

# X-Ray Diffraction: Examining Crystal Structure

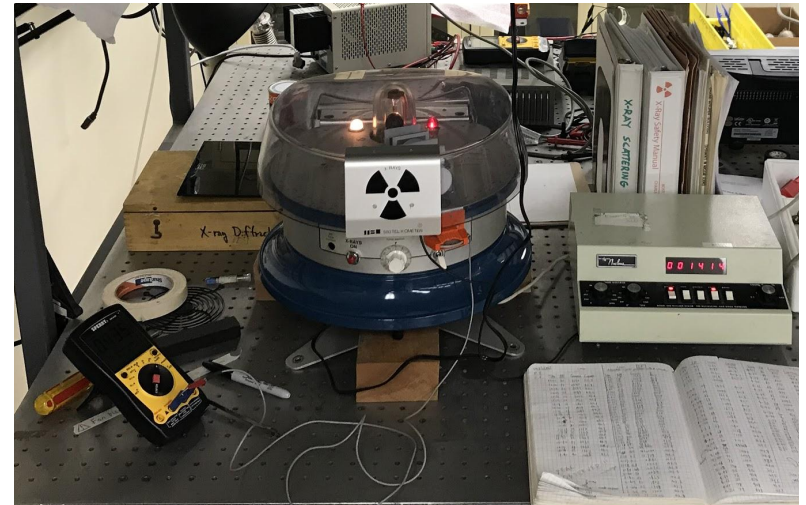
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Lab Partner: Jack Zheng

Advanced Lab Seminar: November 27, 2017

# Overview

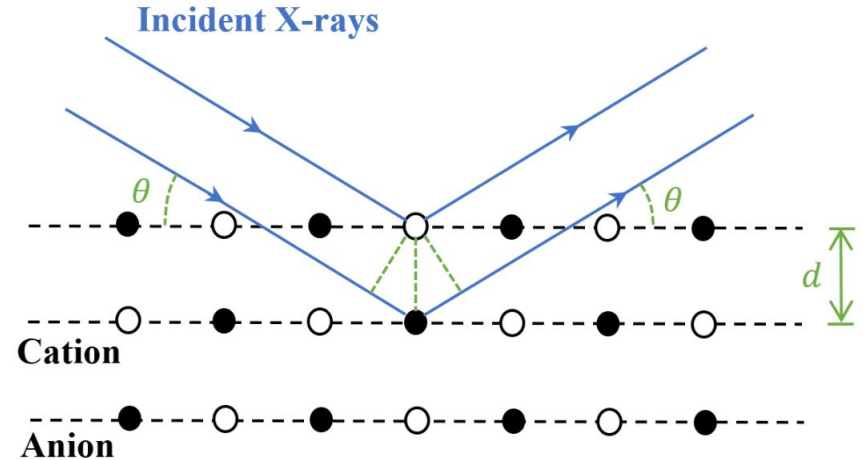
- Bragg diffraction
- Producing X-rays
- Apparatus: Tel-X-Ometer, Geiger-Muller Tube
- Procedure
- Results and Systematics
- Future Work and Improvements



# Bragg Diffraction

- Bragg Diffraction: Diffraction of X-rays on crystal lattices

$$\lambda \sim d$$



- Bragg condition describes where diffracted waves constructively interfere:

