MME SEE CONGRESS 2023

5th Metallurgical & Materials Engineering Congress of South-East Europe
Trebinje, Bosnia and Herzegovina
7-10th June 2023

CONGRESS PROCEEDINGS

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The Association of Metallurgical Engineers of Serbia

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The Faculty of Technology and Metallurgy at the University of Belgrade, Serbia;
The Faculty of Technology at the University of Banja Luka, Bosnia and Herzegovina;
The Faculty of Metallurgy at the University of Zagreb in Sisak, Croatia;
The Faculty of Natural Sciences and Engineering at the University of Ljubljana, Slovenia;
The Faculty of metallurgy and technology at the University of Podgorica, Montenegro.

CONGRESS PROCEEDINGS - MME SEE 2023
5th Metallurgical & Materials Engineering Congress of South-East Europe

Editors:

Dr. Miroslav Sokić,
Institute for Technology of Nuclear and Other Mineral Raw Materials

Dr. Branislav Marković
Institute for Technology of Nuclear and Other Mineral Raw Materials

prof. Dr. Vaso Manojlović
Faculty of Technology and Metallurgy, University of Belgrade

Technical editor:

M. Sc. Gvozden Jovanović
Institute for Technology of Nuclear and Other Mineral Raw Materials

Published and printed by:
Association of Metallurgical Engineers of Serbia (AMES)
Kneza Miloša 9/IV,
11000 Belgrade
Serbia

For the publisher:

AMES president Dr. Miroslav Sokić

Circulation:

120 copies

ISBN 978-86-87183-32-2

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PREFACE

On behalf of the Scientific and Organizing Committee, it is a great honor and pleasure to wish all the participants a warm welcome to the Fifth Metallurgical & Materials Engineering Congress of South-East Europe (MME SEE 2023) which is being held in Trebinje, Bosnia and Hercegovina, 07 - 10 June 2023.

The MME SEE 2023 is a biannual meeting of scientists, professionals, and specialists working in the fields of metallurgical and materials engineering. The aim of the Congress is to present current research results related to processing/structure/property relationships, advances in processing, characterization, and applications of modern materials. Congress encompasses a wide range of related topics and presents the current views from both academia and industry: Future of metals/materials industry in South-East European countries; Raw materials; New industrial achievements, developments and trends in metals/materials; Ferrous and nonferrous metals production; Metal forming, casting, refractories and powder metallurgy; New and advanced ceramics, polymers, and composites; Characterization and structure of materials; Recycling and waste minimization; Corrosion, coating, and protection of materials; Process control and modeling; Nanotechnology; Sustainable development; Welding; Environmental protection; Education; Accreditation & certification.

The editors hope that Congress will stimulate new ideas and improve knowledge in the field of metallurgical and materials engineering. The Congress has been organized by the Association of Metallurgical Engineers of Serbia, with the co-organization of the Institute for Technology of Nuclear and Other Mineral Raw Materials, Belgrade, Serbia, Faculty of Technology and Metallurgy, University of Belgrade, Serbia, Faculty of Technology, University of Banja Luka, Bosnia and Herzegovina; the Faculty of Metallurgy, University of Zagreb, Sisak, Croatia; the Faculty of Natural Sciences and Engineering, University of Ljubljana, Slovenia; and the Faculty of Metallurgy and technology, University of Podgorica, Montenegro.

Financial support from the Ministry of Science, Technological Development and Innovation of the Republic of Serbia to researchers from Serbia for attending the congress is gratefully acknowledged. The support of the sponsors and their willingness to cooperate have been of great importance for the success of MME SEE 2023. The Organizing Committee would like to extend their appreciation and gratitude to all sponsors and friends of the conference for their donations and support.

We would like to thank all the authors who have contributed to this book of abstracts and also the members of the scientific and organizing committees, reviewers, speakers, chairpersons, and all the conference participants for their support of MME SEE 2023. Sincere thanks to all the people who have contributed to the successful organization of MME SEE 2023.

