UNIVERSITY OF BELGRADE
Faculty of Technology and Metallurgy

TO THE ACADEMIC AND SCIENTIFIC COUNCIL

Subject: Report on the completed doctoral dissertation of the candidate Gordana D. Marković.

By Decision No. 2026-35/367 dated August 27, 2026, we were appointed members of the Committee for the Evaluation of the Doctoral Dissertation of the candidate Gordana D. Marković, entitled "Development and Design of New Titanium Alloys Using Advanced Computational Methods" (Развој и дизајн нових легура титана применом напредних рачунарских метода).
Having reviewed the submitted dissertation and other accompanying materials, and following a discussion with the candidate, the Committee has prepared the following

REPORT

1. INTRODUCTION

1.1. Chronology of the approval and preparation of the dissertation

On March 12, 2025, the candidate submitted to the Faculty the application for the topic of her doctoral dissertation, entitled: "Development and Design of New Titanium Alloys Using Advanced Computational Methods" (Развој и дизајн нових легура титана применом напредних рачунарских метода).
On March 20, 2025, the Academic and Scientific Council of the Faculty of Technology and Metallurgy, at its session, adopted Decision No. 35/40 appointing the Committee for the Evaluation of the Eligibility of the Topic and the Candidate for the preparation of the doctoral dissertation, composed of: Dr. Željko Kamberović, Full Professor, University of Belgrade, Faculty of Technology and Metallurgy; Dr. Veljko Đokić, Principal Research Fellow, Innovation Center of the Faculty of Technology and Metallurgy; Dr. Stefan Dikić, Assistant Professor, University of Belgrade, Faculty of Technology and Metallurgy; Dr. Gvozden Jovanović, Research Associate, Institute for Technology of Nuclear and Other Mineral Raw Materials; and Dr. Francisco Javier Dominguez Gutierrez, Associate Professor, National Centre for Nuclear Research, Otwock, Poland.
On April 24, 2025, the Academic and Scientific Council of the Faculty of Technology and Metallurgy, at its session, adopted Decision No. 35/90 accepting the Report of the Committee for the Evaluation of the Eligibility of the Topic and the Candidate for the preparation of the doctoral dissertation, and appointed as supervisors Dr. Vaso Manojlović, Associate Professor of the Faculty of Technology and Metallurgy, and Dr. Jovana Ružić, Senior Research Associate of the "Vinča" Institute of Nuclear Sciences – National Institute of the Republic of Serbia.
On May 27, 2025, the Council of Technical Sciences of the University of Belgrade, at its session, adopted Decision No. 61206/2-25 granting consent to the decision of the Academic and Scientific Council of the Faculty of Technology and Metallurgy on the acceptance of the doctoral dissertation topic of the candidate Gordana D. Marković, entitled "Development and Design of New Titanium Alloys Using Advanced Computational Methods" (Развој и дизајн нових легура титана применом напредних рачунарских метода), and confirming Dr. Vaso Manojlović, Associate Professor of the Faculty of Technology and Metallurgy, and Dr. Jovana Ružić, Senior Research Associate of the "Vinča" Institute of Nuclear Sciences – National Institute of the Republic of Serbia, as supervisors.
On August 27, 2026, the Academic and Scientific Council of the Faculty of Technology and Metallurgy, at its session, adopted Decision No. 2026-35/367 appointing the Committee for the Evaluation of the Doctoral Dissertation, composed of: Dr. Željko Kamberović, Full Professor, University of Belgrade, Faculty of Technology and Metallurgy; Dr. Stefan Dikić, Assistant Professor, University of Belgrade, Faculty of Technology and Metallurgy; Dr. Gvozden Jovanović, Research Associate, Institute for Technology of Nuclear and Other Mineral Raw Materials; and Dr. Francisco Javier Dominguez Gutierrez, Associate Professor, National Centre for Nuclear Research, Otwock, Poland.