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

$$n = 1, 2, 3, \dots$$

$d$ : interplanar spacing

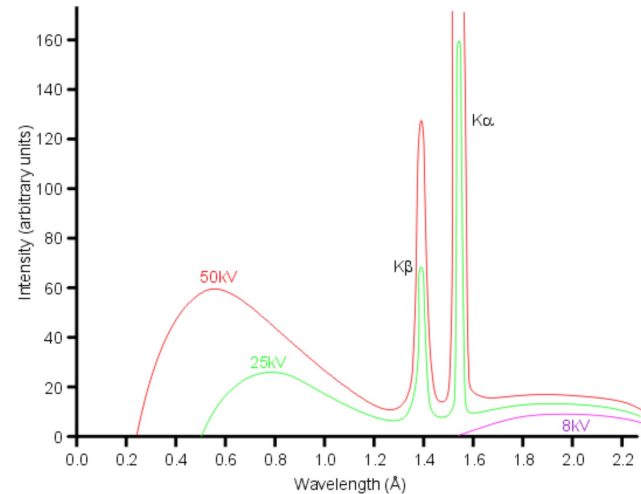
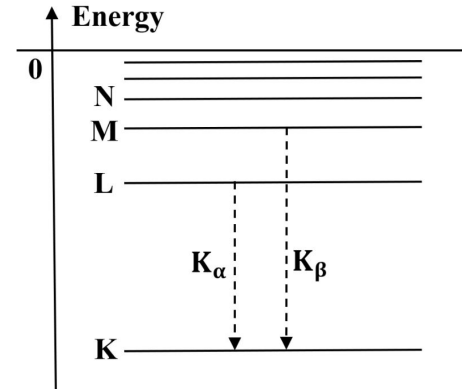
# Producing X-Rays

$$E = eV = \frac{hc}{\lambda}$$

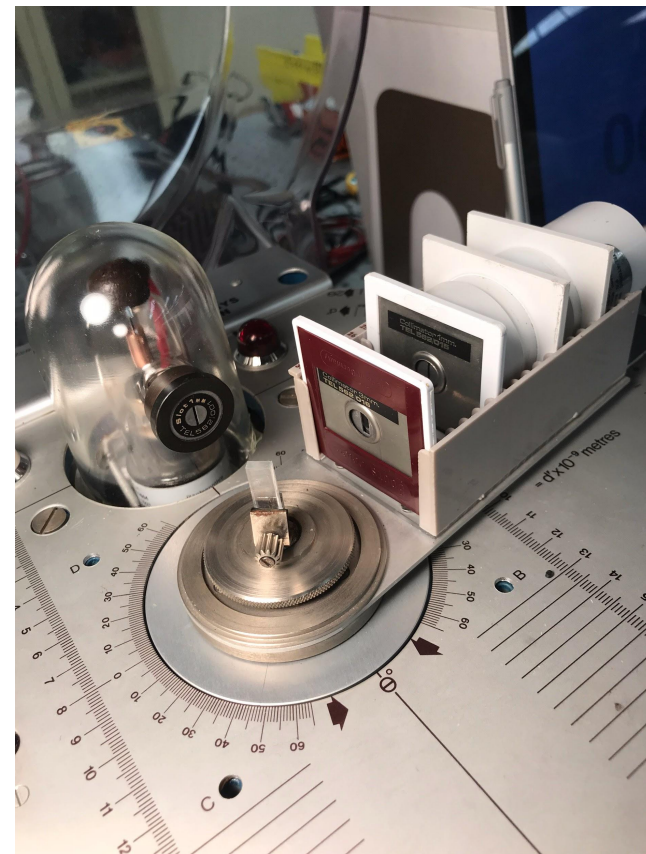
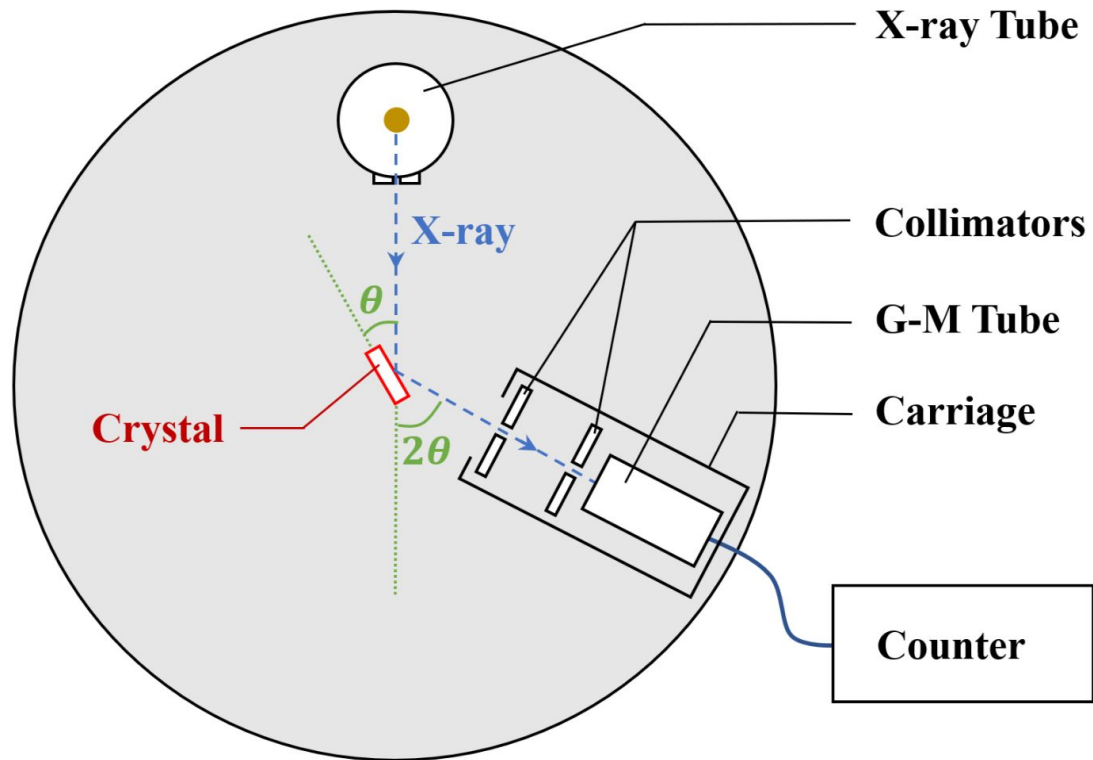
- Higher potential creates shorter wavelength photons
- Apparatus applies 30 kV to a copper source

