated with the following model:

$f(x) = p_1\ x + p_2$
Coefficients (with 95% confidence bounds):
p_1 = 1.049 (1.02, 1.079)
p_2 = -0.7788 (-1.521, -0.03616)

Goodness of fit:
SSE: 0.1129
R-square: 0.9996
Adjusted R-square: 0.9995
RMSE: 0.168

There was no variation in the threshold voltage for the different amounts of current.

2. Question: How does the maximum intensity vary with voltage; with current? In principle the formula is $I = A(V - V_T)^{\alpha} i$. However the GM-tube (your X-ray detector) saturates at relatively modest counts rates. A reasonable expression to model this is $I = ic(1 - \Delta tci)$ where c is the scaling factor and Δt is the dead time . Use your I vs. i measurement to correct for the detector deadtime and then identify V_T and the exponent. (You should assume the actual intensity is linear with tube current.)
1) Perform a linear least squares fit of I/i. The intercept is c and the slope is $-c^2\Delta t$. Use the formula $I' = I/(1 - I\Delta t)$ to correct your data for dead-time.
2) Fit $\log I'/i = \log A + \alpha \log(V - V_T)$ to a line but adjust V_T to get the best straight line (where I' is the corrected intensity).

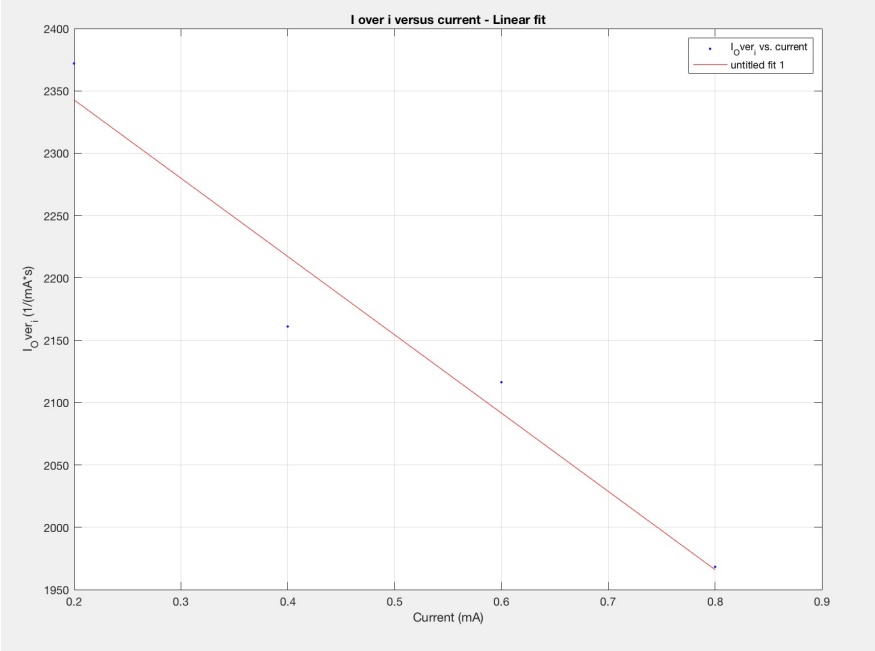

Figure 4: I/i (Intensity over current) versus current (i)

