PHYS 2320 Summary of Weekly Diary Entries

Remedios,Samuel (py23sr2)

Report on Week 1 Report

Progress

Week1 - This week I've done the main planning needed for the whole 8 weeks.

I've not written any code as of right now, but I've been reading the task sheet and appropriate functions so that next week when I start coding, I'll be better prepared with more of an understanding of the task.

Plan

Overall Project Plan

Week 1: Understanding the Project & Planning

- Read the task sheet and marking criteria carefully.
- Download and inspect the data files.
- Analyse the file format, metadata structure, and expected outputs.
- Create an initial project plan with clear milestones.
- Make the first weekly diary entry.

Week 2: Data Handling & Visualization

- Write Python code to read the data file and extract relevant sections.
- Generate a basic intensity / 2 theta plot with proper labels, a log-scale intensity axis, and your login name in the title.
- Identify and handle metadata extraction, including the wavelength of the X-rays.
- Test with practice datasets to ensure correct data reading.
- Update the project plan and weekly diary.

Week 3: Peak Detection & Background Removal

- Implement peak-finding using SciPy’s find_peask() or Gaussian fitting.
- Annotate detected peaks on the plot for clarity.
- Implement background subtraction if applicable. (Depends on how much noise isused)
- Test with different dataset
- Update the weekly diary with progress and any necessary adjustments.

Week 4: Peak Characterization

- Write functions to determine:
  - Peak positions (interpolating between data points if needed).
  - Full-Width at Half-Maximum (FWHM) using Gaussian fits.
  - Integrated intensity (area under each peak).
- Validate results with the practice dataset and refine the methods.
- Start adding docstrings and comments to my code.
- Update the project plan and weekly diary.

Week 5: Lattice Parameter Calculation

- Implement Bragg's law to calculate d-spacing for each peak.
- Determine the lattice parameter aa using multiple peaks.
- Calculate alloy composition
- Apply uncertainty propagation to get error estimates
- Test and refine the calculations for accuracy.
- Update the weekly diary and continue improving documentation.

Week 6: Crystallite Size Estimation & Final Testing

- Use Scherrer's equation to estimate grain size from diffraction peak widths.
- Compute uncertainties for grain size estimates.
- Run final tests with different datasets to confirm thecode is robust.
- Ensure the code has error chekcing
- Finalize the ProcessData() function to match submission requirements.
- Update the project plan and weekly diary.

Week 7: Report Writing & Code Refinement

- Start drafting the report:
  - Create a well-formatted results table.
  - Generate final annotated figures.
  - Make a flowchart explaining the structure of mycode
- Perform final tests to confirm correctness.
- Update the weekly diary with reflections on the progress made

Week 8: Final Review & Submission

- Review the report for clarity, formatting, and correctness.
- Ensure all required files are ready:
  - Python script (issid.py)
  - Report (PDF)

    - Assessment data file
- Use the coursework checker to validate the code format
- Make a final weekly diary entry summarizing mywork.

Submit everything before the March 27, 2025, deadline!!

Report on Week 2 Report

Progress

This week, I have managed to write code to fit multiple peaks with variable metadata extraction and also plot the data and the peaks fits. (3 Hours) I've written a function to determine the FWHM (1.5 Hours) and I've been struggling to plot the data with semilogx as it gives a crazy scale. Perhaps there are some boundaries I can introduce but I have not looked into that yet. There has also been some trouble reading the data file: currently I'm having to convert it into a csv before running the code as it seems to merge both columns of the .dat file into one, even when explicitly changing the delimiter to a space/tab. I am slightly further ahead than anticipated, so in Week 3, I shall attempt to incorporate the quadratic background signal, fix the log x issue as well as the initial data loading issue.

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Week 3: Peak Detection & Background Removal

- Implement background subtraction if applicable. (Depends on how much noise isused)

- Extract the wavelength of the X-rays.
- Test with different dataset
- add log axis...
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Report on Week 3 Report

Progress

I have been unable to implement the log scale as it gives a ridiculous range for the y-axis down to 1x10^-281... Removing the background noise has also been tricky, but I did manage to write a function to determine the FWHM of each peak. The code seems to work with different data sets and metadata lengths, and I am in the process of extracting the wavelength from the file. I am not sure whether I0 is the integrated intensity or not, as I used scipy.quad to manully compute the integral under each curve and it gave essentially the same result. I'll put a query in the forum and see if that is correct.