$$K_{\alpha} = 154 \pm 1.0 \text{ pm}$$

$$K_{\beta} = 138 \pm 1.0 \text{ pm}$$

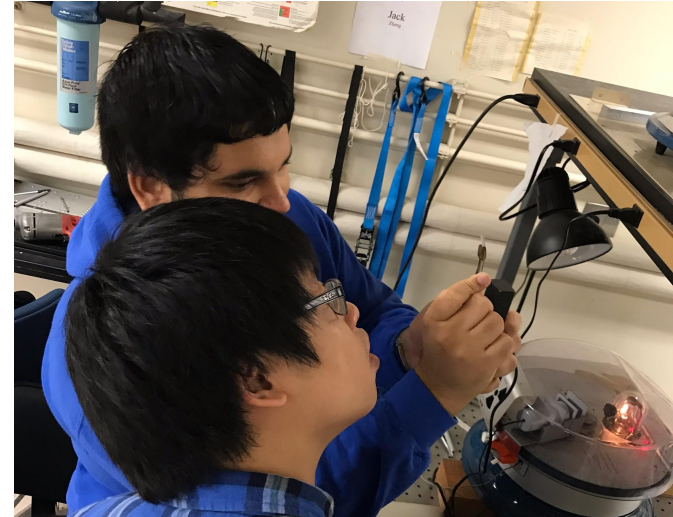


# Tel-X-Ometer Setup



# Procedure

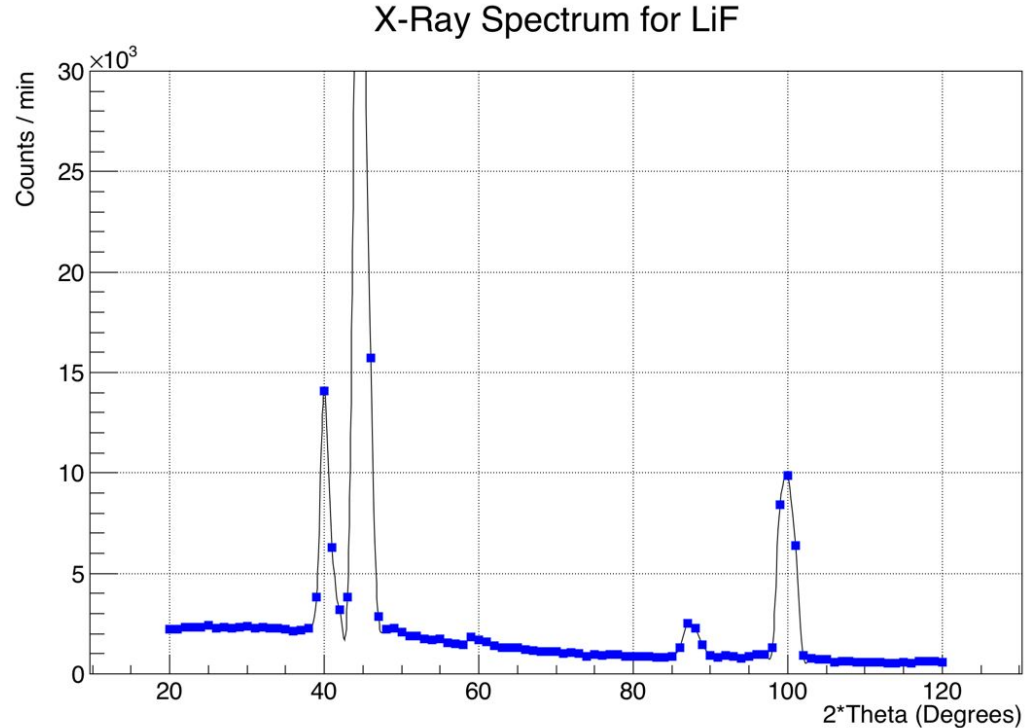
- Use a *clean* crystal: surface should be smooth and clear
- Count x-rays for 1 minute at each degree of  $2\theta$
- Check that Tel-X-Ometer does not overheat