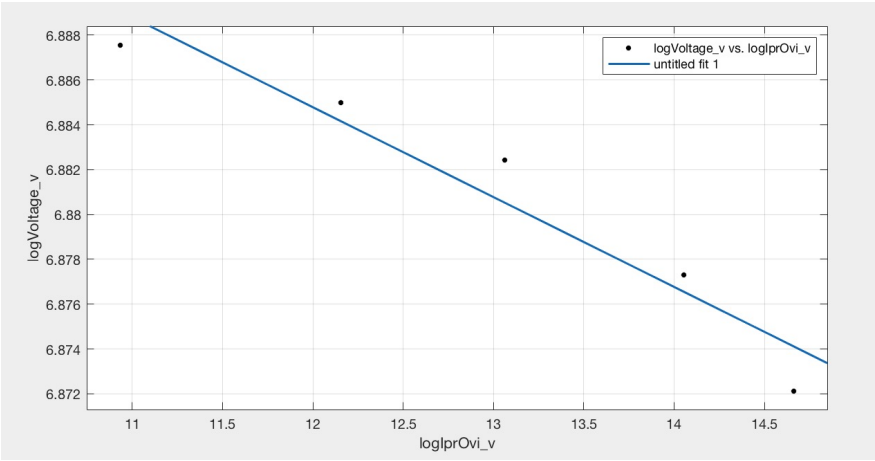

Figure 5: Log I/i (Intensity over current) versus $\log A + \alpha \log(V - V_T)$

Figure 4 shows our linear fit of I/i versus i. From out fit equation, we determined the scaling factor

to be 2468, and the dead time to be 0.103 milliseconds. Figure 5 shows our corrected intensity values. From the linear fit, we found the value for log(A) to be 6.881 and the value of α to be -0.005963. The value of V_T did not have a significant affect on our curve fit, so we chose $V_T = 0$.

3. Question: Do the wavelengths of the characteristic radiation from molybdenum vary with voltage or current? Find the characteristic energies. How do your results vary with the known values?

   The characteristic wavelengths did not change for either voltage or current variations. Our measured values were 17.3keV for K_α and 19.7keV for K_β, which are within 0.6% percent of their true values of 17.4 keV and 19.6 keV respectively.

4. Question: If the NaCl crystal is misaligned how will this affect your results? Does anything in your results suggests this effect?

   If the crystal is misaligned, then the $n\lambda/2$ Bragg relationship will be offset by a constant. The calculated radiation energies will be slightly off, but the linear relationship between $n\lambda/2$ and the sine of the angle will be reserved. Our offset constants were -2.40E-13, -1.77E-12, -2.60E-12, so our data is correct to three significant figures $\pm$ 0.02Å. This is enough precision for our purposes, so we can consider the crystal to be aligned.

6 Conclusion

The count rate for K_α and K_β radiation varies with both tube voltage and tube current, but the energy of the peaks are unaffected. The threshold radiation values for the bremsstrahlung depends only on tube voltage, although the count rate depends on both tube voltage and current. Our calculated values for the lattice spacing did not match the accepted values, likely due to the large error associated with only using 2-3 data points. If time allowed, I would have liked to repeat the scans for each crystal to verify the data points and figure out what caused this discrepancy.

