Indexing of the X-Ray Diffraction Peaks of Copper

Yacine Benkirane

Eloise Chakour

Yukuan Zhao

McGill University Department of Physics

Supervisor: Prof. Kenneth Regan and Prof. Dominic Ryan

March 14, 2021

good start

8.5

nice clean abstract, no claim of structure?

Abstract

The X-ray diffraction of Copper was observed in this experiment. A k_α X-ray beam was pointed at a powder sample. The intensity of the diffraction was recorded at different angles and the peaks were fitted with a Voigt profile. The peaks were indexed using Miller indices and the five indexed peaks were found to have indices (h, k, l) of $(1, 1, 1), (2, 0, 0), (2, 2, 0), (3, 1, 1)$, and $(2, 2, 2)$. Subsequently, the lattice parameter of copper was found with a value of $a = (3.6164 \pm 0.0003)$ Å, and a goodness of fit parameter $\chi_r^2 = (2.7 \pm 0.8)$. The value of a obtained is within the known value. value?

Contents

1 Introduction

may be scattered, diffraction requires conditions be met

An electromagnetic wave encountering a disturbance will be diffracted. An interaction is observed when the size of the disturbance is of similar magnitude to the wavelength [1]. This effect can be observed by diffracting x-rays on crystals. The wavelength of the light λ, the diffraction angle θ and the inter-planar distance d are related by Bragg's Law [2]:

$$n\lambda = 2d\sin(\theta) \tag{1}$$

with $n = 1$ for crystals. The inter-planar distance d is related to the physical structure of the crystal; it is characterized by its diffraction planes, which are indexed using the Miller indices (h, k, l) [2]. Copper's crystalline structure is a face-centered cube (FCC) [3]. This lattice structure has an inter-planar distance d with indices (h, k, l) [4] :

$$\frac{1}{d^2} = \frac{h^2 + k^2 + l^2}{a^2} \tag{2}$$

where a is the length of one side of the cubic lattice, also called the lattice parameter. For a crystal with the FCC structure, the Miller indices must either be all even or all odd.

1.1 Apparatus

monochromator?

An angled x-ray tube emitting a combination of $K_{\alpha 1}$ and $K_{\alpha 2}$ radiation was aimed towards a rotating powdered copper crystal sample.

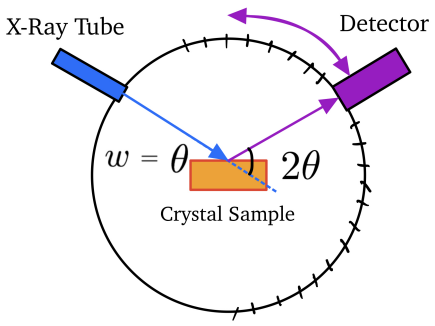


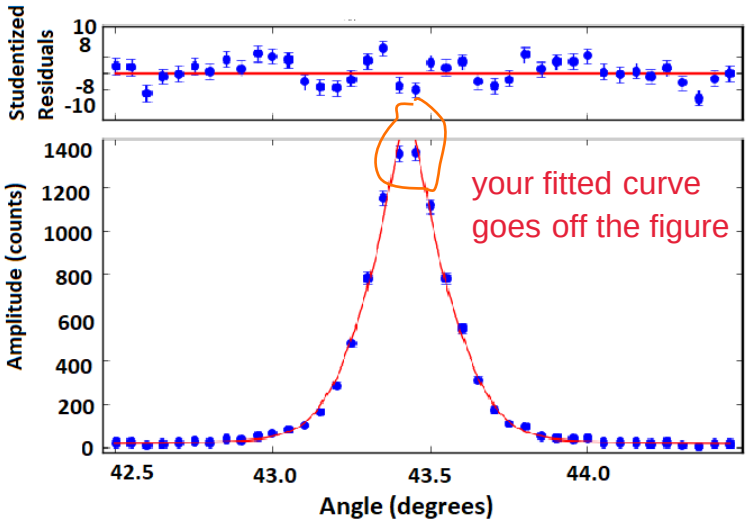
Figure 1: The detection of the waves' intensities is performed by an automated diffractometer rotating about the sample target in $\theta - 2\theta$ mode at twice the rate of the crystal's rotation ω.

it is a step-scan - not clear that you get that from this description

An automatic diffractometer, acting as the detector, measured diffracted wave intensities while rotating about the crystal from $0 - 2\theta$ at twice the crystal's rotation rate.

2 Methods and Results

To index the peaks in a pure copper sample, the intensity of the diffracted x-rays was measured as a function of their angular position. All peaks were then fit using a Voight profile with a flat background, as seen in Figure 2.



index?

Figure 2: Bragg angle fit for the left-most peak of the pure copper sample using a Voight profile with a flat background, with $\theta = (21.7136 \pm 0.0007)$ degrees and a goodness of fit parameter $\chi_r^2 = (2.6 \pm 0.6)$.