# Results: Lithium Fluoride (LiF)

- Each peak gives value for  $d$  using Bragg equation
- $n = 1, 2$  peaks are observed
- Averaging over all values:

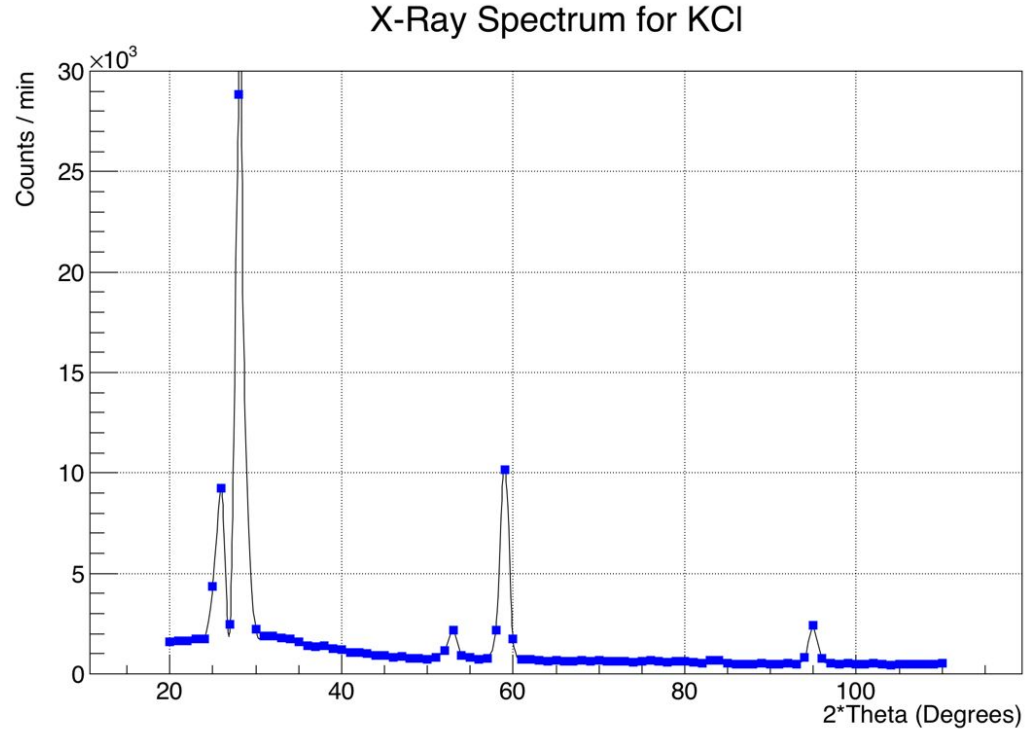
$$d_{LiF} = 201 \pm 2.9 \text{ pm}$$



# Results: Potassium Chloride (KCl)

- Each peak gives value for  $d$  using Bragg equation
- $n = 1, 2,$  and  $3$  peaks are observed
- Averaging over all values:

