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PREDICTION OF ELASTIC MODULUS, YIELD STRENGTH, AND TENSILE STRENGTH IN BIOCOMPATIBLE TITANIUM ALLOYS

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Abstract

Biocompatible titanium alloys possess a balanced set of improved mechanical properties and good biocompatibility, making them crucial materials in biomedical engineering. There is an increasing demand for these new alloys with superior properties. Furthermore, there is a need to understand the relationship between parameters and properties, and machine learning is being applied to make the whole process cheaper and more efficient. The aim of this study is to develop accurate machine learning models for predicting mechanical properties: modulus of elasticity, tensile strength, and yield strength, specifically using the Extra Trees Regressor model. Compared to the previous results, an improvement of the elastic modulus prediction model was observed after the inclusion of data on heat treatment parameters and Poisson's ratio, as seen in the reduced MAE from 7.402 to 7.160 GPa. Models were built to predict the values of tensile strength and yield strength, where iron and tin were shown as most important features respectively, while the correlation coefficients for the test set were 0.893 and 0.868.

Keywords: *Modulus of elasticity; Tensile strength; Yield strength; Biocompatibility; Machine learning*

1. Introduction

Titanium alloys have been the most widely used metallic materials in the field of biomedical engineering, for decades [1, 2]. Owing to their excellent mechanical and physical properties such as high strength, corrosion and wear resistance, and low modulus of elasticity, as well as their exceptional biocompatiblity , titanium alloys have become essential materials for medical implant production [3-7]. Titanium implants are used in orthopedics (joint replacement surgery on shoulders, knees and hips), and dentistry (tooth replacement) [3, 8]. Even though titanium and its alloy exhibit the highest biocompatibility among biomaterials, they are considered bioinert materials due to the osteogenesis trend. In general, titanium implants are manufactured by traditional metallurgical techniques such as powder metallurgy and casting. Lately, few studies are reporting on titanium implant production using additive manufacturing [9, 10].

The presence of different alloying elements is crucial for their biomechanical compatibility. The alloying elements used in this study are classified as non-toxic or neutral to the human body and include: Nb, Zr, Ta, Sn, Fe, Mn, Si, Mo, O, N and H. Among them, Nb, Zr, Ta, Sn, Fe, Mn and Mo are β stabilizers, which, by lowering the β-transus temperature, favor the formation of the β phase (which is characterized by low elastic modulus values). In contrast, O, H and C are α stabilizers, predominantly present as impurities. The remaining elements are considered neutral within this classification. As the number of alloying elements increases, the interactions between the alloying elements become increasingly complex, requiring detailed investigations of the enormously large number of combined effects on mechanical properties [11, 12].

Increasing the Nb content in binary Ti-Nb alloys decreases the modulus of elasticity due to increased porosity while increasing the tensile strength and yield strength through the formation of titanium carbide [13]. Similarly, the Ti-30Ta alloy achieves an optimal modulus-to-strength ratio due to its acicular phase [14]. Zr increases strength in Ti-Zr binary dental alloys through solution strengthening, grain refinement, and FCC phase introduction [15]. Sn, especially in concentrations above 10 wt.%, leads to

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the formation of the Ti3Sn intermetallic phase, increasing the elastic modulus [16]. The Ti-9Mn alloy is known for its low modulus and high yield strength, which is attributed to the reduction of the ω phase and solid solution strengthening [17]. Mo in alloys such as Ti-15Mo shows similar advantages [18]. Small intentional additions, such as in TNTZ alloys with O, Fe and Si, can maintain a modulus of about 75 GPa while increasing the yield stress above 1000 MPa [19].

According to the latest global biomaterials market analysis reported in 2023, the global biomaterials market size is estimated at USD 106.51 billion, and is projected to USD 619.27 billion by 2031, which implies that biomaterials possess significant commercial potential. The biomaterials market is divided by product material (natural materials, bimetallic, bioceramics, and biopolymers) or by product application (dentistry, orthopedics, cardiovascular, ophthalmology, tissue engineering, etc.). The highest market share belongs to biomaterials used for orthopedics, which is estimated to reach a compound annual growth rate (CAGR) of 16.4% up to 2031. Implant fabrication is a challenging and expansive process for both, traditional metallurgy and additive manufacturing [20].

