Laboratory Report

X Ray Diffraction

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Report presented for the
Advanced Physics Laboratory Course (PL 701)

School of Physical Sciences
UM-DAE Centre for Excellence in Basic Sciences
Mumbai, MH, India
November 6, 2024

Objectives:

1. To study the theory of X Ray diffraction, and use it on the given crystal (Lithium Fluoride)
2. To use different X-Rays (Copper and Molybdenum) and obtain the spectrum and hence the wavelength
3. To use a filter (Nickel for Copper and Zirconium for Molybdenum) and find out it's effects on the spectrum
4. To find out the structure of the given material (Copper).

Apparatus required

X Ray diffractometer, a crystal of Li-F, Cu and Mo metal targets, Computer for analysis and measuring.

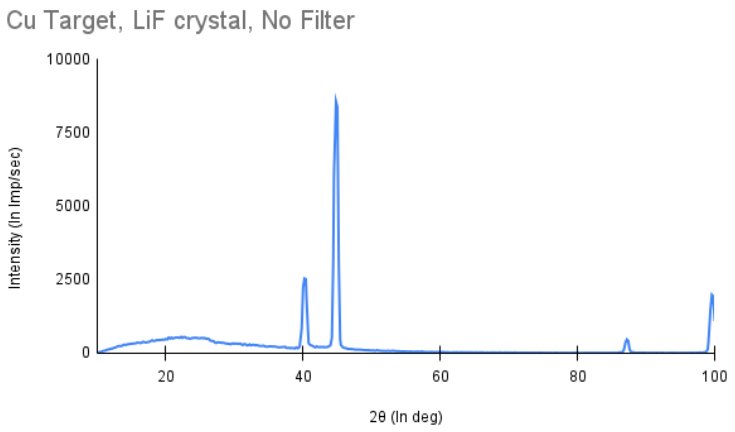
Theory

X Ray diffraction is a technique used to find atomic and molecular structures of a crystal. The atoms of a crystal, by virtue of their uniform spacing, cause an interference pattern of the waves present in an incident beam of X-rays.

Observations

Target:Copper, Crystal:LiF, Filter: None

We obtain a spectrum like this



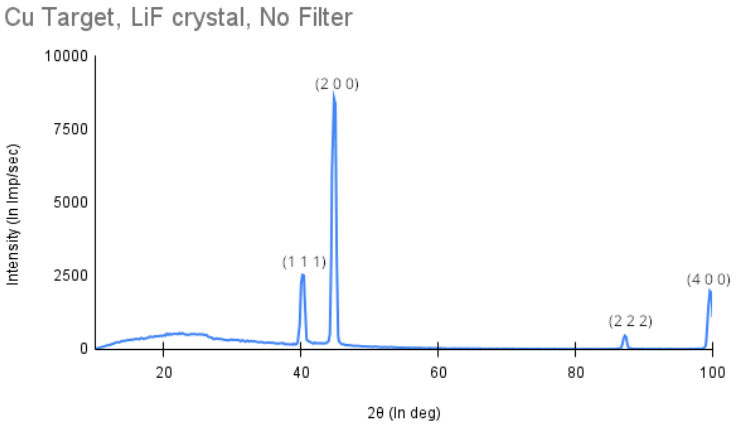
Spectrum of LiF XRD with Copper Target and no filter

We try to match it with the table given to us

2 θ	Intensity	h	k	l
38.696	95	1	1	1
44.996	100	2	0	0
65.494	48	2	2	0
78.765	10	3	1	1
82.998	11	2	2	2
99.628	3	4	0	0
112.967	4	3	3	1
117.606	14	4	2	0
139.134	13	4	2	2

2θ vs Intensity data for Lithium Fluoride

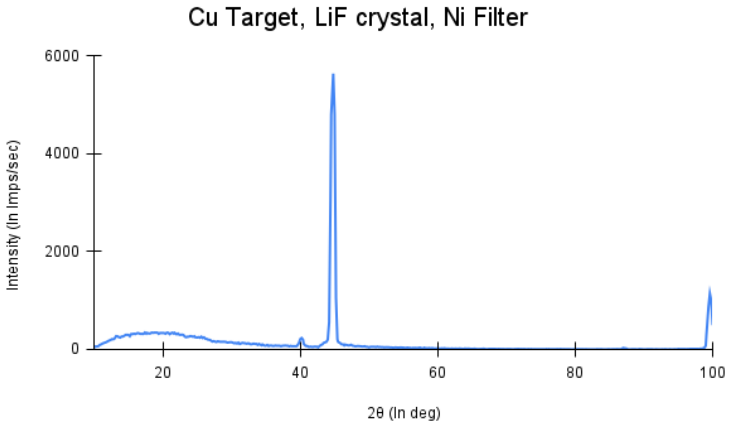
At the first thought, it seems like the 38.696, 44.996, to an extent 82.998 and 99.628 bands are visible. So we mark that.