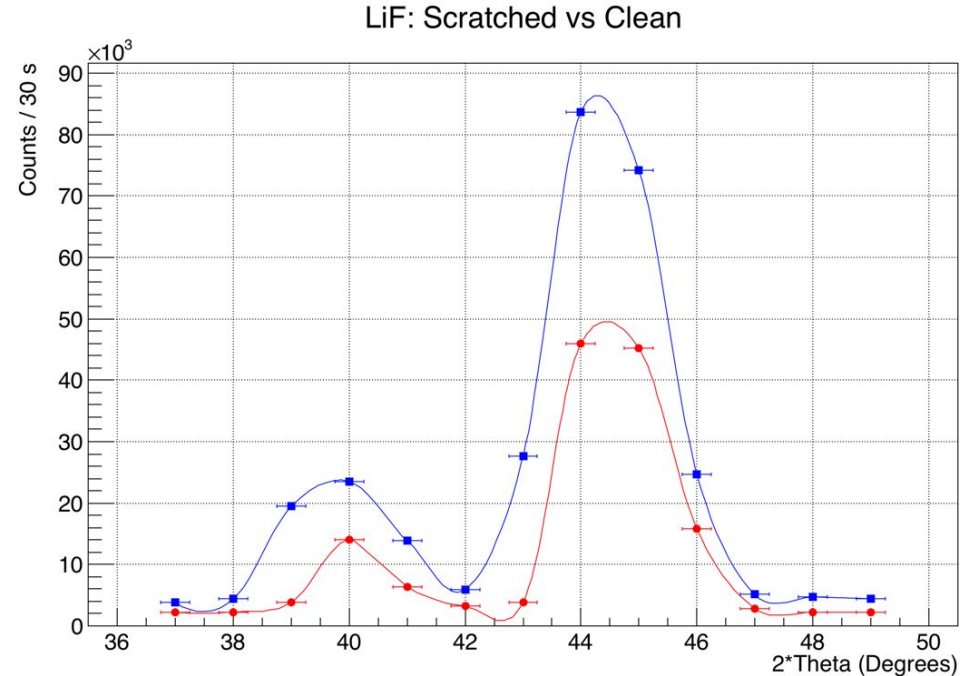
$$d_{KCl} = 311 \pm 6.4 \text{ pm}$$





# Systematics

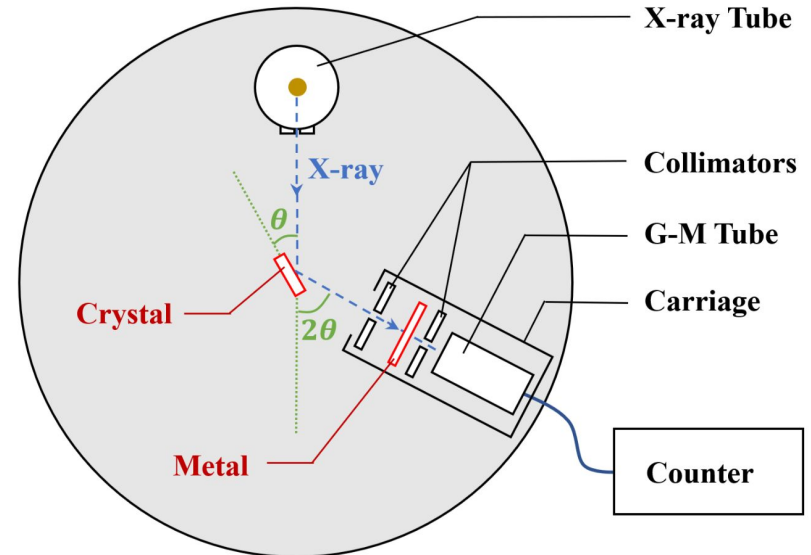
- Scratched (dirty) crystal
  - Peaks are smeared
- Operating voltage of Tel-X-Ometer and GM Tube
  - No noticeable effect
- Alignment of crystal
  - Shift of peak
- Fluctuations of counts day to day
  - Affected width of peak
  - Cause unknown: Temperature fluctuations?