It is well-known that many years of research and development of any material, especially a biomaterial, are necessary to obtain a desirable material appropriate for biological applications. These days, many researchers employ machine learning methods for designing biomaterials to improve their performances, shorten the time for material development, and decrease production costs [21-25]. In most studies, machine learning models are employed to predict hardness, corrosion resistance, modulus of elasticity, tensile, and yield strength of biocompatible materials.

As the parameters-microstructure-properties relationship cannot be fully described by physical models, statistical models are often applied [26]. One of the groundbreaking studies on predicting the mechanical properties of titanium alloys using artificial neural networks was performed by S. Milanov. He used data on alloy composition, heat treatment parameters and operating temperatures to predict nine mechanical properties, including tensile strength and yield strength [27]. In addition, several studies have evaluated the influence of various parameters on the yield strength and tensile strength of the well-known Ti6Al4V alloy. For instance, S. Kar used microstructural parameters to predict the yield strength and tensile strength values, identifying that an increase in the thickness of the alpha lamellae decreases the strength, while the volume of this phase increases strength [28]. Junaidi Sjarif analyzed the values of tensile strength and yield strength using heat treatment parameters for Ti6Al4V alloys, concluding that water quenching and the degree of deformation enhance both tensile strength and yield strength [29]. P. S. Nuri Banu used the alloy composition and processing parameters to predict the mechanical properties of titanium alloys, finding that the model is highly sensitive to high concentrations of Ta and Nb. He determined the optimal combination for the Ti-xNb-yTa ternary alloy, which provides the best combination of high tensile strength, yield strength, and low modulus of elasticity [30].

However, these results refer to widely used alloys with extensive data and results, but many of their constituent elements, such as V, Al, Ni, Co, Cu and Cr, are cytotoxic. This study addresses this shortcoming by focusing on the optimization of biocompatible titanium alloys, thus making a new contribution to the field.

The main objective of this study is to build a credible machine learning model to predict the key mechanical properties of biocompatible titanium alloys: elastic modulus, tensile strength and yield strength. A comprehensive database of biocompatible titanium alloys was established. By introducing Poisson's ratio and heat treatment parameters (temperature and time) into the model for predicting the modulus of elasticity, significant improvements were observed compared to previously published results. It is important to note that the study identified iron and tin as important features of tensile strength and yield strength, respectively. Also, the accuracy of both models for the test set was over 85%.

2. Methods

2.1. Database

These data sets, obtained from the literature, include alloying mass fractions, along with experimental values for modulus of elasticity, tensile strength, yield strength, and hardness. Furthermore, the datasets include information on mechanical treatments, deformations, thermal treatments and corresponding temperatures and durations [23]. In addition to the parameters derived from the literature, the calculated parameters obtained with the help of imported dictionaries were also integrated, and the calculation scripts were published on the Zenoodo platform [31].

The Poisson's ratio is calculated using two methods: summing Poisson's ratios of individual elements and applying a formula based on the bulk and shear modulus. The theoretical modulus of elasticity is determined in three ways, using the "least squares" coefficient optimization method, using the formula that relates the modulus of elasticity to the specific heat, and the formula that relates bulk and shear modulus.

2.2. Data preparation

Different models were developed to predict various biocompatible titanium alloys properties: modulus of elasticity, tensile strength, and yield strength. Correspondingly, the approach to data preprocessing varied. Before data processing, thorough preparation of the dataset was crucial. Columns containing product information, references, or similar data were initially excluded from the prediction model due to their unsuitability. Furthermore, the column detailing the specifics of heat treatment has been replaced with a simplified numerical representation to facilitate data processing in regression analysis.

