Lab Book: X-Ray Diffraction

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09/01:

- Learnt how to use the x-ray diffractometer and set up the programs
- Samples need to be analysed
    - 1 mystery sample
    - 2 Cu3Au alloys
    - CuNi and PbSn alloys

- Diffractometer parameter1 (param1 from now on) file:
    - Scantype: locked coupled
    - Scan mode : step scan
    - step size (for 2 theta): 0.05deg / 2s
    - initial 2 theta angle: 10 deg
    - final 2 theta angle: 110 deg
    - default generator: 40kV and 40mA

- Wavelength of the diffractometer that is incident upon our sample is: lambda = 0.154nm

Data Collection Step #1:

- Obtain the data for CuNi and PbSn alloys using parameter 1 set-up
    - The data we obtain from the x-ray diffractometer is: the number of x-rays incident upon the detector when the detector is at a particular angle relative to the sample.
    - We call the angle of the detector 2 theta.
    - The way in which we set up the equipment, the detector moves in increments of 0.05 degrees and counts the x-rays for 2 seconds at each position.

Data Collection Step #2:

- Collect data for the rest of the samples: 2 Cu3Au samples and 1 mystery sample with parameter1 set-up

Data Collection Step #3:

- If we need to, do another run of data collection on all samples by focusing the diffractometer to collect more data points around the peaks.

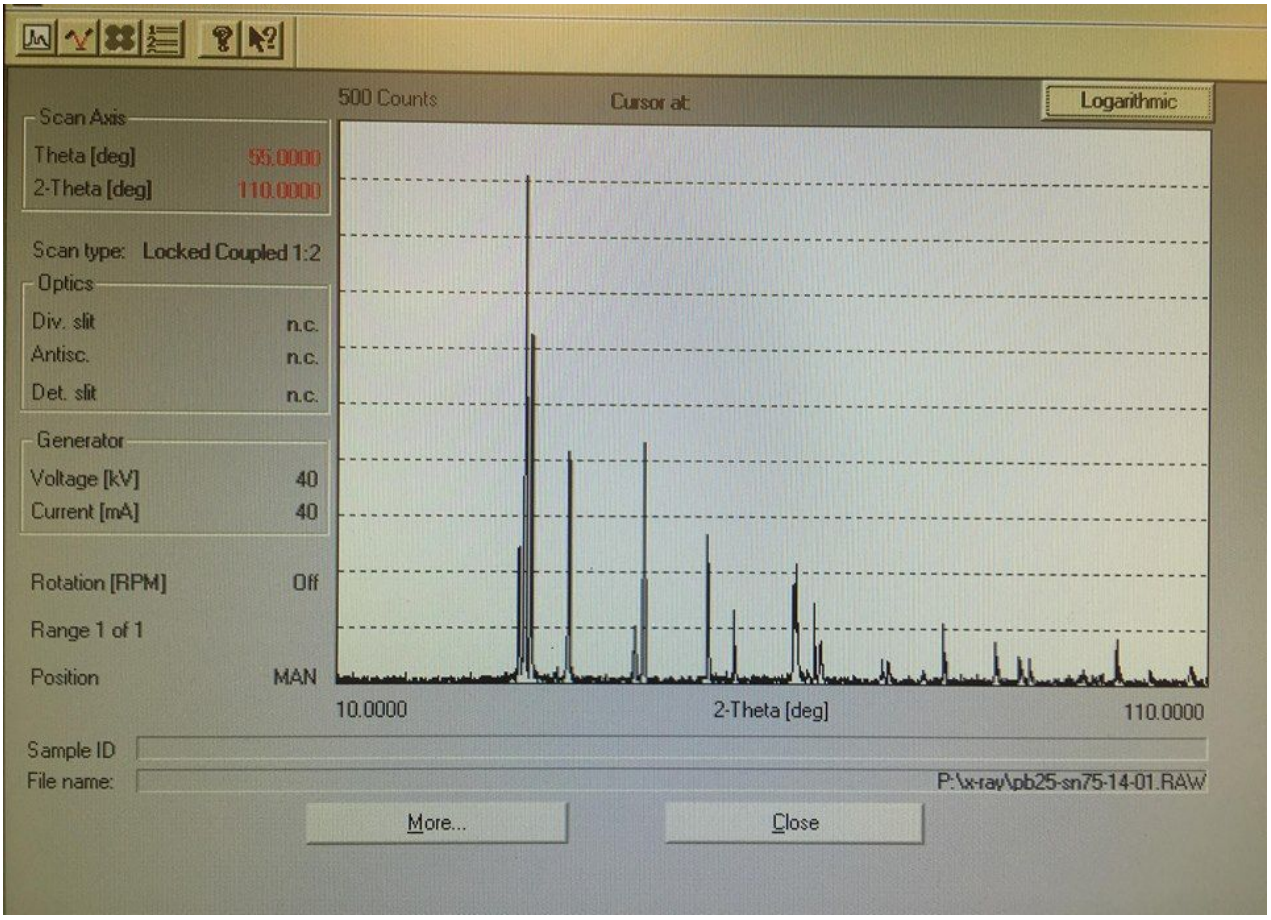
Data Analysis Step #1:

- Solve for the lattice structure of the CuNi and PbSn alloys :
    - Calculate “a”: the lattice constant
    - The data will show peaks in counts at particular values of 2*theta. From this, we can solve for “a” and for the miller indices.
- Need to get an idea of how the different concentrations of metals within the alloy reflects on the data and miller indices / lattice constants. -> place to start: plot the counts vs angle for each alloy on the same set of axes to compare.
- Starting point: conduct analysis for 100% Cu to get the code running and the fit working. (Work on automating the process for the other trials).

Samples run in the day : (using param1)

- Cu 100%
- Ni 100%
- Cu 75% , Ni 25%
- Cu 50%, Ni 50%

Example of monitoring data as diffractometer is running:



- The angle 2 theta at each peak is what we will need in order to solve for the lattice constant and miller indices.

10/01:

Samples run in the day : (using param1)

- Cu 25%, Ni 75%
- Pb 100%
- Sn 100%
- Pb 75%, Sn 25%

14/01:

Samples run in the day: (using param1)

- Pb 50%, Sn 50%
- Pb 25%, Sn 75%
- Cu3Au sample A

- Cu3Au sample B

Miller Indices and Characterisation of lattices:

Copper is FCC
Nikel is FCC
Lead is FCC
Gold is FCC

For FCC, h, k and l must be either all odd or all even to have peaks
Combinations are: 111, 200, 220, 222