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Report on Week 4 Report

Progress

Have spent around 6/7 hours this week on removing the background intensity, and I have finally done it i think, the integrated intensities are around 1% off. FWHMs and peak positions are very accurate. Some docstrings have been added, but I urgently need to figure out how to change the y log axis as it still gives a stupid scale. I also havent extracted the wavelength from the data for calculations but this is a simple matter which i shall do next week. Next week I'll also try to calculate d for each peak and determine their respective lattice parameters.

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Report on Week 5 Report

Progress

Due to unforseen circumstances, little progress has been made this week mostly due to the culmination of other work. However, since I have finished my lab report really early this time, extr awork shall be done on tuesday next week, catching up to the correct week in the original plan.

I did manage to extend the function that skips the metadata and extracts the counts vs 2theta data, so that it now also extracts the wavelength and determines the allow composition and lattice parameter I THINK IT WORKS, I'm not sure I need to test with different files.

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Report on Week 6 Report

Progress

On track with the initial plan:

- Determined grain size, hkl values, and alloy compositions with uncertainties.
- Process data function works with the checker file; some error checking implemented (needs improvement next week).

Next week follows the initial plan, plus adding a log scale for intensity (y). The graph looks strange with noise, possibly due to the quadratic background fit—needs refinement.

Plan

Weeks 1-6: What's Done

So far, I've worked through data handling, peak analysis, and lattice/crystallite size calculations. I've:

Read the task sheet, inspected data, and planned the project.

Written Python code to read data files, extract key info, and generate intensity vs. 2-theta plots.

Implemented peak detection, background subtraction, and Gaussian fits for FWHM. Used

Bragg’s law to calculate d-spacing, determined lattice parameters, and estimated alloy composition.

Applied Scherrer’s equation to estimate crystallite size, refining calculations and error handling along the way.

(Only thing left from this is adding the log axis!)

Weeks 7-8:

Add the log axis to the plots.
Finalize code structure and improve documentation.
Put together the report with results, figures, and a flowchart.
Double-check everything and submit before the March 27 deadline!

Report on Week 7 Report

Progress

Coding is fully complete: I have spent around 5/6 hours on completing it this week **except for the comments and some docstrings**

Log-axis has been added and the plot has been changed in line with the example plot on minerva

I have noticed that the crystal size is around 10% out but my code determines that it has a large uncertainty so perhaps this is not musch of an issue. I've spent around an hour attempting to improve this.

Next week will be just putting together a high quality report and flow-chart, as I have more time because I have finished my self-guided labs a week early. This will take me around 5-6 hours roughly, maybe a little more as I haven't made a flowchart in a long time... Hopefully this project shall be completed **and** submitted by the weekend.

Plan

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Weeks 7-8:

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Report on Week 8 Report

Progress

Everything has been completed, log axis has been added and the plot formatted to look like to example. I've also added a few extra comments than I had before and used Spyder's docstring generator to give each function an appropriate docstring. The report was compiled with the Plot, tables of results and the flowchart which I made with drawio. I had trouble with calculating the some of the uncertainties, as it kept returning really high and most certainly incorrect results. However, it now returns far more reasonable results but I'm not 100% clear on whether the method I've incorporated is entirely correct. Either way I've left it as it is because I've spent far too long (~5 hours) attempting to resolve this error, in favour of submitting the coursework nice and early so that I can focus on the next Experimental lab and Physics Coursework.

Plan

Weeks 1-6: What’s Done

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(Only thing left from this is adding the log axis!)

Weeks 7-8:

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Finalize code structure and improve documentation.
Put together the report with results, figures, and a flowchart.
Double-check everything and submit before the March 27 deadline!

Report on Week 9 Report

Progress

Resubmitted a couple of times as I forgot to add a comment for the module imports at the start and also to cite a useful source which helped me understand what i had to do for the masks around the peaks to isolate them. All resubmitted - fully done :)

Plan

Weeks 1-6: What's Done

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Put together the report with results, figures, and a flowchart.
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