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. Max Hodapp

I confirm the absence of any conflict of interest (Alternatively, Reviewer can formulate a possible conflict)	**Date: DD-MM-YYYY**

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

Reviewers report should contain the following items:

- Brief evaluation of the thesis quality and overall structure of the dissertation.
- The relevance of the topic of dissertation work to its actual content
- The relevance of the methods used in the dissertation
- The scientific significance of the results obtained and their compliance with the international level and current state of the art
- The relevance of the obtained results to applications (if applicable)
- The quality of publications
- The summary of issues to be addressed before/during the thesis defense

The thesis is devoted to the development of molecular dynamics simulations for two topics: 1) grain growth in metals, and 2) evolution of nanobubbles in Van der Waals heterostructures. The two topics are rather different which makes it difficult to assess the thesis as a whole. My comments below mostly revolve around 1) because I am not an expert on 2).

The work on grain growth is devoted to the development of an algorithm that computes the grain boundary migration from atomistic simulations of polycrystalline structures, and compares the results to experiments. I very much enjoyed reading this part and I expect that this algorithm can become very useful in the future as atomistic simulations are more and more approaching more realistic length scales so that results can be compared to higher-scale models or experiments.

Overall, the thesis is mostly well written and the storyline is clear, although the two topics could sometimes be separated a bit better (see my comments at the end). There have been two publications in Q1 journals on each of the two topics; another one is still on arXiv. The proposed methodology advances the state-of-the-art and I therefore consider the PhD candidate as eligible to defend her thesis after the following issues have been addressed.

- one point that appears not to be discussed at all is the difference in time scales between the simulations (nanoseconds) and experiments (minutes). This must be discussed more in-depth, in addition to possible implications on the results.

- While the developed methodology is independent of the interatomic potentials, it is necessary to assess whether improvements are expected when replacing the EAM potential with a more quantitative potential (like machine-learning potentials). For example, are there material properties (e.g., defect energies) that are not sufficiently well captured by your Ni potential that could hint towards errors in the large scale simulations?

- Section 3.2.5 is very confusing because the results are not discussed at all although there is a huge difference in the migration energies as presented in Table 3.2. There is also no discussion on diffusion properties of Cu in Ni, and whether the simulation setup is able capture such effects. Some discussion suddenly pops up in Section 6, but on Al. What is the relation to the Cu-Ni system you studied?

Minor comments:

- Sometimes I got confused while reading because you are talking about grain boundaries, and then suddenly switch to nanobubbles, In particular, in Chapter 1, it was not clear to me whether the two topics are connected, or not. Same in Chapter 6: first you talk about grain boundaries, then about nanobubbles, and then again about grain boundaries, without separating the two topics.

- Also, for me, as a non-expert on Van der Waals heterostructures, the global picture of this topic could have been presented better, like why are these materials interesting, what properties can you achieve, and how does your work fit in?

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*