7 Appendix

7.1 LiF

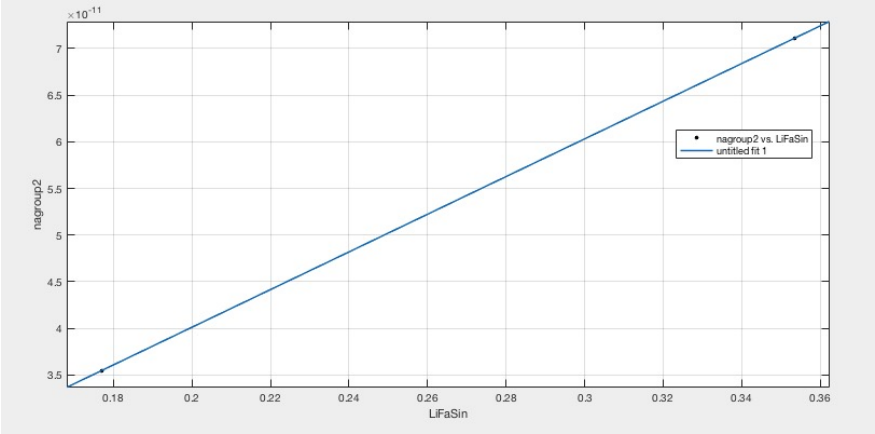

Figure 6: LiF $n\lambda/2$ vs. $\sin(\theta)$ for K_α

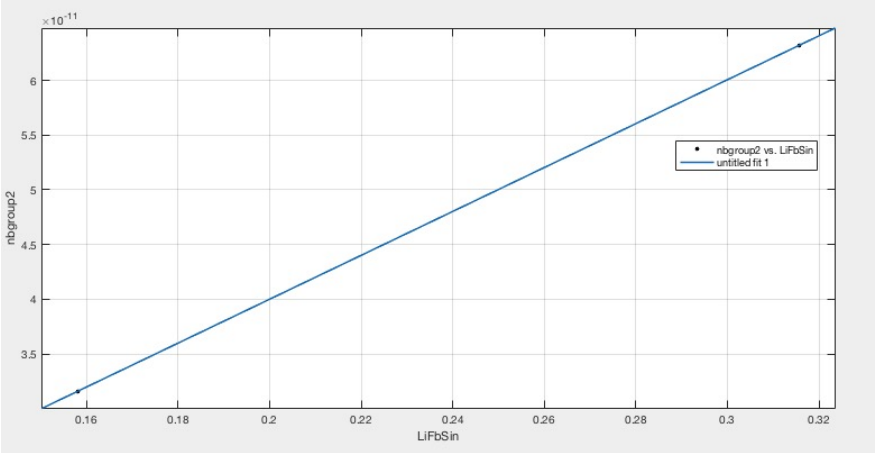

Figure 7: LiF $n\lambda/2$ vs. $\sin(\theta)$ for K_β

Linear model for LiF K_α:
f(x) = p1*x + p2
Coefficients:
p1 = 2.018e-10
p2 = -2.402e-13
R-square: 1

Linear model for LiF K_β:
f(x) = p1*x + p2
Coefficients:
p1 = 2.006e-10
p2 = -1.339e-13
R-square: 1