Blue: Scratched Crystal  
Red: Clean Crystal

# Future Work and Improvements

- Increase resolution by reducing angular spacing
- Why do number of counts changes from day to day?
- Test metal absorption over a range of  $2\theta$  with peaks



# Acknowledgements

I'd like to give special thanks to my lab partner, Jack Zheng, and Yaokun Situ for their help with the experiment. Jack spent time outside of our regular Monday schedule to take data. Situ provided guidance, cleaned crystals, and replaced parts to ensure a smoothly operating apparatus.

I'd also like to thank Professor Larry Sulak and Dan Arcaro for checking in on our experiment, making sure we had everything we need, and giving us the opportunity to work on this experiment.

# References

R. W. James, Optical Principles of the Diffraction of X-Rays, Vol. 2 (G. Bell and Sons, 1962).

TEL-X-OMETER 580 Manual, Teltron Limited.

Instruction Manual, Oxford Instruments Inc.

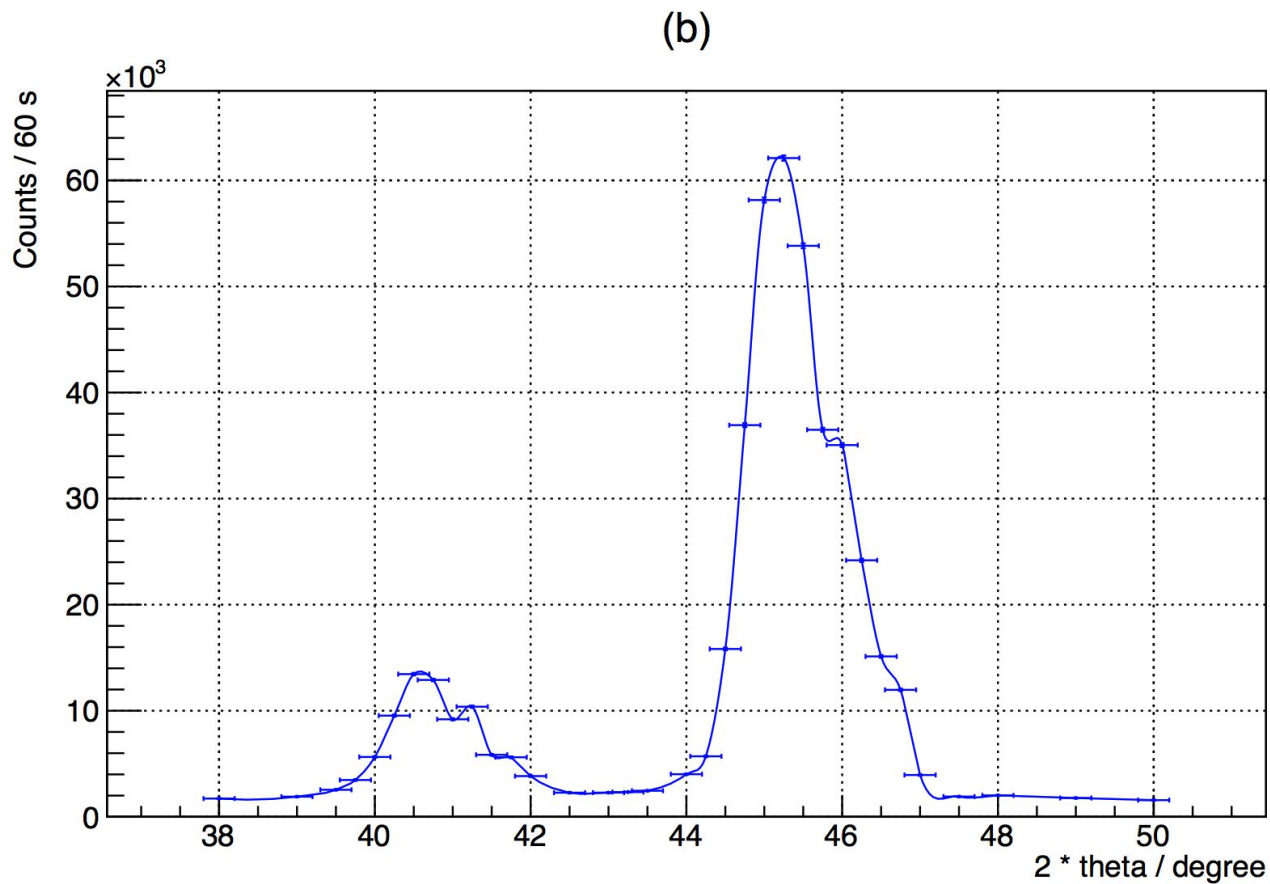
W. D. Sultan LeMarc, Navjeevan Soor, "Investigation of crystal structures and x-ray diffraction," (2012).

