Preliminary Exam Report

Student name: Sam Nittala
Student ID: 260713242

Date and time of the exam: November 18th, 2024 CE

Upon deliberation, the committee concludes that the student
_x_ passes __ fails

Rationale for the conclusion: (Please also attach the written record of the exam which includes the questions asked and comments on the quality of the responses.)

Please see attached written record, which also contains the rationale

Feedback to the student:

Keep up the great work!

Committee member name	Committee member signature
(Committee chair) Adrian Liu	
(Supervisor) Nik Provatas	
(Co-advisor, if applicable)	
(Member) Hong Guo	Digitally signed by Hong Guo Date: 2024.11.18 21:31:49 -05'00'
(Member) David Cooke	

~~**GPD signature:**~~ Department chair signature (because supervisor is GPD)

Sam Nittala Preliminary Exam

Committee: Adrian Liu (chair), Nik Provatas (supervisor), David Cooke, Hong Guo
Date: November 18th, 2024

Presentation

- Plasticity and topological defects during solidification
- Motivated what the theory needs to account for:
    - Must be able to account for equilibrium. Coexistence. Common tangent approach to get phase diagrams. Must be able to make good free energy wells
    - Solidification. Building on old theories like sharp interface model. Sharp interface models really difficult numerically. Spread out sharp interface models to get phase-field models.
    - Discussed length and timescales: nanosecond to microsecond timescales, angstrom to 10s of nanometres. But need to simulate to 100s of nm. Looking a field theory, diffusive(ish) dynamics that can make good free energy well.
    - Need to account for topological defects.
- Classical density functional theory fits the bill.
    - Went through some of the timescale and lengthscale technical difficulties.
- Paper 1. Dislocations keep showing up during rapid solidifications. Where are they coming from?
    - Discussed interface morphology
    - Dislocation Nucleation from Atomically Rough Solid-Liquid Interfaces
    - Progress thus far: When/Why does a given cusp nucleate a dislocation?
    - Also asking (in progress): Why cusps past absolute stability?
- Paper 2. Atomistic Perspective on Banding

Questions:

Nik: what do physicists call common tangent?

Assessment: Presentation was excellent, with occasional background slides inserted for the astrophysicist on the committee. Addressed many of the committee's questions that came up during the written part of the prelim.

Q&A Session

The following standard rubric was used in assessing the candidate's answers during the Q&A period:

1. *Answered the question to the committee's satisfaction without help.*
2. *Answered the question to the committee's satisfaction with some help and direction provided from the questioner or committee.*
3. *Didn't answer the question to the committee's satisfaction, even after receiving help and direction from the questioner or committee.*
4. *Didn't answer the question at all, and was not knowledgeable enough to make any reasonable progress, or exhibits a fundamental misconception about basic knowledge.*

Adrian Liu

- Q: Can you talk generally about the concept of free energy, discussing how it is useful and how it differs from the internal energy? Also discuss different types of free energy (e.g., Helmholtz free energy, Gibbs free energy, etc.), how they're defined, and how they're useful.
    - A: In an isolated system, any work that's done goes into internal energy. E.g., keeping fixed temperature, needs to account for heating. Helmholtz free energy. Etc.
    - **Score: 1**
- Q: Corresponding to which ensembles?
    - A: canonical <-> Helmholtz, etc.
    - **Score: 1**
- Q: Correlation functions. Can you define this?
    - A: <Defined correctly in terms of covariance matrices; provided intuition on this>
    - **Score: 1**
- Q: You talked about the covariance matrix as quantifying independence. Is it dependence or is it correlation?
    - A: Technically it's correlation, but most of the time in condensed matter they'll be synonymous.
    - **Score: 1**

Hong Guo

- Q: Let's look at the correlation function. This looks like a liquid to me. Why does this give you a solid? Suppose I wanted a BCC lattice, could I get it?
    - A: For simple lattices (particularly cubic lattices), it is in principle enough. The reason the liquid side says something about liquid side, it depends on the
    - **Score: 1**
- Q: Paper 2. You talked about linear stability analysis, maybe that's enough?
    - A: I won't be able to get that.
- Q: What about nonlinear amplitude stability analysis.
    - A: Not sure it'd give new analysis
    - **Score: 1**
- Q: Sharp interface…why is it a hard problem?
    - A: Still need to worry about diffusive effects.
    - A: Sharp interface models are really important because of pencil-and-paper accessibility. Phase-field theory more versatile.
    - **Score: 1**
- Q: Suppose I want to insist that you do 3D theory. What are difficulties?
    - A: Simulation timescales. Two fundamental issues. First is Fourier methods, aperiodicity. Need to simulate thick blocks in 3D, which is hard.
    - **Score: 1**