Marked spectrum of LiF XRD with Copper Target and no filter

Target:Copper, Crystal:LiF, Filter:Ni

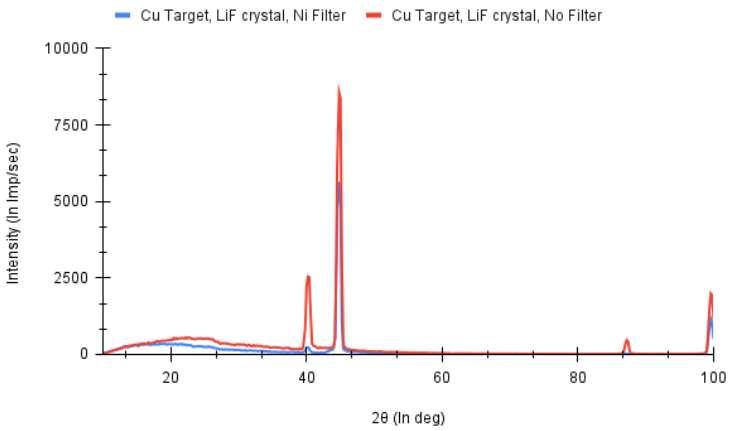
We obtain a spectrum like this



Spectrum of LiF XRD with Copper Target and Ni filter

This comes as a surprise for us as

1. There is no (1 1 1) band or (2 2 2) band in the filtered one
2. There are bands of only one kind predominant, that is the (h,0,0) type bands. We present the combined two graphs together for a better inference



Combined spectrum of LiF XRD and Copper Target, with and without filter

Inferences

- The presence of just (h,0,0) bands should imply the crystal lattice is oriented in a single direction, hence it is a mono-crystalline solid.
- We can find out the wavelength of the X-Ray with this spectrum. We know

$$2dsin\theta = n\lambda$$

We have

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

We have a to be 402 pm or 4.02 Å which is the lattice constant of LiF. Calculating the λ of the X-Ray, we get

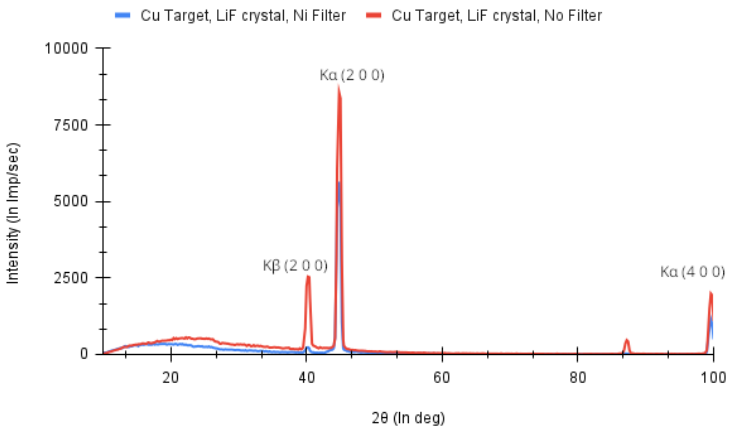
$$\lambda = \frac{2 \times 4.02 \times 10^{-10}}{\sqrt{2^2 + 0^2 + 0^2}} sin(44.8/2)$$
$$\lambda = 1.531\mathring{A}$$

The uncertainty stems up from the least count of the machine (0.2 degrees). Accounting that
λ = **1.531 ± 0.007 Å**

- So the line which we incorrectly marked as (1 1 1) was actually the K_β line, the major one being the K_α line. Doing the similar calculations for the K_β line, we get

$$\lambda = \frac{2 \times 4.02 \times 10^{-10}}{\sqrt{2^2 + 0^2 + 0^2}} sin(40.2/2)$$
$$\lambda = 1.381\mathring{A}$$

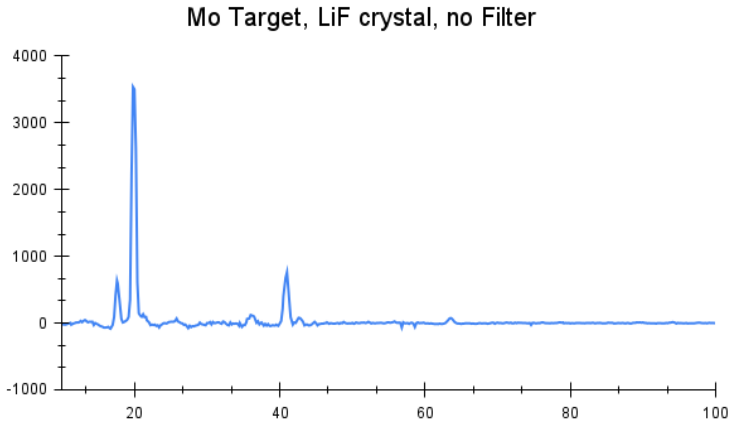
With uncertainty, λ = **1.381 ± 0.007 Å** Now finally marking both the spectrum with the correct markings



- The role of the filter is that it shunts away the K_β line, hence we get only the K_α spectrum.