D. Sirdeshmukh, L. Sirdeshmukh, and K. Subhadra, Alkali Halides: A Handbook of Physical Properties (Springer Science and Business Media, 2013).

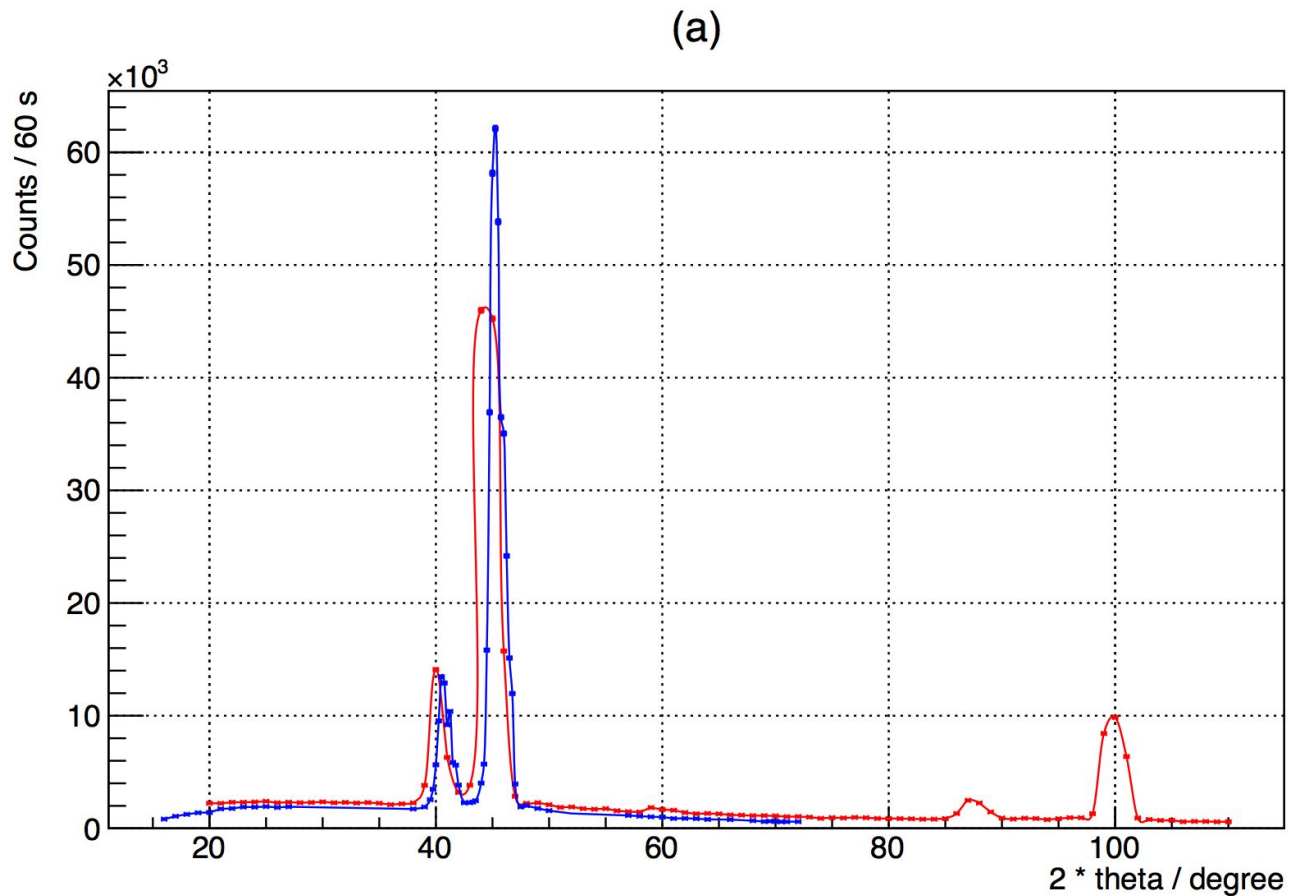
<http://pd.chem.ucl.ac.uk/pdnn/inst1/xrays.htm>

