X-Ray Diffraction Title

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The abstract is still a work in progress.

I. INTRODUCTION

In early 1913, proposals were put forth that it may be possible to observe diffraction due to the light wave, spin-orbit interaction in crystalline lattices in an effect which is known well known as Bragg Diffraction. In the century since, application of such physics has been applied to pioneer crystallography and metrology, and in this work we aim characterize the x-radiation of molybdenum by imaging the bragg reflection upon NaCl crystals.

The emission spectra of molybdenum observed in this work arises from the fine structure of the L shell, and subsequently the spin-orbit interaction of the electrons with x-radiation [1]. Furthermore, there exist three sub-shells, L_{I}, L_{II}, L_{III}, which are subject to emission rules:

$$\Delta I = \pm 1, \qquad \Delta j = 0, \pm 1$$

Where I is the orbital angular momentum, and j the total angular momentum, therefore, two transitions from the L-shell to the K-shell are permitted.

We aim to directly measure these by first directing electrons from a source to the molybdenum anode, bombarding it with electrons and ionizing electrons in the inner K shell. This prompts the formation of a hole which is immediately relaxed by the electrons in the upper L orbital, emitting x-radiation. Our machine operates using Bragg-Brentano geometry, such that the substrate is flat relative to the incident x-rays which are fired into a detector (see figure 1). A photon sensitive detector is equipped to orbit the sample in increments of $0.5°$. The detector sees a powder diffraction pattern, appearing as a series of rings, where brightness peaks will occur at characteristic $K_\alpha, K_\beta, K_\gamma$ lines [2].

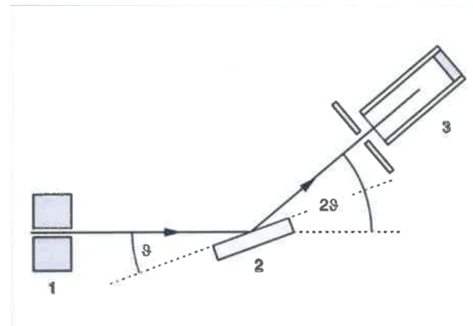

FIG. 1. Bragg-Brentano reflection geometry, where x-rays are emitted from a collimator (1), reflect off the sample (2) and are detected by the PSD (3).

II. CHARACTERIZATION OF BRAGG PEAKS

It is essential to accurately characterize the peaks in the resulting powder diffraction spectra. We accomplish this by fitting a standard gaussian function in the domain of candidate peaks. This alone is surprisingly challenging for the 5^{th} order diffraction peaks where there is severe noise in the region neighboring the K_β and K_γ peaks. Several options exist to reduce noise, namely using wider slit sizes to increase flux (results in lower resolution), and using a longer counting time (results in lower signal to noise ratio). With a similar motivation to the latter, we choose to take several scans of our sample. Because background noise is approximately white, the average between scans will result in curves that overlap about the peaks but have no discernible trend. This allows us to easily fit our peaks without the need for sophisticated techniques to isolate the background [3].

III. LATTICE RECONSTRUCTION

I would like to talk about how now we could use this reference to reconstruct a crystal lattice using Bragg diffraction, and prepare a figure of the lattice of NaCl using literature lattice spacing, or alternatively do a scan of another crystal.

IV. DISCUSSION

In this paper, we directly measure the x-ray emission spectra of a molybdenum anode and demonstrate how it

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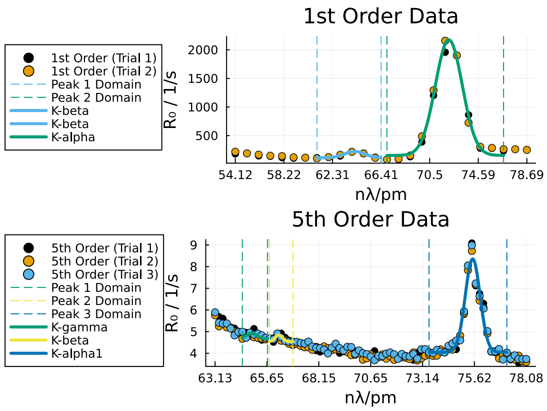

FIG. 2.

is possible to use this characteristic spectra to determine lattice parameters in unknown materials. Our parameters are found to be within 1.7% for first-order diffraction, and within 6.29% for fifth-order diffraction, when compared to literature values [4], shown in table I.

Literature notes an additional $K_{\alpha 2}$ peak neighboring the fifth-order $K_{\alpha 1}$ peak. Due to the angular resolution limitations, we were unable to image this peak, instead we observe a perceptual widening of the larger $K_{\alpha 1}$ peak. Future work on the subject would benefit from sub 0.5° angular resolution as well as a narrower collimator and longer counting times in this very narrow band.

I would like to have a short discussion about why we observe more discrepancy in 5th order data than 1st order

Type	μ	μ (Literature Value)	Order
$K_{\beta+K_\gamma}$	64.1741±0.0064	63.09	1
K_α	72.1129±0.00039	71.08	1
K_γ	64.9000 ±0.6	62.09	5
K_β	66.2100 ±0.42	63.26	5
$K_{\alpha 1}$	75.5330 ±0.037	70.93	5
$K_{\alpha 2}$	N/A	71.36	5

TABLE I. Location of exact emission peaks obtained from gaussian fits compared with literature values [4]. *Note, uncertainty is underestimated.*

Appendix A: Discussion of Precision and Uncertainty

Throughout this work, we use linear propagation theory for the propagation of error via the excellent measurements Julia library [5].

Furthermore, fitting is done using iMinuit and underlying algorithms [6].

We preform several standard statistical assessments of our data, necessary for chi-square testing. *note: information related to detector uncertainty is not yet available at the time of writing.* Goodness of fit (chi-square) parameters can be found in table **??**.

Chi-square values cannot be computed accurately until full uncertainty is understood and characterized.

[1] LD Didactic, *Title of the Manual*, LD Didactic GmbH, Location (if available) (Year of Publication), manufacturer's manual.

[2] M. Taddei, Fundamentals and applications of x-ray diffraction (2015), accessed: 2025-03-29.

[3] Wikipedia contributors, Rietveld refinement — Wikipedia, the free encyclopedia (2024), [Online; accessed 29-March-2025].

[4] D. V. Rao, Table of isotopes, edited by c. m. lederer and v. s. shirley, Medical Physics **6**, 540 (1979), https://aapm.onlinelibrary.wiley.com/doi/pdf/10.1118/1.594620.

[5] M. Giordano, Uncertainty propagation with functionally correlated quantities, ArXiv e-prints (2016), arXiv:1610.08716 [physics.data-an].

[6] F. James and M. Roos, Minuit: A System for Function Minimization and Analysis of the Parameter Errors and Correlations, Comput. Phys. Commun. **10**, 343 (1975).