1.2. Scientific field of the dissertation

The research conducted within this dissertation belongs to the scientific field of Technological Engineering, and to the narrower scientific field of Metallurgical Engineering, for which the parent institution is the Faculty of Technology and Metallurgy of the University of Belgrade. The supervisors, Dr. Vaso Manojlović, Associate Professor at the Department of Metallurgical Engineering of the Faculty of Technology and Metallurgy, University of Belgrade, and Dr. Jovana Ružić, Senior Research Associate of the "Vinča" Institute of Nuclear Sciences – National Institute of the Republic of Serbia, University of Belgrade, are, on the basis of their published scientific work and previous research experience, competent to supervise the preparation of this doctoral dissertation.

1.3. Biographical data on the candidate

Gordana Marković was born on April 21, 1997, in Belgrade. She completed elementary school in Vojka in 2012 and the general-track gymnasium in Stara Pazova in 2016. She enrolled in undergraduate academic studies in the study programme Materials Engineering at the Faculty of Technology and Metallurgy, University of Belgrade, in the 2016/17 academic year, and completed them on September 30, 2021, with a GPA of 8.75. Her bachelor's thesis, entitled "The Influence of the Degree of Deformation on the Size of Crystallized Grains in Al-Mg Alloys for the Automotive Industry", was defended with the highest grade (10), under the supervision of Prof. Dr. Miljana Popović. She completed her master's academic studies in the study programme Metallurgical Engineering on September 30, 2022, with a GPA of 10.00, defending her master's thesis entitled "Prediction of Mechanical Properties of Biocompatible Titanium Alloys Using Machine Learning" under the supervision of Prof. Dr. Vaso Manojlović. She enrolled in doctoral academic studies in the study programme Metallurgical Engineering at the Faculty of Technology and Metallurgy, University of Belgrade, in the 2022/23 academic year. Since November 2022 she has been employed at the Institute for Technology of Nuclear and Other Mineral Raw Materials (ITNMS) in Belgrade, first as a Junior Research Assistant and, since August 2025, as a Research Assistant. Her research activity is focused on the application of modern computational methods, such as machine learning, density functional theory (DFT) and molecular dynamics (MD), in the design and characterization of titanium alloys with improved mechanical properties. The candidate actively participates in international research projects and is a member of four COST Actions: CA22143 – European Materials Informatics Network (EuMINe), CA21121 – European Network for the Mechanics of Matter at the Nano-Scale (MecaNano), CA22154 – Data-driven Applications towards the Engineering of functional Materials (DAEMON), and CA22123 – European Materials Acceleration Center for Energy (EU-MACE). Since November 2024 she has been a member of the modelling team within the international project INNUMAT (Innovative Structural Materials for Fission and Fusion), led by Dr. Francisco Javier Dominguez Gutierrez. Within COST Action CA21121 she carried out a Short-Term Scientific Mission (STSM) at the National Centre for Nuclear Research (NCBJ) in Otwock, Poland, from July 6 to July 20, 2025, including a research visit to the AGH University in Kraków. From April 1 to May 31, 2026, she undertook a two-month research stay at the TechLab laboratory of the Mines Nancy engineering school of the University of Lorraine, France, working on the application of large language models for the extraction of scientific data and knowledge in materials science. In September 2024 she participated in the EuMINe 1st Training School in Belgrade, dedicated to the application of digital tools and artificial intelligence in materials informatics, and in May 2026 in the AccelMAPs school (Accelerating Energy Materials Development: From Legacy Labs to Material Acceleration Platforms), organized within COST Action CA22123 and held at the Instituto Superior Técnico in Lisbon, Portugal. She received the second prize for the best student paper at the BECCSI 2025 conference in Belgrade. She was a member of the organizing team of the international conference 6th Metallurgical & Materials Engineering Congress of South-East Europe (MMECSEE 2025) and is an active member of the Metallurgical Society of Serbia. In her research she uses the simulation packages VASP and LAMMPS and the Python programming language. She is fluent in English and holds a B1-level certificate in Spanish.