On behalf of the 5th MME SEE Scientific and Organizing Committee

Miroslav Sokić, PhD

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PREDICTING THE MODULUS OF ELASTICITY OF BIOCOMPATIBLE TITANIUM ALLOYS USING MACHINE LEARNING

Gordana Marković[1], Vaso Manojlović[1], Miroslav Sokić[1], Jovana Ružić[2], Dušan Milojkov[1], Aleksandra Patarić[1]

e-mail: g.markovic@itnms.ac.rs

1-Institute for Technology of Nuclear and Other Mineral Raw Materials, 11000 Belgrade, Serbia,
2-Faculty of Technology and Metallurgy, University of Belgrade, 11000 Belgrade, Serbia

Titanium alloys are widely employed in various fields, particularly in biomedical engineering, due to their mechanical and corrosion resistance properties combined with good biocompatibility. The modulus of elasticity is a distinguishing feature of this group of materials compared to others used for similar purposes. A database of approximately 238 titanium alloys free of toxic elements was compiled for this study. The influence of different factors (such as alloy element proportions, density, and specific heat) on the modulus of elasticity was predicted using four methods: support vector machine, XGBoost, Neural Network, and Random Forest. The Random Forest mean absolute error (MAE) of 7.33 GPa, falls within the range of experimentally obtained absolute errors in the literature (up to about 11 GPa). A strong correlation (R2 = 0.72) was observed between experimental and predicted data. Lastly, specific alloying element regions were identified for the modulus of elasticity, which can be used to design new biocompatible titanium alloys in the future.

Keywords: titanium alloys, modulus of elasticity, biocompatibility

Introduction

In recent decades, titanium alloys have become popular in biomedical engineering due to their exceptional properties [1]. Significant features include low modulus of elasticity, low density, biocompatibility, good specific strength and corrosion resistance [2]. Unlike materials used for the same purpose, such as stainless steels, titanium alloys have a significantly lower modulus of elasticity and higher specific hardness [3]. These advantages have led to their increased use in the creation of various implants, such as artificial hips, artificial shoulders, and pacemakers [4].

Despite the benefits of these alloys, there are still concerns about their effects on the human body. A high modulus of elasticity compared to bone can lead to stress shielding and other negative consequences, including bone atrophy and implant loosening. For example, the widely used alloy Ti–6Al–4V has a modulus of elasticity around 100 GPa, while the modulus of elasticity of bone ranges from 10 to 40 GPa [5, 6]. In addition, the presence of toxic elements such as aluminum and vanadium in commercial alloys raises concerns about their effects on human health, including neurological disorders, brain damage, and even Alzheimer's disease [7, 8].

In order to solve these problems, the influence of various parameters on the modulus of elasticity was investigated in this paper. A created database contains information on 238 low modulus alloys that do not contain toxic elements [9]. This database has been created on the basis of experimental data from the literature. Modeling was then performed using machine learning.

Materials and methods

Formation of the database

A database comprising 238 titanium alloys, devoid of any toxic elements, has been developed [9]. Each alloy has been entered with its mass and atomic fractions of titanium and alloying elements in addition to 36 parameters, comprising calculated and literature data. These parameters encompass thermal and mechanical processing, atomic mass, theoretical and experimental modulus of elasticity, Mo equivalents, and others.

From the database, 65% were used for the training set, while 35% of the alloys were used for testing the models. The samples were modeled using the 4 aforementioned statistical methods. Coefficient of determination, mean square error, mean absolute error metric, maximum absolute error, mean absolute percentage error for each of these methods, depending on whether it is the training set or the test set, are determined.

Notably, the Y_eq_V coefficient represents the resultant equivalent from this endeavor. By utilizing experimental data of the modulus of elasticity, coefficients for each element were sought to derive the theoretical elasticity value closest to the experimental value. A database search identified the minimum of the sum of all differences between theoretical and experimental values.

Applied statistical methods for predicting mechanical properties

Applied statistical methods for predicting mechanical properties are: Support vector machine, Random Forest, XGBoost and XGBoost. The following parameters were used to define the performance of the given methods: coefficient of determination (R^2), mean square error (RMSE), mean absolute error metric (MAE), maximum absolute mean error (MAX) and mean absolute percentage error (MAPE). These methods are described in detail in literature [10].

Results and discussion

The parameters for which the impact on the accuracy of the modulus of elasticity was examined are shown in Figure 1 in correlation with each other.

The parameters are matched on a one-to-one basis and numerical values are obtained, and each field is colored in different shades of blue and pink. Intense shades of blue indicate a significant correlation. Lighter and paler shades of blue indicate that the dependence of the parameters is weakening. Intense shades of pink indicate a negative dependence of the parameter, while lighter shades of the swarm mean a still negative correlation, only to a lesser extent. For example the value for the density and automatic share of tantalum is 0.82 and the field is colored intense blue, which means that these are parameters that have a significant interdependence.

The smallest errors were observed using the Random Forest method. The mean absolute error (MAE) obtained by the Random Forest method (7.33 GPa) enters the range of experimentally obtained absolute errors in the literature (up to about 11 GPa).

