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OPINION

by Prof. Vassil Guliashki, PhD
Institute of Information and Communication Technologies - BAS
on a dissertation thesis for awarding the educational and scientific degree **"Doctor"**
in professional direction **4.6 "Informatics and Computer Science"**
Doctoral programme **„Informatics"**

titled: "MONTE CARLO APPROACH FOR OPTIMIZATION OF BIMETALLIC NANOSTRUCTURES"

by ROSSEN MIKHOV MIKHOV

By order № 303/28.11.2025 of the Director of the Institute of Information and Communication Technologies – Corr. Member Svetozar Margenov, D.Sc. – in connection with the procedure for acquiring the educational and scientific degree "Doctor" in the professional field 4.6 Informatics and Computer Science, Doctoral programme „Informatics" by Rossen Mikhov Mikhov with a dissertation thesis titled „Monte Carlo approach for optimization of bimetallic nanostructures" I have been included in the Scientific Jury as a member.
As a member of the scientific jury, I received:

1. Dissertation thesis for awarding the educational and scientific degree „Doctor", in Bulgarian.
2. Abstract in Bulgarian.
3. Abstract in English.
4. Scientific publications related to the dissertation.
5. Other documents.

When evaluating the dissertation, the terms of the Law on the development of the academic staff in the Republic of Bulgaria (LDASRB), the Regulations for Implementation of LDASRB (Decree No. 26 of February 13, 2019) and the Regulations of University of Library Studies and Information Technologies for application of the Law for the development of the academic staff in the Republic of Bulgaria are decisive.

1. According to Art. 27 (1) of LDASRB "the dissertation work shall contain scientific or applied research results that represent an original contribution to science. The dissertation shall show that the candidate has profound theoretical knowledge in the respective subject, as well as their abilities of independent scientific research."
2. According to Art. 27 (2) of LDASRB the dissertation work should be presented in a form and volume corresponding to the specific requirements of the primary unit. The dissertation work should contain title page; contents; introduction; presentation; conclusion – summary of the obtained results, accompanied by declaration of originality; bibliography.

The scientific supervisor of the dissertation thesis is Prof. Dr. Leoneed Kirilov.

Relevance of the topic

The topic of the dissertation is very relevant. Modeling of nanoparticles and optimization of bimetallic structures in order to find stable atomic configurations is an important area of research due to its numerous applications in a number of fields such as medicine, biomedicine, cryobiology and reproductive medicine, dentistry, sensor applications, nanoelectronics, telecommunications, information technology, optics, physics and technology of complex crystals, ecology and environmental protection, etc. A large number of researchers are working hard in this field. This dissertation is included and is part of a broader study of nanostructures, which is being conducted in an international multidisciplinary team.

GENERAL CHARACTERISTICS OF THE DISSERTATION THESIS

The dissertation submitted to me for opinion is 124 pages long, structured in an introduction, 6 chapters, conclusion, contributions, list of publications, list of noted citations, declaration of originality of the results and a bibliography of 149 literary sources. Its text includes 34 figures and 7 tables.

The aim of the dissertation is to develop a Monte Carlo simulated annealing approach, using the potential of strong coupling, for the optimization of various types of bimetallic nanostructures, including nanoparticles, nanowires and nanofilms.

To achieve this goal, the **following tasks** have been defined and completed:

1) To propose a method for optimization of bimetallic nanostructures, including nanoparticles, nanowires and nanofilms;

2) To investigate the effectiveness of the proposed method;

3) To propose an appropriate way to determine and adjust the parameters of the method;

4) To determine which of the following factors most significantly influence the optimal choice of the initial temperature of simulated annealing: the chemical element, the size of the nanoparticle, the type of lattice, the size of the lattice;

5) To propose a software architecture and to develop a software system implementing the new method, which allows a high level of optimization of the efficiency of the calculations, flexibility for varying the algorithms and their parameters and good compatibility with external applications for analysis and visualization of the results;

6) To conduct a study applying the proposed method to a specific class of 3000-atom gold-silver nanosheets, which are of interest for many applications, to determine how differences in the Au:Ag ratio and crystal lattice symmetry affect atomic arrangement and surface segregation processes.