# Extra Slides

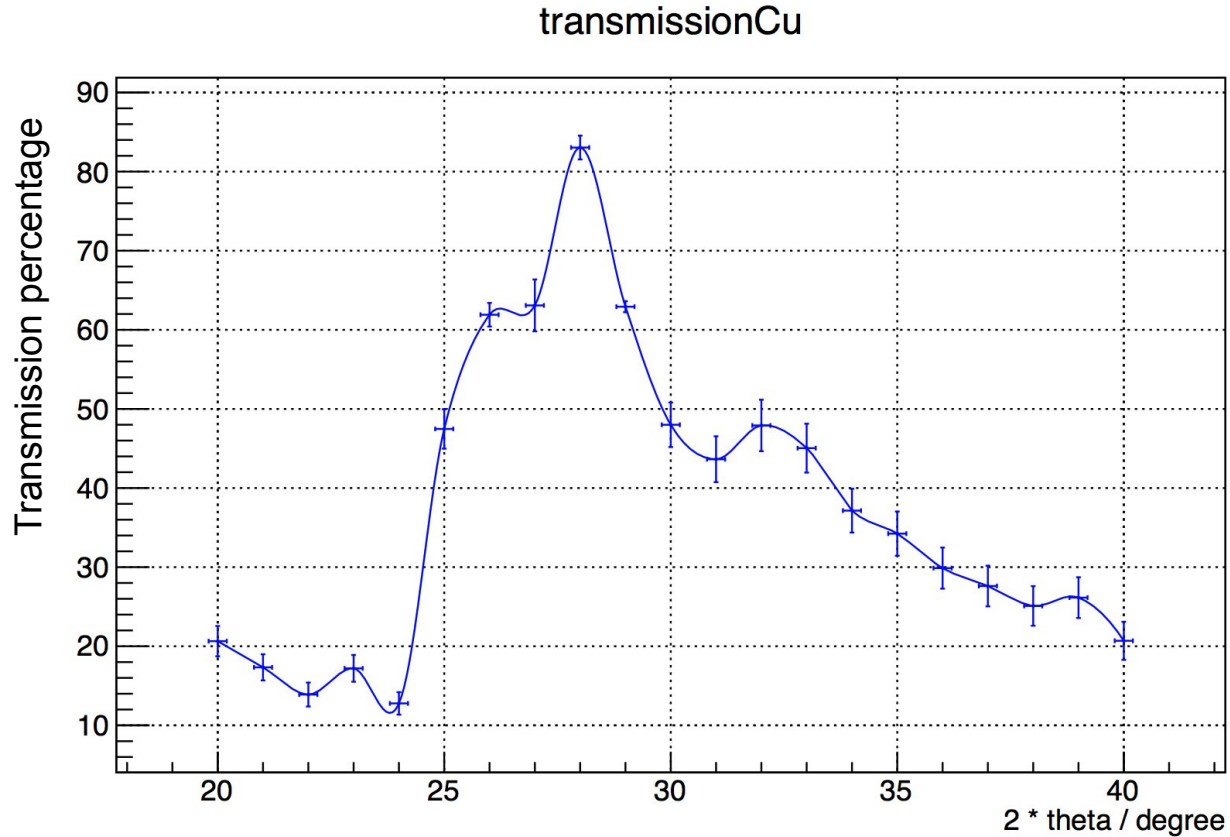
# Increasing the resolution



# Analyzing Increased Resolution



# Transmission/Absorption of Copper





# Transmission/Absorption of Nickel