2. DESCRIPTION OF THE DISSERTATION

2.1. Contents of the dissertation

The doctoral dissertation of the candidate Gordana D. Marković, M.Sc. in Metallurgical Engineering, entitled "Development and Design of New Titanium Alloys Using Advanced Computational Methods" (Развој и дизајн нових легура титана применом напредних рачунарских метода), is written in English on 111 pages,

of which 103 are numbered, and contains 52 figures, 20 tables, and 124 references. The dissertation comprises chapters with the following titles: Introduction, Background and Literature Review, Materials and Methods, Results and Discussion, Conclusions, and References, as well as the author's biography, acknowledgements, and abstracts in Serbian and English. The dissertation also contains annexes with the Statement of Authorship, the Statement on the Identity of the Printed and Electronic Versions of the Doctoral Thesis, and the Statement of Use, as well as the evaluation of the report on the originality check of the doctoral dissertation. In its form and content, the dissertation meets the regulations and standards for doctoral dissertations defended at the University of Belgrade.

2.2. Brief overview of the individual chapters

The Introduction chapter discusses the importance of titanium alloys as metallic biomaterials, with particular attention to biocompatibility, corrosion resistance, and the mechanical compatibility of the implant and bone tissue. The stress shielding effect is explained, which arises from the difference in stiffness between the implant and the bone and represents the main motivation for the development of titanium alloys with a reduced Young's modulus of elasticity, whereby the stiffness mismatch between the implant and the bone tissue is decreased. The introductory chapter formulates the subject and objectives of the research: the compilation of a database of experimental data from the literature, the development of machine-learning models for the prediction of mechanical properties, the computational design of new compositions in the Ti–Mo–Sn system, and their experimental verification. The Background and Literature Review chapter is divided into three parts: Crystal structure and phase transformations in titanium, Deformation mechanisms in titanium alloys, and Approaches to titanium alloy design. The first part describes the α and β phases of titanium, the β-transus temperature, and the role of alloying elements in phase stability. The second part covers slip mechanisms in the structure of α-titanium, twinning and phase transformations, the relationship between structure and mechanical properties, as well as an atomistic view of the deformation mechanisms of α-titanium. The third part provides an overview of empirical and semi-empirical design parameters (the molybdenum equivalent, the electron-to-atom ratio, e/a, and the d-electron concept), the high-throughput experimental approach to alloy development, and computational approaches: the CALPHAD methodology, first-principles calculations, and machine-learning-based alloy design. The Materials and Methods chapter describes the compilation of the database on biocompatible titanium alloys from literature sources, data preprocessing and cleaning, the construction of descriptors based on chemical composition, and the machine-learning methodology with cross-validation, which prevents information leakage between the training and test sets and reduces the risk of model overfitting. The computational design procedure based on a search of the chemical composition space of the Ti–Mo–Sn system is described, followed by the experimental methods: arc melting of the selected alloys, density measurement by the Archimedes method, phase and microstructural characterization (XRD, SEM, and EDS), EBSD analysis, nanoindentation, quantitative analysis of the α-lamellar microstructure using the MIPAR software, thermodynamic calculations in the PANDAT software with the PanHEA thermodynamic database, and atomistic simulations of nanoindentation of single-crystal α-titanium in the LAMMPS code. The Results and Discussion chapter comprises the statistical analysis of the compiled database and the physical interpretation of the derived descriptors, the selection and verification of the dataset for modelling, the prediction of mechanical properties, and the analysis of the model response. The Random Forest model for the prediction of Young's modulus, developed on the basis of 240 experimental records, achieved a coefficient of determination of 0.417 and a mean absolute error of 11.50 GPa under publication-grouped validation, with the d-orbital energy and the β-phase stability descriptors identified as the most significant. For comparison, under the conventional random data split the same model achieved a coefficient of determination of 0.597 and a mean absolute error of 8.93 GPa, showing that the random split overestimates model accuracy. A search of the composition space identified a region of reduced modulus values, and the alloys Ti–6.2Mo–xSn (x = 5, 10, and 15 wt.%) were selected, then synthesized and characterized. The results of chemical and phase analysis, density measurements, EBSD characterization, and nanoindentation are presented, showing a reduction of Young's modulus from 101.02 GPa for the Ti–6.2Mo alloy to 79.26, 85.31, and 83.65 GPa for the alloys with 5, 10, and 15 wt.% Sn. The CALPHAD analysis provided the thermodynamic context of phase stability, while atomistic simulations of nanoindentation explained the dependence of the local modulus on the crystallographic orientation of the α-lamellae. The final part of the chapter presents a comparison of the experimental results with the model predictions and an analysis of the causes of the deviations and the limitations of the composition-based approach. The results confirm the applicability of machine learning for the selection of alloy compositions with targeted mechanical properties, while the microstructure and the processing route remain important factors that determine the final properties of the material.