7.2 NaCl

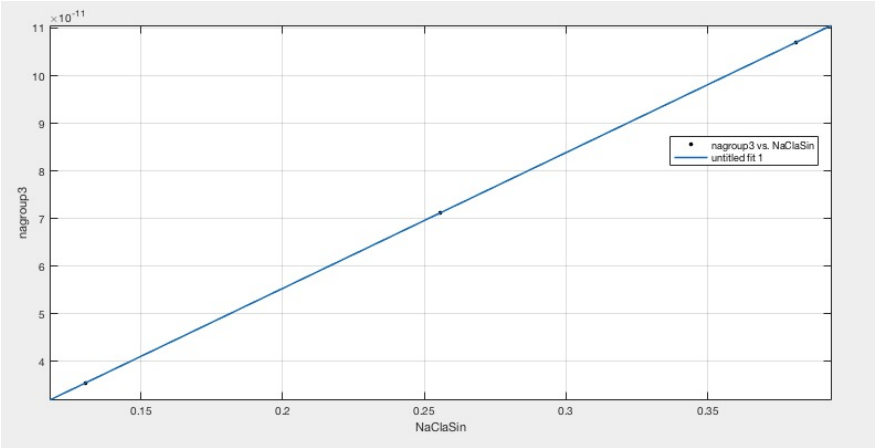

Figure 8: NaCl $n\lambda/2$ vs. $\sin(\theta)$ for K_α

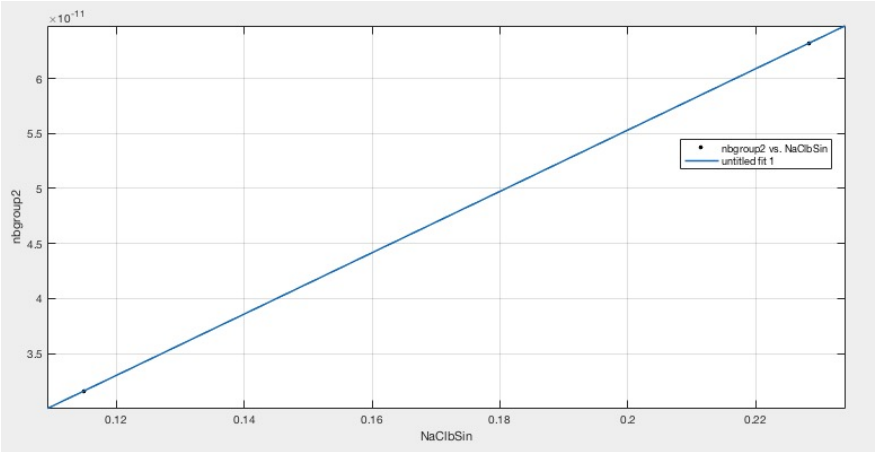

Figure 9: NaCl $n\lambda/2$ vs. $\sin(\theta)$ for K_β

Linear model for NaCl K_α:
f(x) = p1*x + p2
Coefficients (with 95% confidence bounds):
p1 = 2.854e-10 (2.825e-10, 2.883e-10)
p2 = -1.766e-12 (-2.563e-12, -9.694e-13)
R-square: 1

Linear model for NaCl K_β:
f(x) = p1*x + p2
Coefficients:
p1 = 2.786e-10
p2 = -4.245e-13
R-square: 1

7.3 KCl

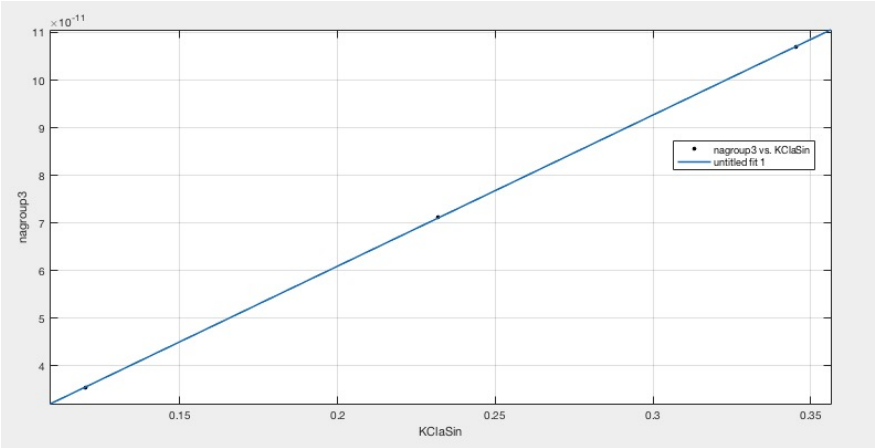

Figure 10: KCl $n\lambda/2$ vs. $\sin(\theta)$ for K_α

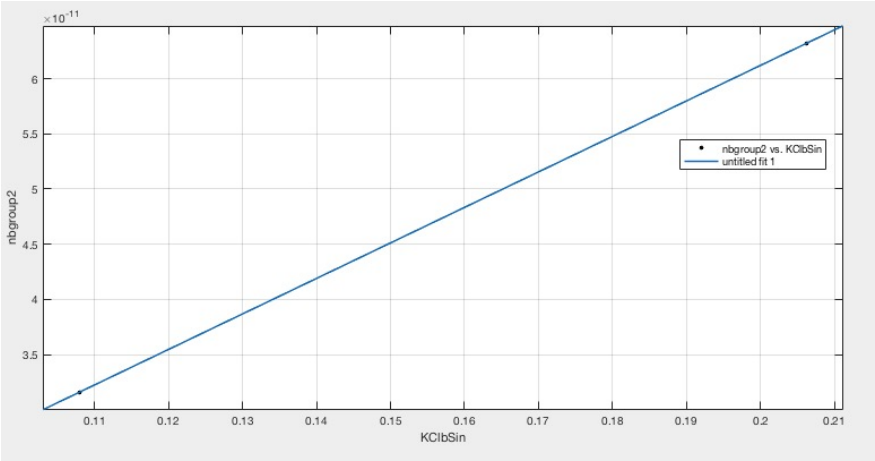

Figure 11: KCl $n\lambda/2$ vs. $\sin(\theta)$ for K_β

Linear model for KCl K_α:
f(x) = p1*x + p2
Coefficients (with 95% confidence bounds):
p1 = 3.175e-10 (3.073e-10, 3.278e-10)
p2 = -2.596e-12 (-5.167e-12, -2.456e-14)
R-square: 1