Afterward, rigorous checks were carried out to ensure the absence of non-numeric entries, followed by outlier detection. Our previous research has shown that the ratio of elastic modulus to specific heat serves as a key criterion for identifying outliers due to its strong correlation [24]. For this purpose, several techniques were used, including linear regression, Z-score analysis, IQR method, local outlier detection, and combined outlier detection.

After removing the outlier alloys, the integration of the calculated parameters and literature data resulted in a refined database consisting of 218 alloys characterized by 62 different parameters for tensile strength and yield strength and 58 parameters for modulus of elasticity. Subsequently, rows with missing data entries for elongation, ultimate tensile strength, and yield strength were excluded, leaving a total of 57 alloys for the analysis of tensile strength and yield strength as target variables (Figure 1).

We utilized Lazy Predict and identified the Extra Trees Regressor as the optimal model for our analysis [32].

The next stage involved the selection of key properties relevant to the target variables. This step aimed to identify the most influential features, thereby increasing the accuracy of the prediction. For all analyses, 65 % of the dataset was allocated for model training, while the remaining 35 % was designated for the test set. The model's accuracy was evaluated using common metrics such as mean absolute error (MAE), mean squared error (MSE), maximum absolute error (MAX), mean absolute percentage error (MAPE), root mean square error (RMSE), and R-squared (R2) [32].

3. Results and discussion

3.1. Model for predicting modulus of elasticity

Prior research examined the accuracy of predicting Young's modulus with the Extra Trees Regression model, resulting in favorable findings [15]. Building upon this foundation, incorporating data on heat treatments, temperature and time variables, resulted in improvements that led to a reduction in mean absolute error (MAE) from the original 7.402 to 7.160 GPa, with improvement in the correlation coefficient from 0.724 to 0.793, for the test set (Table 1). A decrease in MAE indicates a corresponding decrease in the difference between the predicted and actual values of the target parameter. The enhanced correlation coefficient indicates improved linearity in the relationship between predicted and actual values at the same time.

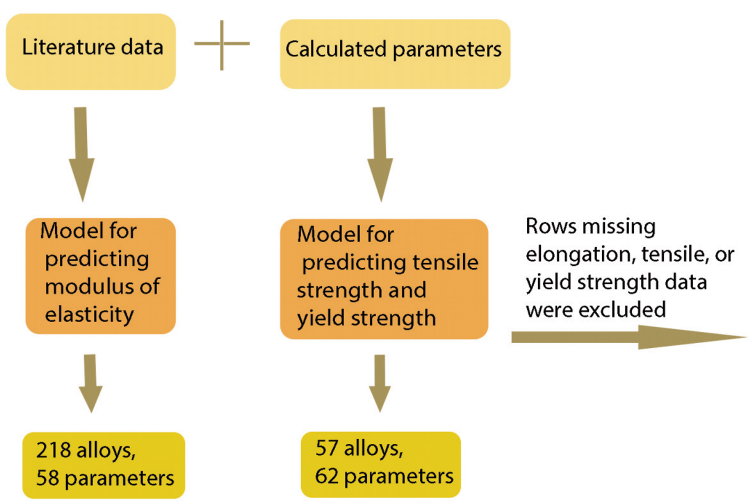

Figure 1. *Refined database overview with filtered alloys and parameters*

Table 1. *Metrics for train and test set for a model predicting Young's modulus with heat treatment data incorporated*

	MAE	R2	MSE	MAX	MAPE
Training set	0.523	0.988	5.052	12.526	0.0008
Test set	7.160	0.793	101.46	38.734	0.108