Target:Molybdenum, Crystal:LiF, Filter: None

We obtain a spectrum like this



Spectrum of LiF XRD with Copper Target and no filter

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2 θ	Intensity	h	k	l
17.548	95	1	1	1
20.295	100	2	0	0
28.843	48	2	2	0
33.971	10	3	1	1
35.525	11	2	2	2
41.251	3	4	0	0
45.146	4	3	3	1
46.387	14	4	2	0
51.119	13	4	2	2

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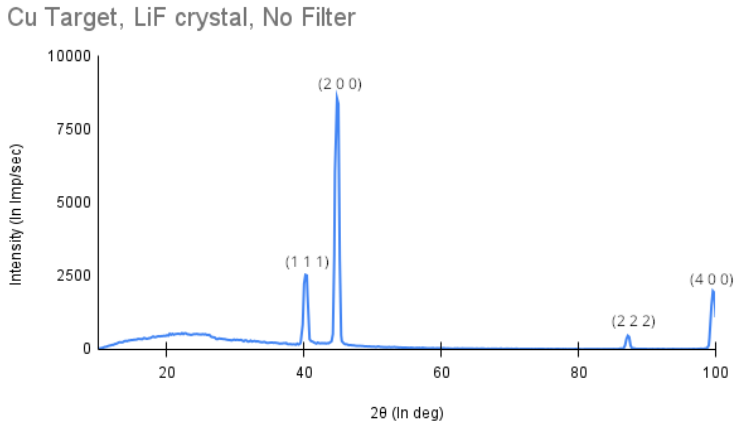

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Target:Molybdenum, Crystal:LiF, Filter:Ni

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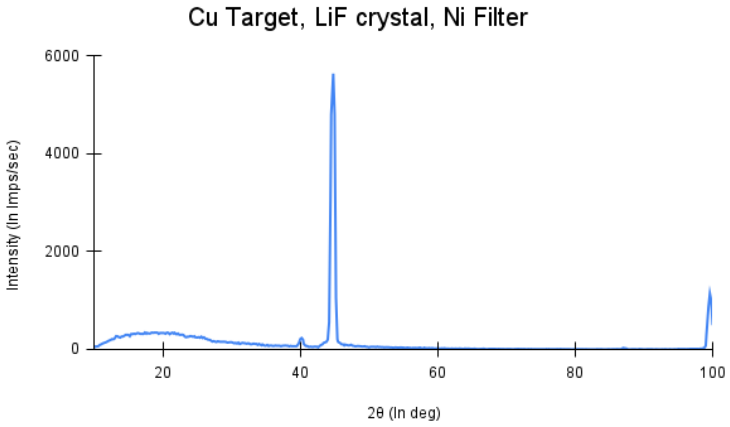

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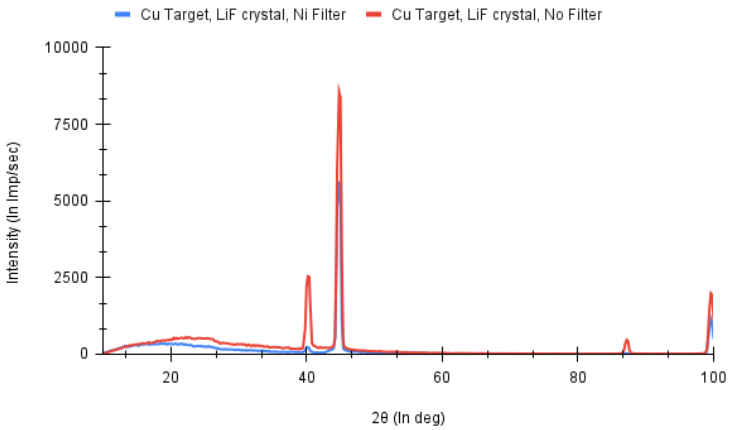

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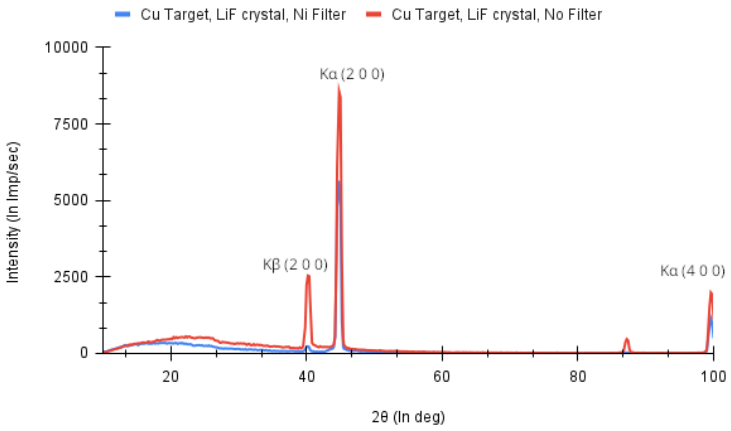

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