Figure 2 presents the dependence between the predicted and experimental values of the samples used for the test. There are certain deviations, but the correlation between the data is good, as indicated by the value of the correlation coefficient, which is $R^2 = 0.72$.

During modeling, 35 parameters were shown to have a positive influence on the accuracy of the modulus of elasticity. Figure 2 shows all those parameters as well as the extent to which they affect the accuracy of Young's modulus. The influence of the parameters shown in the picture was obtained using the random forest method. Among the parameters that showed the most influence are Mo equivalent, Y_eq_V coefficient and atomic mass.

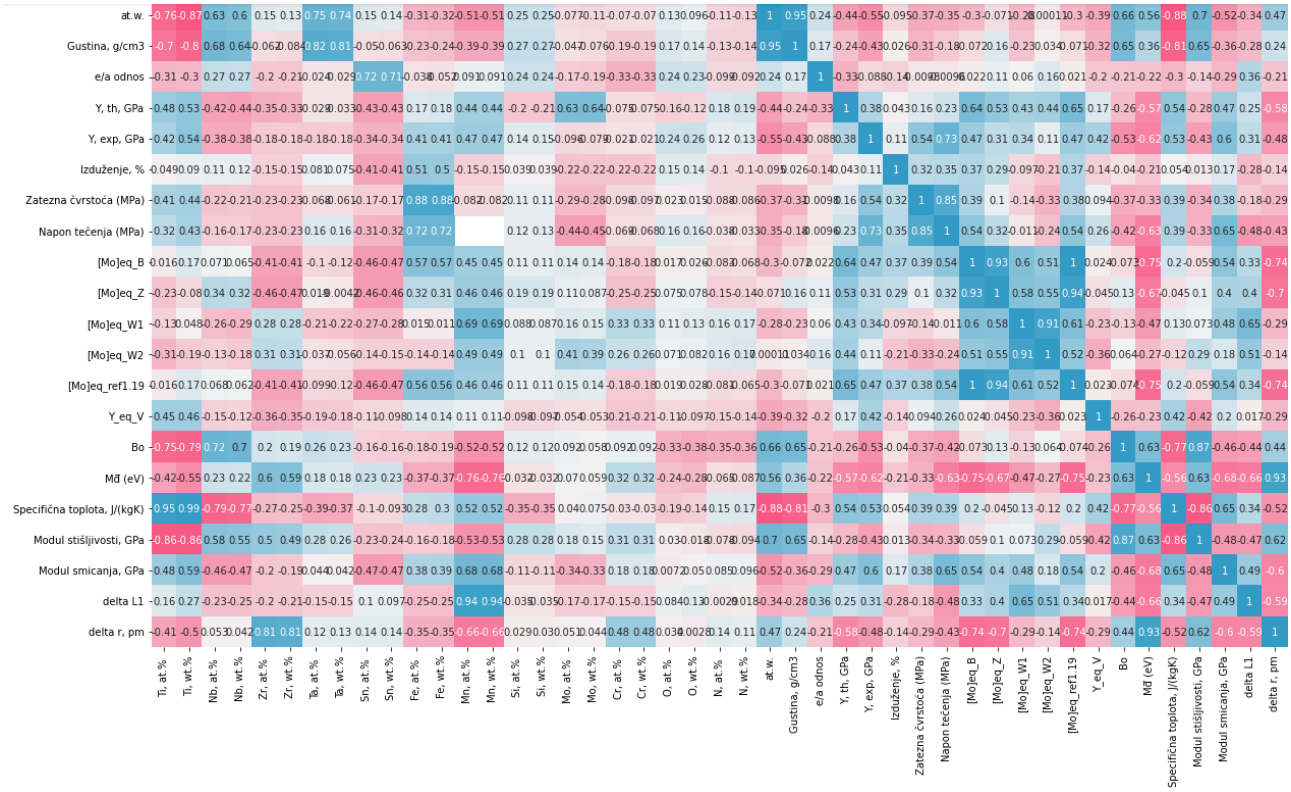

Figure 1 Correlation between studied parameters

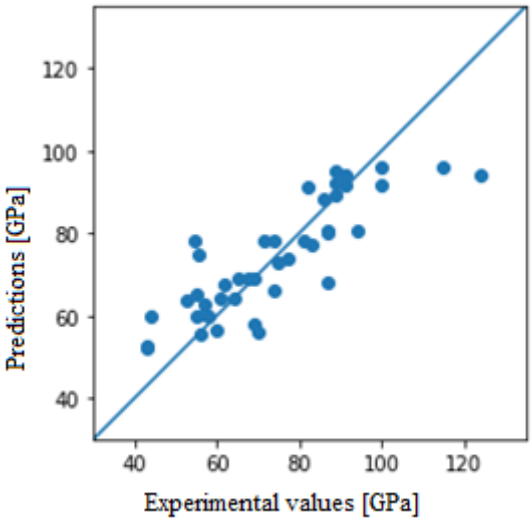

Figure 2 Comparison of data on the test data set: modeled and experimental data

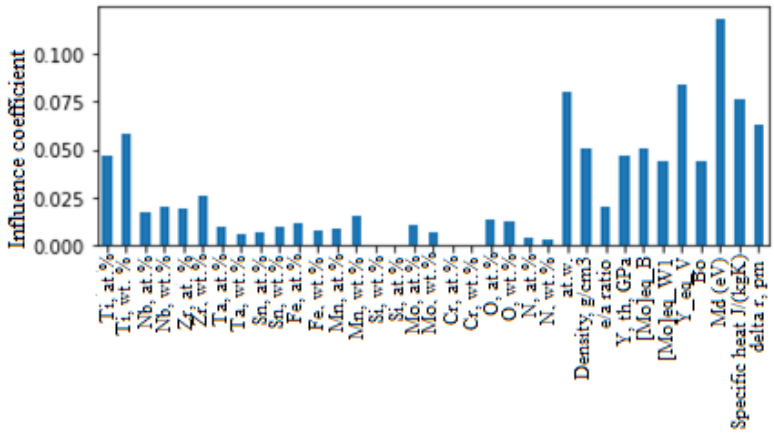

Figure 3 The influence of certain parameters on the accuracy of the modulus of elasticity

In Figure 4 a) b) c) and d) shows the influence of niobium, zirconium, tantalum and tin as alloying elements, depending on the mass fraction, on the modulus of elasticity. The x-axis shows the share of titanium in relation to the maximum value, and the y-axis the share of the alloying element in relation to the maximum value. From these diagrams it is possible to read which areas of alloying elements and titanium have the lowest modulus of elasticity, which enables the design of new dual alloys.

