Skoltech
Skolkovo Institute of Science and Technology

Jury Member Report – Doctor of Philosophy thesis.

Name of Candidate: Mariia Korneva

PhD Program: Mathematics and Mechanics

Title of Thesis: Application of molecular dynamics simulations for the analysis of nanoscale structures

Supervisor: Assistance Professor Dmitry Kolomenskiy

Co-supervisor: Dr. Petr Zhilyaev

Name of the Reviewer: Christian Tantardini

I confirm the absence of any conflict of interest	**Date: 13-11-2024**

The purpose of this report is to obtain an independent review from the members of PhD defense Jury before the thesis defense. The members of PhD defense Jury are asked to submit signed copy of the report at least 30 days prior the thesis defense. The Reviewers are asked to bring a copy of the completed report to the thesis defense and to discuss the contents of each report with each other before the thesis defense.

If the reviewers have any queries about the thesis which they wish to raise in advance, please contact the Chair of the Jury.

Reviewer's Report

1. Brief Evaluation of the Thesis Quality and Overall Structure of the Dissertation

The thesis presents a comprehensive study on the application of Molecular Dynamics (MD) simulations to investigate mechanical processes at the atomic scale, focusing on nanocrystalline nickel (Ni) and graphene nanobubbles (GNB). The document is well-structured, beginning with an introduction to the relevance of MD in materials science and progressing logically through research objectives, methodologies, results, and conclusions. The writing is generally clear and coherent, though minor grammatical errors should be addressed to enhance clarity.

2. The Relevance of the Topic of Dissertation Work to Its Actual Content

The dissertation's topic is highly relevant to its content. It aims to improve MD simulation methodologies to accurately reproduce material properties and eliminate modeling artifacts. The research stays focused on this goal by thoroughly investigating MD simulations in two specific systems—nanocrystalline Ni and GNB-confined argon—thus aligning the actual content with the proposed topic.

3. The Relevance of the Methods Used in the Dissertation

The use of MD simulations is appropriate and effective for studying nanoscale phenomena such as grain boundary (GB) migration and phase transitions under confinement. The selection of four different models to study GB migration in Ni demonstrates a methodical approach to understanding the influence of GB geometry. The development and implementation of an automated method for

analyzing GB evolution in polycrystalline structures showcase innovation in methodology, enhancing the accuracy and efficiency of the results.

4. The Scientific Significance of the Results Obtained and Their Compliance with the International Level and Current State of the Art

The thesis contributes significant insights into the activation energy of GB migration and the behavior of materials under nanoscale confinement. The finding that polycrystalline models yield activation energies closest to experimental values, despite some discrepancies, advances the understanding of GB dynamics. The study on the melting curve of argon in GNBs adds valuable knowledge to the field of nanoconfined phase transitions. These results are pertinent to current international research efforts and reflect a high level of scientific inquiry, contributing to the advancement of materials science.

5. The Relevance of the Obtained Results to Applications (If Applicable)

The findings have potential applications in materials science and nanotechnology. Improved understanding of GB migration can inform the design of materials with enhanced mechanical properties, such as increased strength or ductility. Insights into phase transitions under confinement could influence the development of nanoscale devices, sensors, or storage systems where control of phase behavior at the nanoscale is crucial. While practical implementation may require further research, the results provide a foundational understanding that can be built upon for real-world applications.

6. The Quality of Publications

The candidate has published her research in reputable, peer-reviewed journals, demonstrating the quality and impact of her work:

1. **“Solid–liquid phase transition inside van der Waals nanobubbles: an atomistic perspective”**

Physical Chemistry Chemical Physics, 25(28):18788–18796, 2023

This journal is well-respected in the field of physical chemistry and chemical physics, indicating that the research meets high scientific standards and contributes valuable insights into nanobubble confinement effects on phase transitions.

2. **“Atomistic Modeling of Grain Boundary Migration in Nickel”**

Advanced Engineering Materials, 22(10):2000115, 2020

Published in a reputable journal focusing on advanced materials, this work highlights the candidate’s contribution to understanding GB migration, a topic of significant interest in materials science.

As a co-author, she has also contributed to:

1. **“Disjoining Pressure Oscillations Causing Height Discretization in Graphene Nanobubbles”**

arXiv preprint arXiv:2003.05423, 2020

Although this is a preprint and may not have undergone peer review at the time, it indicates active collaboration and engagement with cutting-edge research topics.

The quality of these publications reflects the candidate's ability to conduct high-level research and effectively communicate her findings to the scientific community.

7. The Summary of Issues to Be Addressed Before/During the Thesis Defense

- **Addressing Discrepancies with Experimental Data**: The candidate should provide a detailed explanation of the discrepancies between simulation results and experimental data, specifically regarding the influence of system size and grain sizes on GB migration activation energy.
- **Methodology Clarification**: More information on the validation of the methodologies used, and how metastable states and modeling artifacts were minimized or accounted for, would strengthen the thesis.
- **Automated GB Analysis Method**: Elaborating on the development, validation, and limitations of the automated method for GB analysis will provide deeper insight into its effectiveness and potential applications.
- **Extrapolation of Results**: Justification for extrapolating results obtained from argon to other van der Waals nanobubbles should be provided, supported by literature or preliminary data.
- **Grammatical and Typographical Errors**: A thorough proofreading to correct minor grammatical errors and improve overall readability is recommended.
- **Future Work and Applications**: Discussing potential future research directions and practical applications of the findings would enhance the thesis, demonstrating the candidate's understanding of the broader impact of her work.

Conclusion

Overall, the thesis is a valuable contribution to the field of materials science, offering significant insights into MD simulation methodologies and their application to nanomaterials. The high quality of the publications in reputable journals underscores the scientific merit and relevance of the research. By addressing the aforementioned issues before the defense, the candidate can strengthen her thesis and be well-prepared to discuss and defend her research findings.

Provisional Recommendation

☐ *I recommend that the candidate should defend the thesis by means of a formal thesis defense*

☑ *I recommend that the candidate should defend the thesis by means of a formal thesis defense only after appropriate changes would be introduced in candidate's thesis according to the recommendations of the present report*

☐ *The thesis is not acceptable and I recommend that the candidate be exempt from the formal thesis defense*

Tantardini Christian