OPINION

from professor Daniela Borissova, D.Sc. at IICT-BAS

Subject: Dissertation by Rossen Mikhov Mikhov,
on the topic "Monte Carlo approach for optimization of bimetallic nanostructures",
submitted for the acquisition of the educational and scientific degree "doctor"
in the professional field 4.6 "Informatics and Computer Science",
doctoral program "Informatics"

According to Order No. 303/28.11.2025 of the Director of IICT-BAS, I was elected as a member of the scientific jury, and at the first meeting of the scientific jury, held on 02.12.2025, I was assigned to prepare a statement on the procedure.

ACTUALITY

The development of reliable and environmentally friendly methods for synthesizing metal nanoparticles is a key step in the development of the field of nanotechnology. In recent years, there has been significant interest in the development of nanoparticles of noble metals such as gold and silver, due to their various biological, chemical and physical characteristics. Nanoparticles with several thousand atoms are one of the most difficult to numerically model, since the nanoparticle is too small and methods for modeling macroscopic metals are not applicable, but on the other hand the nanoparticle is too large to use methods based on quantum physics. Therefore, the numerical modeling of nanoparticles remains a current problem, for which different ways are sought for the synthesis and characterization of the properties of such nanostructures.

KNOWLEDGE OF THE RESEARCH PROBLEM

From the review made, as well as from the published results on the topic of the dissertation, it can easily be established that the doctoral student is well acquainted with the nature of the researched issue. Additional evidence of this is the number of literary sources used, the number of publications and the citations to them.

ANALYTICAL CHARACTERISTIC

The dissertation has a total volume of 124 pages, contains 34 figures, 7 tables and 149 literary sources. It is structured as follows: introduction, 6 chapters, conclusion - summary of the results obtained, contributions, list of publications on the dissertation, list of noted citations of the publications, participation in research projects, declaration of originality of the results and

bibliography. The goal of the dissertation research is formulated on page 25, for the implementation of which 6 additional tasks are formulated.

In Chapter 1, existing methods for modeling the atomic configurations of metallic and bimetallic nanostructures are analyzed. The task of modeling the atomic configurations is presented as a global optimization task using a potential energy function, as well as Monte Carlo simulation as the main tool for realizing configurations.

In Chapter 2, the proposed two-stage Monte Carlo approach for optimization of bimetallic nanostructures is described. This approach is implemented using a mathematical model, three algorithms, and some prerequisites for their software implementation. A two-stage method is proposed - the first stage is based on simulated annealing on a wide lattice, and the second - on simulated diffusion.

In Chapter 3, results from numerical testing of the proposed two-stage method with different ratios for dividing the computational resources between the two stages are presented, and the approach for determining the parameters of the method is experimentally justified.

Chapter 4 presents results of a study of the influence of the initial temperature on the performance of the wide-grid Monte Carlo algorithm, which is a component of the proposed two-stage method. The tested Ag and Co nanoparticles of different sizes, on grids of different types and sizes show how different factors influence the choice of the initial temperature for simulated annealing.

Chapter 5 presents results from the application of the two-step method to study the atomic arrangement and surface segregation processes in Au-Ag nanocells of 3000 atoms. Through a comparative analysis of the results for different Au:Ag ratios and crystal lattices with different symmetries, it is shown how the interaction of these factors determines the local order and their influence on the macroscopic properties of the bimetallic nanocells.

In Chapter 6, a software system is described through which the numerical simulations of the two-step method are implemented.

OBJECT AND METHODOLOGY OF THE RESEARCH

The object of the scientific research is bimetallic nanostructures, and the subject of the research is the methods for optimization of these structures. The methodology used, based on analysis, synthesis, comparison, generalization, and experimental studies, is appropriately selected and contributes to the realization of the set goal and the tasks formulated in the dissertation work.

ABSTRACT AND AUTHOR REFERENCE

The submitted abstracts in Bulgarian and English faithfully reflect the content of the dissertation work and comply with the requirements of the Law on the Development of Academic Staff in the Republic of Bulgaria and the Regulations for its implementation. From the submitted declaration of originality, as well as from the publications on the topic of the dissertation, it can be determined that the described results are the personal work of the author.

ASSESSMENT OF COMPLIANCE WITH THE MINIMUM NATIONAL REQUIREMENTS AND WITH THE ADDITIONAL REQUIREMENTS

A total of 4 publications on the topic of the dissertation work are presented. All publications are indexed in Scopus, 3 of which are SJR, and in 3 of them the doctoral student is the first author. The presented publications on the topic of the dissertation research fully satisfy the requirements for acquiring the educational and scientific degree "Doctor", since the doctoral student has 72 points out of the required 30 points.

The plagiarism check result from the strikeplagiarism.com website showed the following results: Similarity Coefficient 1: 1.76% and Similarity Coefficient 2: 0.15%.

CONTRIBUTIONS

I accept the contributions formulated by the doctoral student, which I evaluate as scientific and applied contributions.

CRITICAL REMARKS AND RECOMMENDATIONS

The dissertation is well balanced. It would be good to present parts of the software implementation in a separate application, and in the text only to schematically present their functional features – such as figures 6.1 to 6.6.

I have the following questions for the doctoral student: How is the high level of optimization of the efficiency of the calculations achieved? With which external applications for analysis and visualization is the proposed software architecture compatible?

FINAL COMPLEX EVALUATION

The results obtained on the topic of the dissertation research convincingly show that Rossen Mikhov Mikhov possesses the necessary theoretical knowledge and practical skills in the field of informatics and computer sciences, as well as proven abilities for independent scientific research. The presented dissertation work meets the requirements of the Law on the Development of Academic Staff in the Republic of Bulgaria, the Regulations for its implementation, as well as the Regulations on the Specific Conditions for Acquiring Scientific Degrees and for Holding Academic Positions at IICT-BAS. **The results obtained on the topic of the dissertation research give me sufficient reason to give a categorically positive assessment of the presented dissertation work and I propose to the esteemed Scientific Jury to award Rossen Mikhov Mikhov the educational and scientific degree "Doctor" in the doctoral program "Informatics", professional field 4.6. "Informatics and Computer Sciences".**

05.01.2026

Member of the Scien
/pro:

На основание

ЗЗЛД