3. EVALUATION OF THE DISSERTATION

3.1. Relevance and originality

The doctoral dissertation addresses the topical subject of developing titanium alloys whose Young's modulus of elasticity is close to that of bone, thereby mitigating the stress shielding effect and reducing the consequent resorption of bone tissue around the implant. The research belongs to the field of metallic biomaterials. At the same time, the dissertation belongs to the field of data-driven materials design, which has been developing rapidly within materials science over the past decade. The application of machine learning in the development of new alloys is increasingly present in contemporary research. The topicality of the subject is also evidenced by the structure of the literature used: approximately two thirds of the cited works were published since 2016, and almost half since 2021, including works published in 2026. The originality of the dissertation is reflected in several aspects. An extensive and critically curated database of experimental data on biocompatible titanium alloys was compiled, applying strict criteria regarding the comparability of the measured quantities and the processing routes. The database is publicly available and represents a useful research resource and a basis for its further extension and enrichment. The critical analysis of the collected data and of the results reported to date also enables the formulation of recommendations for future research, particularly regarding the data and experimental parameters that should be consistently reported in publications in this field so that the results are comparable and suitable for use in machine-learning models. For the assessment of model accuracy, validation based on grouping the data by source publication was applied and compared with the conventional random data split. In this way, a more realistic assessment was obtained of the model's ability to predict alloy properties from data originating from new, previously unseen sources. This methodological approach is still rarely applied in the field of predicting the properties of titanium alloys. The dissertation implements a complete materials design cycle: from database compilation and model development, through the computational search of the composition space and the selection of compositions in the ternary Ti–Mo–Sn system, to the synthesis, characterization, and quantitative comparison of the experimental results with the model predictions. A particular contribution of the dissertation is the linking of results obtained at different levels of the material structure. The local values of the elastic modulus, determined by nanoindentation, were related to the crystallographic orientation determined by EBSD analysis and to the quantitative parameters of the α-lamellar microstructure. The results obtained were also considered in a broader thermodynamic context based on CALPHAD calculations. Finally, the dissertation is also characterized by a critical analysis of the limitations of the applied approach, including the quantification of the influence of individual literature sources on the model predictions. This enables a more objective approach to materials design, as well as a clearer delineation between what the model can predict from chemical composition and the influence of microstructure and processing, which are not fully captured by the data used.

3.2. Review of reference literature used

In preparing this doctoral dissertation, the candidate used 124 literature sources. In addition to the most recent scientific papers in the fields of titanium alloy design and the application of machine learning in materials science, including works published in 2025 and 2026, the sources used include professional books, monographs, and book chapters in the fields of materials science, titanium metallurgy, and biomaterials; review papers presenting the development of these fields over the past decades; fundamental literature on phase transformations, deformation mechanisms, and nanoindentation; as well as methodological literature relating to the computational tools and thermodynamic calculations applied. Publications by the candidate and her collaborators, in which particular aspects of database compilation and the prediction of the mechanical properties of biocompatible titanium alloys had previously been investigated, were also used. The cited sources encompass experimental results, their analysis and interpretation, the conclusions drawn, and the theoretical foundations of the applied testing methods. The candidate has contributed to extending the existing knowledge on the application of machine learning in the design of biocompatible titanium alloys, with particular emphasis on relating the chemical composition and composition-based descriptors to Young's modulus of elasticity, as well as on the experimental verification of the predictions and the investigation of the role of microstructure in the final properties of the Ti–Mo–Sn alloys. Based on the list of the literature used, it can be concluded that the candidate has an adequate knowledge of the subject area and of the current state of research worldwide, with approximately two thirds of the cited sources published within the last ten years. The results presented in the dissertation are consistent with contemporary research in the fields of biocompatible titanium alloy development and data-driven materials design.

