Please look over the homework and grading policies in the syllabus before you begin.

1 Setup

Given an unknown material and some experimental data, your job is to determine three things:

1. The crystal structure, which means lattice vectors, basis, and atomic identity.
2. The electronic gap
3. The speed of sound in the material.

You are given the following information, available at https://courses.grainger.illinois.edu/phys460/sp2021/project/index.html:

- The material was synthesized using pure gallium and pure arsenic in a quartz cell.
- An X-ray diffraction pattern. (diffracion.csv) This diffraction was performed at a wavelength of 1.6 Å.
- Resistivity vs temperature (resistivity.csv)
- Optical absorption (absorption.csv)
- An image of the material. (image.jpg)
- Heat capacity as a function of temperature (heat_capacity.csv)

2 Required sections of the project document

2.1 Revised proposal: methods section

You should revise your proposal based on anything you have learned since then (discussions with Prof. Wagner, issues you encountered when fitting). You don’t need to explain the story of how you got to your final method. The final copy must be a self-contained document that is detailed enough to be verifiable, contain correct references, and be correct.

You should explain the assumptions of that method, and develop a plan to check the assumptions of the method. Your grade will be based on whether, for each quantity, you make a section that does the following, and based on the reasoning in each section.

- Explain a plan to estimate the quantity, using the experimental data. Reference where equations come from, and any manipulations that must be done.

- Explain the assumptions of the plan. If using a model to extract the quantity, explain the assumptions of the model and what evidence you could obtain from the data or by other means to support that these assumptions are accurate.

- Explain what multiple points of comparison you could make to reinforce your conclusions. Can you use several experiments to check the consistency of your conclusions? Is there a range that you expect to obtain a priori?

- If there are unit conversions, make sure to write them down explicitly.
2.2 Execution of the plan: Results

Use your plan to compute the values of each quantity listed above. The purpose of this section is to convince the reader that the correct derived value is the value you obtained.

- Demonstrate the quality of the fit. Plots can help do this.
- Note any choices you made in the fitting procedure. People should be able to reproduce exactly your results from the information provided.
- Estimate the uncertainty in your results.

2.3 Discussion

In this section, you interpret your results.

- Do your results agree with each other, where you have multiple points of comparison, or do they disagree? Keep in mind any uncertainties.
- Do your results agree with a priori estimates from your plan?
- If there is a disagreement, suggest some reasons for it. You do not need to solve the disagreement, only note whether it exists or not.

2.4 Conclusion

Here you should summarize your results and conclusions.

- Did you get results similar to your original expectations in the plan?
- Were there any issues with the method and data obtained here that might be improved later?
- What experiments/calculations might be done in the future to improve your conclusions?

3 Suggested layout

I suggest the following layout:

- Introduction
- Lattice parameters and basis
  - Methods
  - Results
  - Discussion
- Electronic gap
  - Methods
  - Results
  - Discussion
- Speed of sound
  - Methods
  - Results
  - Discussion
- Conclusion
4 Presentation

You will need to make a 4-minute presentation during the exam period (May 7 8AM-11AM Central time). Prof. Wagner will make an upload link available the week of the exam. Your presentation should be 1-2 slides, and focus on one thing, which can be your choice of:

- A demonstration of something you’ve learned while doing the project. This can be physics-related, or methods related (fitting, etc).
- A problem you encountered and how you solved it.
- Something else related to the project that you found interesting.

If you are in a time zone significantly different from Central Time, please let me know.