The formulated aim and tasks have scientific and applied scientific potential for research and application in the field of informatics, information systems and technologies.

The dissertation has resulted in **4 publications**, one of which is in a collection of papers of an international scientific IEEE conference, and 3 are in scientific journals with an impact rank (SJR). All publications are co-authored, but in 3 of them Roscen Mikhov is the first author. So far, they have been cited 7 times. These publications meet and exceed the requirements for awarding the educational and scientific degree "Doctor". The presented publications give reason to assume that the research has the necessary publicity.

CONTRIBUTIONS

The contributions are formulated as follows:

1. A two-stage lattice Monte Carlo method is proposed for the optimization of bimetallic nanostructures, including nanoparticles, nanowires and nanofilms, with the first stage simulated annealing on a wide lattice and the second stage simulated diffusion. The method is implemented using data structures and a preprocessing strategy that significantly increase its efficiency, and allow to optimize nanostructures from several hundred to several thousand atoms on a standard personal computer.

2. It has been experimentally established that an effective strategy for distributing the computational resources between the two stages of the method is to use 30% of the time for the first stage and 70% of the time for the second stage.

3. It has been experimentally established that the specific way in which the method is formulated in 5 steps is appropriate and leads to successful parameter tuning.

4. The influence of the initial temperature on the performance of the wide-lattice Monte Carlo algorithm for different lattices and chemical elements has been studied. It has been experimentally established that for the selection of a suitable initial temperature, the most important factor is the size of the lattice, with the highest temperatures required when placing a small particle on a large lattice. The type of chemical element also has some importance, and the type of lattice does not have a significant influence.

5. An adaptation of the proposed two-step method for working with nanocells has been made. It has been used to study the atomic arrangement and surface segregation processes in gold-silver nanocells of 3000 atoms. A comparative analysis of the results for three compositions (Au:Ag = 1:1, 1:3, 3:1) and two lattices (fcc and icosahedral) shows that fcc nanocells have thinner walls, a cavity with a larger radius and more low-coordinate atoms on the surface compared to icosahedral ones. Ag atoms show a tendency to migrate to both surfaces of the nanocell, due to which the inner layers of Au-enriched alloys are practically devoid of Ag and Au-Au bonds prevail. Ag-enriched alloys have a maximum number of mixed Ag-Au bonds and a more uniform local order of both crystal lattices.

6. A software architecture is proposed for the implementation of the two-stage method, which allows a high level of optimization of the efficiency of calculations, flexible parallel launch with a combination of composite algorithms under different conditions and good compatibility with external applications for analysis and visualization of the results.

It can be assumed that the presented results sufficiently cover the scope of the set goals and objectives.

The abstract in Bulgarian, 47 pages long, presents the dissertation work.

The abstract in English, 44 pages long, presents the dissertation work.

CRITICAL NOTES

I have no significant remarks. I would only suggest that the contributions be formulated a little more concisely. Also, a small number of stylistic errors have been noticed in the text of the dissertation, which should be corrected.

Overall, the structure and layout of the dissertation make a very pleasant impression. In scientific terms, the research has a completely finished appearance. The applied methodology is clear and logical. It has been followed consistently. The results obtained are very interesting and useful.

FINAL COMPLEX ASSESSMENT

The technical remarks made do not belittle the contributions of the dissertation. I believe that the presented dissertation work meets the requirements of the Law on the Development of the Academic Staff in the Republic of Bulgaria. The achieved results give me reason to propose to the esteemed Scientific Jury to grant the educational and scientific degree "Doctor" to **Rossen Mikhov** in the professional field - 4.6 Informatics and Computer Sciences, doctoral program - "Informatics".

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Sofia city /Pr

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