3.3. Description and adequacy of the applied scientific methods

The research within this dissertation is based on a combination of computational and experimental methods. The database was compiled by the systematic collection of experimental results from the literature, applying strict inclusion criteria that ensured the uniformity of the measured quantity and the processing route, so that the dataset for modelling Young's modulus comprises 240 experimental records from 77 publications. The model inputs consist of 30 features: the contents of 12 alloying elements, 16 composition-based descriptors derived from the electronic and atomic parameters of the alloying elements, and two categorical variables. Several machine-learning algorithms were compared for property prediction, among which the Random Forest model was selected as the most suitable. The model accuracy was assessed by publication-grouped cross-validation, which reduced the possibility of overestimating the accuracy due to the relatedness of data from the same source and provided a more realistic assessment of the model's ability to predict alloy properties from data originating from new sources. The importance of individual descriptors was determined by permutation analysis, while the share of variance associated with the belonging of the alloys to particular alloy systems was quantified. The computational design of new compositions was performed by a search of the composition space of the Ti–Mo–Sn system, in which the Mo and Sn contents were varied from 0 to 16 wt.% in steps of 0.2 wt.%, whereby 6561 candidate compositions were evaluated and the alloy series Ti–6.2Mo–xSn (x = 5, 10, and 15 wt.%) was selected. The selected alloys were produced by arc melting, homogenized at 1000 °C for 2 h in evacuated quartz tubes, water quenched, and cold rolled with a thickness reduction of approximately 20%. The density was determined by the Archimedes method, the phase composition by X-ray diffraction (XRD), and the chemical homogeneity and microstructure by scanning electron microscopy with energy-dispersive spectroscopy (SEM/EDS). The crystallographic orientation of the α-lamellae was determined by EBSD analysis, while their morphology and orientation distribution were quantified by processing the micrographs in the MIPAR software, enabling the objective determination of the microstructural parameters. The reduced elastic modulus and hardness were determined by nanoindentation, and the values of Young's modulus were calculated using the Oliver–Pharr method. Combining nanoindentation with EBSD analysis enabled the direct correlation of the local modulus with the crystallographic orientation. The thermodynamic context of phase stability was obtained by CALPHAD calculations of the Ti–Mo and Ti–Sn binary diagrams and of the isothermal sections of the ternary Ti–Mo–Sn system at 1000 and 100 °C, performed in the PANDAT software with the PanHEA database. The mechanisms of the orientation dependence of the local properties were investigated by atomistic simulations of nanoindentation of single-crystal α-titanium in the LAMMPS code. This approach, in which the model predictions were verified by experiment and the experimental results were considered across several spatial scales, enabled a comprehensive evaluation of the investigated alloys and the achievement of the objectives of the dissertation.

3.4. Applicability of the achieved results

The topic of the doctoral dissertation was chosen with the possibility of practical application of the expected results in mind. The research results can be viewed through several units: (1) the compiled and publicly available database of experimental data on biocompatible titanium alloys, with strictly defined inclusion criteria, represents a lasting resource that can be directly used in future research and for the development of new models; (2) the developed methodology for predicting mechanical properties, based on composition-derived descriptors and publication-grouped validation, is applicable as a tool for the pre-selection of promising compositions, thereby reducing the number of required experiments, accelerating the development of new alloys, and lowering costs; (3) the experimentally confirmed series of Ti–6.2Mo–xSn alloys with a Young's modulus of elasticity from 79.26 to 85.31 GPa, considerably lower than the modulus of conventional titanium alloys, represents a starting point for the further development of alloys intended for medical applications; and (4) the established procedure for relating the local elastic modulus to the crystallographic orientation of the α-lamellae, by combining nanoindentation, EBSD analysis, quantitative microstructure analysis, and atomistic simulations, represents a methodological framework applicable to other alloy systems as well. The investigations carried out, combined with the analysis of the available literature data, have enabled significant progress in understanding the relationship between the chemical composition, microstructure, and Young's modulus of elasticity of titanium alloys, as well as in the objective assessment of the scope of the composition-based approach to alloy design. Alloys with a reduced elastic modulus of this type have potential applications in medical technology, primarily for orthopaedic and dental implants where a reduction of the stress shielding effect is required, whereby further investigations of biocompatibility, corrosion resistance, and

behaviour under cyclic loading are necessary for clinical application, while the developed data-driven design methodology has broader applicability in the development of metallic materials in general.