The inter-planar distance was found for each peak using Bragg's Law (Equation 1). This was done using the average K_α wavelength taken from [2]. Then, the reciprocal of the square of these values was found and their smallest common factor was computed. Dividing the $1/d^2$ values by this factor, a set of integers was obtained and used to find the Miller indices for each peak. This was done algebraically, producing the integers $(3, 4, 8, 11, 12)$. The Miller indices (h, k, l) were then assigned by inspection, according to FCC indexing with $h^2 + k^2 + l^2$ equal to these integers and were found to be $(1, 1, 1), (2, 0, 0), (2, 2, 0), (3, 1, 1)$, and $(2, 2, 2)$, listed in order from the left-most peak to the to right-most peak. show an indexed plot?

In order to obtain a value for the lattice parameter of copper, the Bragg angle was plotted

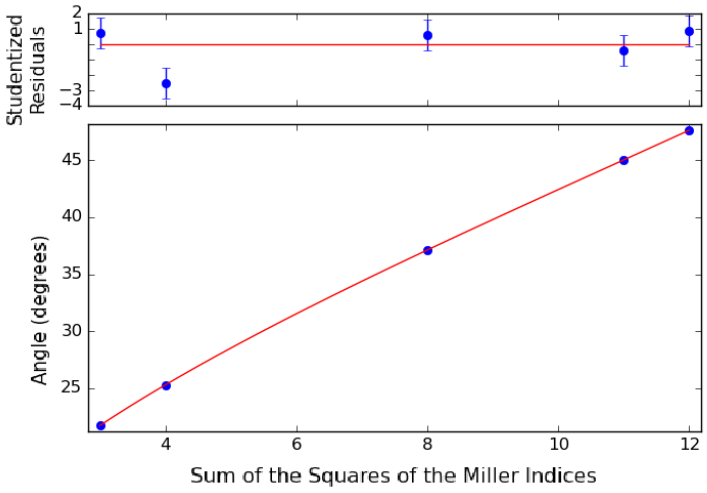


Figure 3: Bragg angles as a function of the sum of the squares of the Miller indices, with a lattice parameter of $a = (3.6164 \pm 0.0003)$ Å, with a goodness of fit parameter $\chi_r^2 = (2.7 \pm 0.8)$.

no value for "z"?

as a function of the sum of the squares of the Miller indices found. The fit function was obtained by solving for the inter-planer distance in Bragg's Law (Equation 1) and substituting this into Equation 2. This yields $\theta = z + \arcsin \frac{\lambda\sqrt{h^2+k^2+l^2}}{2a}$, where the angle z is to take into account the offset due to the zero angle point of the apparatus. The obtained lattice parameter $a = (3.6164 \pm 0.0003)$ Å, with a goodness of fit parameter $\chi_r^2 = (2.7 \pm 0.8)$, is not within error of the known value $a = (3.6146 \pm 0.0002)$ Å [5]. This is probably due to the second diffraction peak from the left, which is the only point that doesn't intersect with the fit. In fact, when examining at that specific peak, it seems to be asymmetrical and differently shaped as compared to the other peaks. We believe that this discrepancy is due to a measurement issue, which could be resolved by taking additional measurements.

use indices!

3 Conclusion

The diffraction peaks of a copper sample were indexed, and the Miller indices (h, k, l) were found to be $(1, 1, 1), (2, 0, 0), (2, 2, 0), (3, 1, 1)$, and $(2, 2, 2)$. The lattice parameter of copper was found to be $a = (3.6164 \pm 0.0003)$ Å, with a goodness of fit parameter $\chi_r^2 = (2.7 \pm 0.8)$, which did not agree with the known value. We attribute this to a shape discrepancy in one of the peaks. The goal following this experiment is to acquire more data to refine this analysis and then, to index the peaks of a pure Nickel sample, as well as a series of CuNi alloys.

4 Progress Summary

- Diffraction peaks for Cu were fit using Gaussian, Lorentzian and Voight fit functions to find the best function to use;
- Diffraction peaks for Cu, Ni and Cu25Ni75 were fit using Lorentzian functions (before the Voight profile was considered);
- Peaks for Ni were indexed using the data from the Lorentzian fit (very similar to Voight for Cu) and its lattice parameter was found - this will be redone and checked with Voight profile fits;
- Changed experiment from Drum 1 to x-ray on March 10^{th}.

5 Plan

- Refit the peaks for Ni and Cu25Ni75 using Voight profiles;
- Index the peaks from these samples and the remaining CuNi alloy samples, and find their lattice parameters using Vegard's law for alloys;
- Repeat this process for the other metals and alloys available.

References

[1] F. P. M. Bernstein, J and S. Gasiorowicz, *Modern Physics*. Prentice Hall, 2000. 1

[2] C. Kittel, *Introduction to solid state physics (8th Ed.)*. John Wiley Sons, 2004. 1, 2

[3] C. D. A. Inc. (2013) General, atomic and crystallographic properties and features of copper. [Online]. Available: https://www.copper.org/resources/properties/atomic_properties.html 1

[4] B. Cullity, *Elements of X-Ray Diffraction*. Addison-Wesley Publishing Company, 1956. 1

[5] E. A. Pasteka, L.F., "Material size dependence on fundamental constants," *Physical Review Letters*, 2019. 3