Linear model for KCl K_β:
f(x) = p1*x + p2
Coefficients:
p1 = 3.218e-10
p2 = -3.152e-12
R-square: 1

7.4 Mica

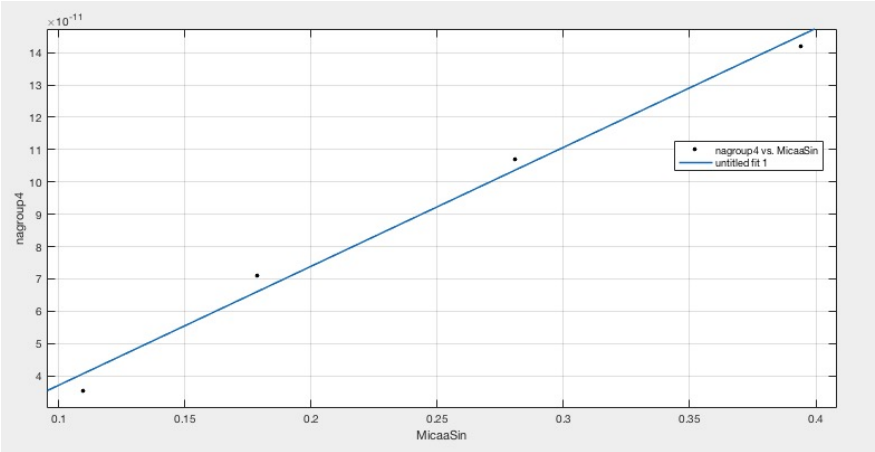

Figure 12: Mica $n\lambda/2$ vs. $\sin(\theta)$ for K_α

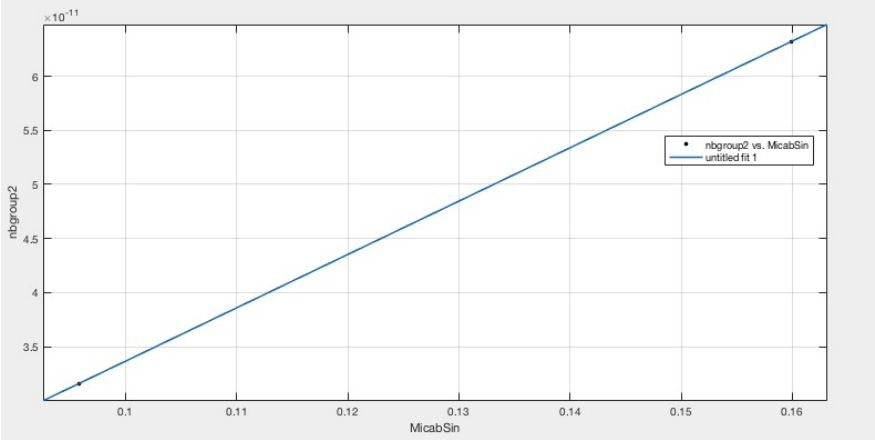

Figure 13: Mica $n\lambda/2$ vs. $\sin(\theta)$ for K_β

Linear model for Mica K_α:
f(x) = p1*x + p2
Coefficients (with 95% confidence bounds):
p1 = 3.681e-10 (2.46e-10, 4.902e-10)
p2 = 2.675e-13 (-3.193e-11, 3.246e-11)
R-square: 0.9882

Linear model for Mica K_β:
f(x) = p1*x + p2
Coefficients:
p1 = 4.935e-10
p2 = -1.57e-11
R-square: 1