3.5. Evaluation of the candidate's ability for independent scientific work

During her doctoral studies to date and her active involvement in scientific research work on projects, Gordana Marković, M.Sc. in Metallurgical Engineering, has demonstrated a high level of independence and maturity in scientific research. The candidate has mastered all stages of the research process, from the critical review of the literature and the formulation of research questions, through the independent planning and realization of experiments and computational simulations, to the analysis, interpretation, and presentation of the obtained results. In her scientific research work to date she has published, as author and co-author, one paper in a top international journal (M21), two papers in prominent international journals (M22), and one paper in a journal of national importance (M52), whereby the M21 paper and both M22 papers resulted from the research within this doctoral dissertation. In addition, she has presented the results of her research through three conference papers published in full (M33) and four conference abstracts (M34) at scientific conferences of international importance. Based on all of the above, the Committee concludes that the candidate Gordana Marković, through her professional competence, continuous dedication, and the quality of her published scientific results, fully meets all the requirements for independent scientific research work.

4. ACHIEVED SCIENTIFIC CONTRIBUTION

4.1. Overview of the achieved scientific contributions

The scientific contributions arising from the research in the doctoral dissertation of the candidate Gordana D. Marković relate to:

− the compilation of a new, critically curated, and publicly available database of experimental data on biocompatible titanium alloys, which encompasses the chemical composition, processing routes, and mechanical properties and represents a basis for the further development and application of machine-learning models in alloy design;
− the development of machine-learning models for the prediction of the Young's modulus of elasticity, yield strength, and tensile strength of titanium alloys, with the application of publication-grouped validation, which provided a realistic assessment of the models' ability to predict the properties of new alloys;
− the determination of the influence of the electronic and atomic parameters of the alloying elements on the prediction of Young's modulus, with the d-orbital energy and the β-phase stability parameters identified as the most significant indicators;
− the development of new alloys in the Ti–Mo–Sn system with a reduced Young's modulus of elasticity, whereby Young's modulus values of 79 to 85 GPa were achieved through the computational selection of compositions and the synthesis and experimental characterization of the Ti–6.2Mo–xSn alloys (x = 5, 10, and 15 wt.%);
− the establishment of the relationship between the local mechanical properties, crystallographic orientation, and microstructure of titanium alloys by applying nanoindentation, EBSD analysis, quantitative microstructure analysis, and atomistic simulations, together with a thermodynamic analysis of phase stability using CALPHAD calculations;
− the determination of the possibilities and limitations of composition-based models for the selection of alloys with targeted mechanical properties, and the demonstration of the importance of including microstructure and processing parameters in the further development of the models.

4.2 Critical analysis of the research results

The review of the literature in the field of titanium alloy design shows an increasing application of machine learning for the prediction of mechanical properties, but also considerable differences in the quality and structure of the available data, in the manner of model validation, and in the degree of experimental verification of the obtained predictions. In this dissertation, particular attention is devoted precisely to these limitations. Validation with data grouped by publication showed that a random data split can lead to an overestimation of model accuracy, while the applied approach provides a stricter and more realistic assessment of its ability to predict the properties of new alloys. The obtained model accuracy values indicate that the chemical

composition and the derived descriptors contain significant information on the mechanical properties of the alloys, but at the same time show that they cannot fully describe the variability of the Young's modulus, yield strength, and tensile strength. A significant part of the deviations can be related to the microstructure, thermomechanical history, phase composition, and testing conditions, which are not uniformly available in the literature sources. This limitation represents an important result of the dissertation, as it points to directions for the further development of databases and machine-learning models in this field. The experimental verification of the selected compositions in the Ti–Mo–Sn system confirmed that machine learning can successfully guide the selection of alloys with a reduced Young's modulus of elasticity. At the same time, the differences between the predicted and the experimentally determined values show that, for more precise prediction, it is necessary to include microstructure and processing parameters. The results of nanoindentation, EBSD analysis, and atomistic simulations additionally demonstrated the importance of the crystallographic orientation and the local microstructure for the values of the mechanical properties. From the application standpoint, the developed alloys represent a promising basis for further research on materials with a reduced elastic modulus. For the assessment of their actual suitability for medical application, additional investigations of the mechanical behaviour under cyclic loading, corrosion resistance, and biocompatibility are necessary. The developed database and methodology at the same time represent a basis for the further extension of the dataset, the inclusion of microstructural and processing parameters, and the development of more reliable models for the selection of alloy compositions with targeted mechanical properties.

