

## Thesis Changes Log

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**PhD Program:** Mathematics and Mechanics

**Title of Thesis:** Application of molecular dynamics simulations for the analysis of nanoscale structures

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

The references to figures are changed to the format like “Figure 1-10” and “Figure 1-10(a)”. The notation (a), (b), etc. is used on subfigures.

The references to equations are changed to the format like “equation/relation/rule (1.10)”; only referenced equations are numerated.

The references to tables are changed to the format like “Table 1-10”.

The references to paragraphs are changed to “paragraph/section 1.1”.

All left “we” mentions are changed to the passive voice or 3<sup>rd</sup> person perspective.

### **Chapter 1: Introduction**

The 2<sup>nd</sup> abstract of ‘zero’ paragraph is corrected.

Added reference to the OVITO software

The misprints are fixed.

The text in “Objectives” is corrected.

p.17: removed "Grain is a part of"

“to study physical properties of polycrystals, the following characteristics are used / defined” – changed to “The following characteristics are usually considered in the framework of studying polycrystallines”

### **Chapter 2**

#### **Section 2.1**

**Par. 2.1.1** The 1<sup>st</sup> paragraph is corrected, the bullet points are corrected.

**Par. 2.1.2** Corrected format of text in bullet points

#### **Section 2.3**

Corrected numeration of equations.

Zero paragraph: corrected description in the “bullet points” list.

**Par. 2.3.4** – corrected text in a part about LJ potentials.

Page 39: "It consists of repellent and attractive parts" changed to "It consists of core repulsion and long-range attraction branches"

Page 39: inversily changed to inversely

#### **Par. 2.3.5**

"The temperature was calculated during MD calculations as a part of LAMMPS code, this value was used to provide Nose-Hoover thermostat integration (??)" – the link is fixed.

**Par. 2.3.6** – corrected numeration, rewritten text for local stress calculation.

**Par. 2.3.7** – corrected text.

## **Chapter 3**

### **Section 3.1**

Corrected numeration of equations.

Replaced figures 3-1,3-2, 3-3.

References to the paragraphs, describing thermostat, potentials and initialization are added where appropriate.

#### **Par. 3.1.2**

– text with the description of initialized bicrystalline is corrected;

– reference to Figure 3-9 is corrected (misprint), instead of this, the reference to a Figure 3-1 is given.

#### **Par. 3.1.3**

Added information.

### **Section 3.2**

**Par. 3.2.1** – details added in the description; added units to  $d_{\text{cutoff}}=10\text{\AA}$ ; numeration of equations is checked and removed for  $M=vP$

**Par. 3.2.2** – details added in the description; Figure 3-8 corrected.

**Par. 3.2.3** – details are added to the text. Numeration of equation is removed.

**Par. 3.2.4** – text is corrected, numeration of equations for  $R(t)$  and  $v_{\text{gb}}$  are removed.

**Par. 3.2.5** – changed order of Figure 3-17 and 3-17.

### **Section 3.3**

Fixed missing reference in conclusions.

## **Chapter 4**

Subscriptions for Figures 4-3, 4-4, 4-6 are corrected; the equation for  $R_1$  and  $R_2$  are re-enumerated and referenced.

## **Chapter 5**

### **Section**

**Par. 5.1.2** – descriptions for Figures 5-1, 5-2 are corrected including “graphene outer layer” changed to “graphene top layer”;

**Par. 5.1.3** – text is corrected; numeration of equations is corrected.

Rearrangement of sections is done: a separate section is created: **5.2 Detection of phase transition of trapped argon**. It contains former **Par. 5.1.3** (former “Search for a phase transition”) and **Par. 5.2** (former “Results and discussion”).

#### **Par. 5.1.4 (current par. 5.2.1) 4**

text is corrected;

description for Figure 5-4 is corrected;

figure with mixing atoms is moved before phase transition to Figure 5-6, the corresponding text is moved to paragraph 5.1.4 from 5.3.

#### **Par. 5.2 (current par. 5.2.2) –**

text is corrected, including “outer membrane: changed to “external membrane”

Figure 5-7 and its description is corrected

**Section 5.3** – text and numeration are corrected,

**Figure 5-7** – corrected: added points (1),(2), (3) and (4) denoting phase transitions and highlighted areas for (1) and (2) for H/R ratios.

