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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. Vasily Pisarev, leading research fellow, HSE University

I confirm the absence of any conflict of interest (Alternatively, Reviewer can formulate a possible conflict)	**Date: 14-11-2024**

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

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

Maria Korneva's PhD thesis is devoted to atomistic modeling of nanostructured materials. The dissertation is well structured, describing motivation, background of the problems, then methods, then providing results for nanocrystalline metals, then for graphene nanobubbles, and ending with conclusions. The topic of the dissertation reflects well the actual problems considered therein. The methods are appropriate for the modeling of nanoscale objects, and there is also comparison between molecular simulations results and the classical elastic theory for nanobubbles pressure, confirming that results are self-consistent. The results are important for the theoretical understanding of the nanostructured materials. In particular, the phase diagram of nanobubbles shows interlinked nature between size, pressure and temperature at phase transition. The results correspond to the current state of art in the area of nanocrystal and low-dimensional materials modeling by classical molecular dynamics. The main results are published in 2 peer-reviewed papers in high-ranking journals.

There are several comments on the dissertation contents and text, which are summarized below.

1. Page 27, last bullet:

It is said that other time integrators can be used, such as RK, multistep, Gear's method, SHAKE and rRESPA.

Out of those:

- SHAKE is not a time integration algorithm. Rather, it is algorithm to apply constraints on distances between certain particles and/or angles

- RK, multistep and Gear's methods, although used for general-purpose differential equations, are not used nowadays in MD simulations, as they are non-symplectic and lead to energy drift in long simulations.

Only rRESPA is a time integrator that is used in practice alongside Verlet algorithm.

Also, it appears that citations are missing in that paragraph.

2. Page 35.

It is written that the LJ potential describes dipole-dipole interaction. That is not correct, as (a) the dipole-dipole interaction energy scales as r^{-3} at large distances and (b) LJ potential includes repulsive term. The correct formulation must be that it combines interaction of fluctuating atomic dipoles at large distances and core repulsion at short distances.

Further, it is written that «Lennard-Jones … showed that powers 6 and 12 in general better describe such potential», which is incorrect. The power 6 comes from the London's theory of atomic interaction, and the power 12 is purely for convenience of calculation.

3. Section 3.2

Although the assumption that «main reason for such discrepancy (between experimental and computed GB migration barriers) is the size of the modeled system as well as the sizes of grains» seems plausible, there is no attempt of its verification. Potentially, the systems with different grain sizes could be simulated for at least one of the investigated temperatures, which would do some evidence in favor or against that assumption.

4. Section 5.2

It appears that the size of the nanobubble is uniquely linked to the melting temperature and pressure. If so, it would be reasonable to add another projection of the phase diagram, in the coordinates temperature-bubble radius (similar to the T-V projection of bulk phase diagrams).

5. Section 5.3.

The goals and results for this chapter are not clearly stated. In the Conclusions for Section 5, it is stated that «The results of MD simulations of pancake-shaped bubbles are in correspondence

with the membrane theory». However, no theoretical results and no explicit comparison between the theory and simulations are provided. Either Section 5.3 must be complemented with proper comparison, or removed from the thesis.

There are some typos in the text, listed below:

Page 15: «The MD modelling of Graphene nanobubble differs by its accuracy...» - «stands out by its accuracy» is more correct

«make calculations shorter but not to loose in quality» - «make calculations shorter without losing in quality»

Page 16: First bullet: «polycrystalls» - «polycrystals»

Page 20, last line: «bicrystalls» - «bicrystals»

Page 32, Eq. (2.18) — must have $F_i(t)$

Also, the numerical scheme is typically called «velocity Verlet» to distinguish from the «coordinate Verlet» algorithm which used coordinates on two previous time steps to propagate in time and does not use the velocities per se.

Page 32, last paragraph: missing citation.

Page 35: missing table reference

Page 52: in $d_{cutoff} = 10$, the measurement units are not provided

Page 70, Fig. 4-3 caption: «grain determination» - «grain identification»

Page 77: Poisson's ratio is missing after Eq. (5.7)

Page 83, Fig. 5-6 caption: «ration» - ratio

Page 84: «depressed» - «reduced» or «lowered»

Page 86: last paragraph ends abruptly

Page 87, first paragraph: «paragraph 5.1.1» - «section 5.1.1»

Page 88, Fig.5-8. Caption says about a graphene nanobubble, the figure itself indicates it's hBN.

Overall, the dissertation satisfies the requirements for the PhD thesis and the Candidate deserves the PhD degree.

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*