
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: Assistant Professor Dmitry Kolomenskiy

Co-supervisor: Dr. Petr Zhilyaev

Name of the Reviewer: Professor Oleg V. Vasilyev, Skoltech

I confirm the absence of any conflict of interest

November 15, 2024

Reviewer's Report

Brief evaluation of the thesis quality and overall structure of the dissertation:

The objectives of this dissertation are to develop a molecular dynamics model capable of producing grain boundary migration energy values consistent with experimental observations and avoiding metastable states during phase transitions in Van der Waals heterostructures. The developed approach has been implemented within the LAMMPS simulation software package and applied to study multiple mechanisms affecting grain boundary migration energies. These mechanisms include the effects of triple junctions, the distribution of interstitial atoms, the possible occurrence of metastable states, the influence of impurities, the mutual orientation of grain boundaries, and the choice of potential used in molecular dynamics simulations. The computationally obtained migration energy is consistent with experimental measurements. Additionally, the study revealed a novel semi-liquid state of trapped argon (Ar).

The scope of the dissertation is comprehensive, addressing a wide range of relevant problems. Except for the abstract and conclusion (summary) sections, the dissertation is well-written and well-organized.

The relevance of the topic of dissertation work to its actual content:

The topic of the dissertation accurately reflects its content.

The relevance of the methods used in the dissertation:

The primary method employed in the dissertation is Molecular Dynamics simulation, implemented using the LAMMPS software package. Additionally, custom Python-based codes were developed to analyze the results and post-processing, while OVITO software was utilized for visualization, preprocessing, and generating atomistic structures. All methods were appropriately chosen, effectively complementing one another and forming a cohesive and comprehensive research framework.

The scientific significance of the results obtained and their compliance with the international level and current state of the art:

The main scientific significance of the dissertation lies in developing a molecular dynamics simulation approach capable of accurately predicting grain boundary migration energy and modeling phase transitions within Van der Waals heterostructures with significantly enhanced computational efficiency. The methodology is built on

the state-of-the-art LAMMPS simulation software package, which is widely used by the research community for molecular dynamics simulations.

The relevance of the obtained results to applications (if applicable):

The methodology developed in this dissertation holds significant practical value, as it can be applied to predicting the properties of polycrystalline materials across a wide range of temperatures and pressures, as well as under external influences such as temperature fluctuations, deformation, electromagnetic fields, and more. The methods and results presented in the dissertation provide a solid foundation for future research into polycrystalline structures and nanobubbles, including various 2D materials such as hexagonal boron nitride, molybdenum disulfide, tungsten diselenide, and others.

The quality of publications:

The quality of the publications is very high and meets the graduation requirements, with all three papers published in WoS-indexed journals.

The summary of issues to be addressed before/during the thesis defense:

Below is the list of major suggestions to incorporate to the PhD dissertation:

- The Abstract should be rewritten to provide a clear and comprehensive overview of the dissertation, including its goals, methodologies, and key findings. It should be logically organized and explicitly state what was studied. In essence, it should give the reader a solid understanding of the dissertation's content, which is not easily achieved in its current form. Furthermore, the abstract should be written in the third-person perspective, as the use of "we" is inappropriate in this context. Lastly, the use of abbreviations in the abstract is highly discouraged and should be limited to cases where the phrase appears multiple times.
- The dissertation lacks a dedicated Conclusion section. I strongly recommend adding one or renaming Chapter 6 to "Summary of Main Results and Conclusions." The Conclusion should offer a comprehensive discussion of the research findings, with an in-depth, systematic, and logically organized analysis for readers who have reviewed the entire dissertation. The Conclusion should address which aspects or properties were studied, highlight those found to be more or less significant, and note any that had minimal influence. Given the comprehensive nature of the research, the Conclusion should reflect this depth and feature a clear, well-organized structure that is easy to follow. Simply listing the main findings without synthesizing the results leaves an impression of superficiality. Considering that the author has invested four years in this dissertation, the results should be presented logically and cohesively, rather than simply listing the findings.
- The use of "we" in the body of the dissertation is somewhat unusual. This likely originates from co-authored papers, where "we" is appropriate. However, since the dissertation reflects the work of a single individual, using "we" may feel awkward. I recommend rephrasing sentences that include "we" to adopt the third-person perspective.
- Many equations in the dissertation are numbered but never referenced. Equations that are not referenced in the text should not be numbered. For example, none of the 57 equations in Chapter 2 are referenced in the body of the dissertation, which is highly unusual. I recommend revising the flow of discussion to reference the equations where relevant and removing the numbering from equations that are used solely for intermediate derivations.

These major issues are critical and need to be addressed in the final version of the dissertation.

Below is the list of minor suggestions to incorporate to the PhD dissertation:

- When writing scientific papers or reports, the use of emotionally charged words (e.g., nice, great, good, tricky) is highly discouraged. Science is quantitative, and the language used in a scientific paper or dissertation

should reflect this.

- Starting sentences with "And" is not good style. I recommend restructuring such sentences.
- On page 49, Figure 3.8 is referenced only once after Figure 3.1. It should be moved to appear before Figure 3.2.
- On page 70, there is a missing space between "Figure 4-4" and "shows."
- References to figures are inconsistent throughout the dissertation, with three different styles used: "Figure," "Fig.," and "fig." The author should select one style and use it consistently.
- The notation for subfigures is inconsistent across labels, captions, and references in the text. Variations such as ".a," "(a)," and "(A)" are used. The author should choose one notation and apply it consistently.
- The dissertation contains numerous spelling errors, such as "dynamincs", "dimentional", "properites", "heterostrucutres", "imperically", "inversily", etc. I recommend running the dissertation through a spell checker to address these issues.
- The dissertation requires reformatting to address excessive half-empty pages. New pages should only begin with a new chapter, while subsections should continue without page breaks.

These minor issues are not critical and do not affect the overall quality of the dissertation. I leave it to the author to decide whether to incorporate them into the final version.

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.