- Q: High temperature alloys, people try to make turbines, high strengths etc. How do I grow such a thing? Seems hard to do, but maybe you guys can do this? Microstructures that look like rectangles.
    - A: <Answer revolving around "this could be interesting"…pretty mature scientific discussion>
    - **Score: 1**

David Cooke

- Q: Formation of these cusps as the interface flows. Is there a type of Reynolds type number that determines whether you form these cusps?
    - A: There isn't a single number, but there is an algorithmic analysis that you can do. <Elaborates on some of those algorithmic analyses>.
- Q: The analogy of turbulence is the roughness of the front?
    - A: I'd go with the width of the Gaussian of the Fourier space correlation function.
    - **Score: 1**
- Q: <Question about vorticies in 2D superconductivity, the analogy to the curl equation N_b = b-hat.(del times sigma) . l-hat . Does the sign matter?
    - A: Yes, it tells you which way the cusps pinch.
    - **Score: 1**
- Q: The experimental goal is to eventually describe additive manufacturing. What are the experimental tools to characterize the quality of the product?
    - A: X-ray diffraction is the gold standard, X-ray transmission microscopy is the next thing. These can't be done *in situ* in real time.
    - Q: Is that true? I think there is some work.
    - A: Might not work in this solidification context.
    - Q: Can you do diffraction with electrons?
    - A: Yes, but penetration depth issues…
    - **Score: 1 (this was basically a scientific discussion)**
- Q: Why is a 2D sim representative of a 3D dislocation problem?
    - A: If it's thin, should still be decent. But there's a ~5nm-ish regime, where it's qualitatively ok, but will be off by factor of ~2. <Talked about a qualitative physical argument>
    - **Score: 1**

Nik Provatas

- Q: Quession about BCC, FCC, and how many peaks in the correlation function
    - A: <Answered some integers that seemed to be correct, and also talked about whether additional lengthscales are needed>
    - **Score: 1**
- Q: If we wanted graphene, would this be enough?
    - A: We'd need 3-pt functions
    - **Score: 1**
- Q: Is the sharp interface model correct in the limit that you're working in?

    - A: No sharp interface models are good in the limit. Just because of the atomic scale fluctuations. I can't ignore thermal diffusion and not vacancy diffusion.
    - **Score: 1 to 1.5**
- Q: Can you tell me about Gibbs-Duheim relation, and Gibbs phase rule?
    - A: Former say intensive variables can be written in terms of intensive variables. Start with thermodynamic identity, do enough Legendre transform to get potential with only intensive variables. But that must be equal to zero.
    - **Score: 1**
- Q: Relation of this to Gibbs phase rule?
    - A: <This notetaker couldn't see the board properly because the applicant accidentally blocked the board, but the manipulations seemed correct verbally!>
    - Q: And what does this give you?
    - Q & A: <Ensuing discussion about degrees of freedom, coexistence curves>
    - Q: In chemistry books we show idealized crystals. Why are vacancies the norm rather than the exception at finite temperature?
    - A: Assuming finite pressure, the entropic gain to have those vacancies is great.
    - Q: How does the vacancy concentration go like?
    - A: <Manipulations minimizing Gibbs free energy>
    - **Score: 1**

Adrian Liu

- Q: How do you know your codes are correct.
    - A: Free energy minimized in fixed box. Check it's consistent with your phase diagrams. Convergence tests to check the right dt.
    - **Score: 1**

Hong Guo

- Q: Suppose I do DFT, how do I calculate the entropy?
    - A: If you have the density matrix, just do rho log rho.
    - Q: I've got the electron density matrix, but I need the phonon density matrix.
    - **Score: 2**

Nik Provatas

- Q: Motivate relation between local temperature and velocity.
    - A: Slow case not trivial. For fast case, want Model A…<more manipulations, very confident exposition that was met with Nik's approval>
    - **Score: 1 (impressively, the derivation was slicker than the standard ways Nik and Hong knew about!)**

Overall Assessment

A very clear pass with flying colours

Recommendations

The committee recommends that the candidate keep going on the awesome trajectory he's on!