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Skolkovo Institute of Science and Technology

Thesis Changes Log

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: Asst. Prof. Dmitry Kolomenskiy

Co-Supervisor: Dr. Petr Zhilyaev

The thesis document includes the following changes in answer to the external review process.

1. Explanation of the discrepancies between simulation results and experimental data
In Chapter 2 (background) I have added the overview on this topic. In paragraph 3.3 and 3.4 I have added comparison of my results and experiment and their discussion.

2. Section 3.2.5 and discussion of the Cu-Ni system
The Section 3.2.5 is enhanced with extra information and figure.
Extra references are added to the paragraph 2.1.5 "Background. State of the art for polycrystalline". Added section "Discussion to the Chapter 3" where additional references and information are provided.
Some discussion suddenly pops up in Section 6, but on Al. What is the relation to the Cu-Ni system you studied? The comment on Ni-Al system approves the theoretical results showing that impurities increase the activation energy of grain boundary migration.

3. 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?
The discussion on the potentials and comparison of Em for 3 potentials for the case of pure Ni is added to the new section "Discussion to the Chapter 3".

4. Methodology Clarification: More information on the validation of the methodologies used, and how metastable states and modeling artifacts were minimized or accounted for, would strengthen the thesis.
The extra description is added to the paragraph 5.1.4

5. Automated GB Analysis Method: Elaborating on the development, validation, and limitations of the automated method for GB analysis will provide deeper insight into its effectiveness and potential applications.
The Chapter 4 is checked on misprints. The section 4.2.2 is corrected and fulfilled with details on the algorithm. Also, I added extra illustrations showing issues. The section "Discussion" is added.

6. Extrapolation of Results: Justification for extrapolating results obtained from argon to other van der Waals nanobubbles should be provided, supported by literature or preliminary data.
In the abstract to the Chapter 5 changed "The observed effects can be extrapolated" to "The developed methodology can be extrapolated" because it better describes the idea of the statement (the idea was that the elasticity theory and developed MD approach can be implemented to the variety of possible VdW heterostructures, like MSO2 with water of HBN with water or CH4). Also, I corrected introduction in Chapter 5, corresponding part in abstract and conclusions.

7. Future Work and Applications: Discussing potential future research directions and practical applications of the findings would enhance the thesis, demonstrating the candidate's understanding of the broader impact of her work.
Added discussion on the possible continuation in chapter conclusions. Added the description of peculiarities of nanocrystallines: references to literature and comment on volume occupied by grain boundary.

8. The abstract: the abstract is rewritten, extra information is added
9. Summary of main results and conclusions: corrected
10. Paragraph 2.2 (Van der Waals heterostructures): added details
11. Could the h/r ratio replace pressure for the correct determination of the phase diagram of argon trapped in graphene nanobubble? Added discussion
12. Added subsection 3.1.5 - Driving force method on the explanation of the nature of elasticity driving force in considered bicrystal.
13. Added discussion 3.4 for Chapter 3
14. Added summary and discussion for Chapter 4

Other corrections
Figure 3-15: corrected the description.
Added subsection 3.1.5 - Driving force method
Introduction in Chapter 5 – corrected
Usage of 'we' – rewritten in the third-person
Spell-check