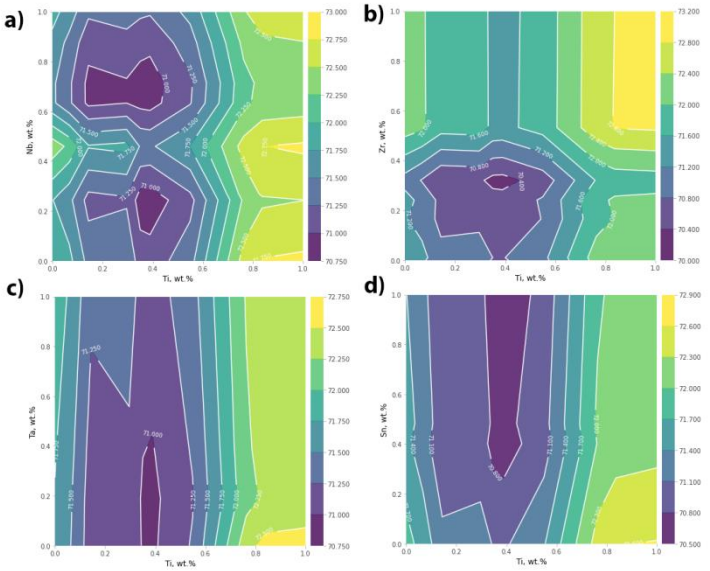

Figure 4 The influence of individual alloying elements a) Nb; b) Zr; c) Ta; d) Sn

on the modulus of elasticity for dual alloys

It should be acknowledged that some parameters have been omitted during modeling, owing to the impracticality of completing all parameters for each alloy. Future work will involve expanding the database to evaluate the impact of additional parameters such as mechanical and thermal processing, yield stress, tensile strength, and elongation.

Conclusion

On the basis of the given data, the modeling was executed employing four statistical techniques, out of which the Random Forest method resulted in the lowest mean error is 7.33 GPa.

Random Forest method show that the most influential parameters on the modulus of elasticity were: atomic weight, Y_eq_V coefficient and Mo equivalent, where the influence coefficients are respectively 0.080, 0.085, 0.120. A significant correlation was obtained between experimental and predicted data which shows value of the correlation coefficient, $R^2 = 0.72$. Areas of certain alloying elements in combination with titanium give minimum values for the modulus of elasticity, which is significant for the design of new alloys, have been determined.

Acknowledgement

This investigation was financed by the Ministry of Science, Technological Developments and Innovation of the Republic of Serbia (Contract number: 451-03-47/2023-01/200023; 451-03-47/2023-01/200135).

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