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: Dr. Nikolay Kondratyuk

I confirm the absence of any conflict of interest	**Date: 12-11-2024**

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

The quality of the thesis is of excellent level. The thesis is well structured: review, theoretical part, methodology, results and discussion are presented in separate chapters. The overall structure and logics of presentation help to understand the key ideas, the bottlenecks of this study and to switch from the description of computer experiment to the theoretical proof of the relevance of used formulae and approaches for both polycrystalline structures and nanobubbles studies.

The topic of dissertation corresponds to the methodologies and results obtained in this work. In the framework of this research the main method was Molecular dynamics simulations and the objects of investigation – polycrystalline structures and nanobubbles formed by Van der Waals heterostructures, both having characteristic sizes of several to hundred nanometers. The systems of such sizes have outstanding properties; therefore, it is worth to be emphasized. Also, the author has developed the automized approach for the analysis of grain growth as an additional module for the OVITO software.

In the framework of this work, the novel approaches were used to investigate grain boundaries' migration and phase transition of the substance inside graphene nanobubbles. Also, the obtained result for the

graphene nanobubble was firstly mentioned – a novel state of the trapped substance was detected. The methods are up-to-date and are commonly used on the international level. Thus, the research complies with the international level and current state of the art.

The obtained results could be applied for the development of multi-scale methods for the materials properties prediction, especially, from the atomistic level of description. The atomistic level of modeling, considered in the PhD thesis, allows to obtain the grain boundary migration energies of polycrystalline structures. Combined with the experimental investigations (Electron backscatter diffraction, which provide limited data) and theory, the results of M. Korneva should be used for the better understanding of the grain growth in polycrystals.

The results of the study are published in 2 scientific papers of excellent quality in Physical Chemistry Chemical Physics and Advanced Engineering Materials. The journals are indexed by the international citation systems Scopus and Web of Science. Also, the paper on the graphene nanobubles is presented on the arXiv website and still is not published in the peer-reviewed journal.

The summary of issues to be addressed during the thesis defense is the following:

1) Has the author considered the dependence of the migration energy on pressure (or density of phases) during the simulations? Also, the clearer conclusion on the results for different interatomic potentials should be provided during the defense.

2) How does the phase diagram of argon depend on the pore size and shape of the confinement? Could the h/r ratio replace pressure for the correct determination of the phase diagram of argon trapped in graphene nanobubble? Or it should be considered as independent additional variable for the phase diagram?

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*