

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: Alexander Kvashnin

| | |
|--|-------------------------|
| I confirm the absence of any conflict of interest (Alternatively, Reviewer can formulate a possible conflict) | 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

Thesis is well structured, it contains an Introduction section, Background, which is basically the literature review in this field of study, and the rest of sections are devoted to results. The main part of the thesis is devoted to investigation of polycrystalline structures by using molecular dynamical approaches. Section 5 differs from the main part with the only common lying in applied approach for simulations.

Content of dissertation is relevant with the topic and the title of the thesis. Applied methods represent the modern methods for simulations of complex structures like polycrystals, and they are widely used in atomistic simulations.

The scientific significance of the work lies in the study of non-single crystal structures, in contrast to the majority of work devoted to atomistic modelling. This is important because real materials are usually synthesized in non-crystalline form. Understanding the behaviour of physical properties of materials as a function of geometrical and structural parameters is an important direction of investigation.

The presented results are performed at a good scientific level and published in good journals belonging to Q1 and Q2 quartiles.

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