4.3. Verification of the scientific contributions

Category M21:

1. Marković, G., Manojlović, V., Ružić, J., Sokić, M. (2023). Predicting Low-Modulus Biocompatible Titanium Alloys Using Machine Learning. Materials, 16(19), 6355. (IF=3.1) (ISSN: 1996-1944) (https://doi.org/10.3390/ma16196355)

Category M22:

1. Marković, G., Ružić, J., Sokić, M., Milojkov, D., Manojlović, V. (2024). Prediction of elastic modulus, yield strength, and tensile strength in biocompatible titanium alloys. Journal of Mining and Metallurgy, Section B: Metallurgy, 60(2), 273-282. (IF=1.0) (ISSN: 1450-5339) (https://doi.org/10.2298/JMMB240221019M)
2. Marković, G., Dominguez-Gutierrez, F. J. (2026). Thermally activated plasticity in single-crystal titanium: a molecular dynamics study of nanoscale deformation. Modelling and Simulation in Materials Science and Engineering, 34(1), 015018. (IF=2.3) (ISSN: 0965-0393) (https://doi.org/10.1088/1361-651x/ae2f77)

5. ORIGINALITY CHECK OF THE DOCTORAL DISSERTATION

In accordance with the Rulebook on the Procedure for the Originality Check of Doctoral Dissertations Defended at the University of Belgrade ("Glasnik Univerziteta u Beogradu", No. 204/18), the originality check of the doctoral dissertation of the candidate Gordana D. Marković, entitled "Development and Design of New Titanium Alloys Using Advanced Computational Methods", was performed using the iThenticate software. It was established that the text similarity amounts to 13%. This degree of similarity is the consequence of common expressions, personal names and titles, definitions, established phrases, references, and professional terms. Based on all of the above, the Committee considers that the doctoral dissertation of the candidate Gordana D. Marković is original and that the academic rules of citation have been fully respected, and therefore the prescribed procedure of preparation for its defence may continue.

6. CONCLUSION AND PROPOSAL

The research conducted within this dissertation belongs to the scientific field of Technological Engineering, and to the narrower scientific field of Metallurgical Engineering, for which the parent institution is the Faculty of Technology and Metallurgy of the University of Belgrade. The doctoral dissertation was prepared under the supervision of Dr. Vaso Manojlović, Associate Professor of the Faculty of Technology and Metallurgy, University of Belgrade, and Dr. Jovana Ružić, Senior Research Associate of the "Vinča" Institute of Nuclear Sciences – National Institute of the Republic of Serbia, University of Belgrade. Based on the detailed analysis, presented above, of the results achieved in the doctoral dissertation of the candidate Gordana D. Marković, entitled "Development and Design of New Titanium Alloys Using Advanced Computational Methods" (Развој

и дизајн нових легура титана применом напредних рачунарских метода), the Committee considers that this doctoral dissertation represents a significant and original scientific contribution to the development and design of biocompatible titanium alloys with a reduced Young's modulus of elasticity, through the integration of machine learning, computational composition selection, experimental characterization, and the analysis of the influence of microstructure on mechanical properties. The subject of the research is clearly defined, the set objectives have been achieved, and the research carried out follows contemporary scientific trends and contributes new knowledge to this field. The Committee therefore considers that the doctoral dissertation meets all the prescribed criteria and proposes to the Academic and Scientific Council of the Faculty of Technology and Metallurgy to adopt this Report and to make it, together with the doctoral dissertation of the candidate Gordana D. Marković, entitled "Development and Design of New Titanium Alloys Using Advanced Computational Methods" (Развој и дизајн нових легура титана применом напредних рачунарских метода), available for public inspection within the period prescribed by law, and thereafter to forward it to the Council of Technical Sciences of the University of Belgrade for final adoption.

September 3, 2026

MEMBERS OF THE COMMITTEE

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Dr. Željko Kamberović, Full Professor
University of Belgrade, Faculty of Technology and Metallurgy

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Dr. Stefan Dikić, Assistant Professor
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