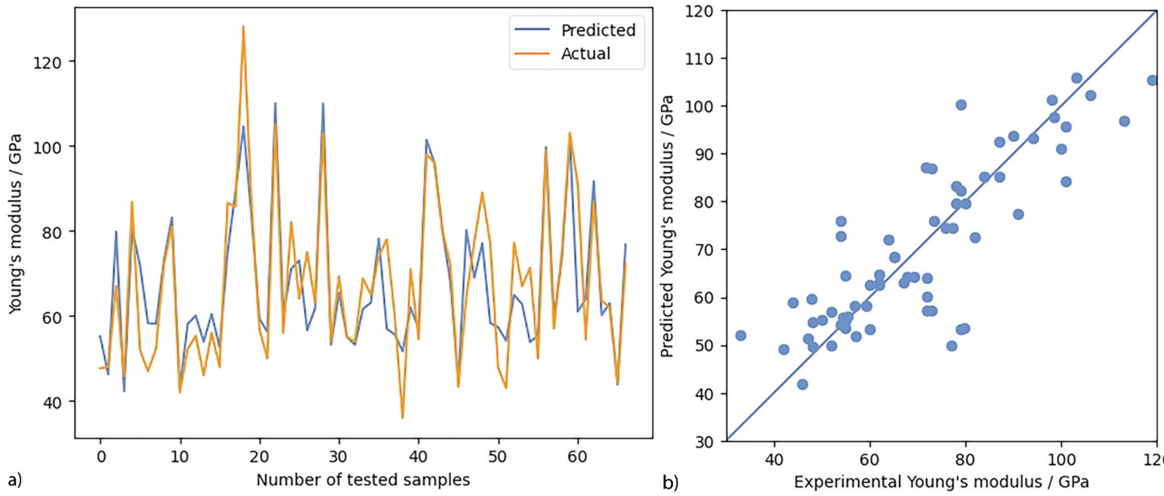

Figure 2. *Comparison of predicted and actual Young's modulus (a) by the number of tested samples and (b) deviation from linearity*

Figure 2 (a) shows the actual and predicted values of Young's modulus of elasticity by the number of tested samples. The largest prediction errors are observed when the true value exceeds 120 GPa or is less than 40 GPa, as these extreme values do not conform to the typical pattern. Additionally, Figure 2 (b) illustrates the deviation from the linear relationship between predicted and actual values.

Understanding important features is crucial for comprehending the factors contributing to the predictions, reducing their dimensionality, and emphasizing key parameters for the final prediction model.

As can be seen from Figure 3, Nb is highlighted as the most influential feature in the elastic modulus prediction model. As previously mentioned, Nb belongs to β stabilizers. A. Thoemmes investigated its influence using 13 binary titanium alloys in which the Nb content varied 10-45 wt.%. He observed that, after rapid cooling, for low Nb contents (less than 17.5 wt.%), formation of α' from the β phase is characteristic. Up to 30 wt.% isolates α'', and somewhere between 30 and 35 wt.% only the β phase or a mixture of β and ω phases occurs. Another interesting observation is that the 37.5 and 45 wt% Nb samples showed the existence of two types of β phase (the main difference is in the size of the lattice parameters). Besides influencing microstructure formation, the Nb content also affects the orthorhombicity and c/a ratio of the α'' phase, and the low value of 48 GPa in Ti-17.5Nb is attributed to the low c/a ratio and high orthorhombic of the α'' phase [33].

The elastic modulus prediction model identified the slip_tw_group parameter as the second most influential. This parameter defines the deformation mechanism present in the observed titanium alloy. When we talk about the deformation mechanism, we refer to the slip and twinning mechanisms and their effects on the properties of Ti alloys. Stable β titanium alloys correspond to the slip mechanism, while metastable β Ti alloys, which are the focus of our research and are defined by lower elastic modulus values, are on the border of the slip/twinning mechanism [34].

In our previous work, we found that specific heat significantly influences the modulus of elasticity, as demonstrated by their relationship formula [24, 35]:

$$c_p \cdot s = \frac{E_a}{1-4\cdot\sigma^2}\cdot\alpha \tag{1}$$

where c_p is specific heat at constant pressure per kilogram (J/(kg·K)); s is density (kg/m^3); E_a is Young's modulus (GPa); α is the linear coefficient of thermal expansion (1/K), and σ is Poisson's ratio. The presence of Poisson's ratio in this formula prompted an examination of its influence on predicting the modulus of elasticity, revealing it to be an influential variable, as shown in Figure 2. Poisson's ratio is expressed by the equation [36]:

$$\sigma = \frac{3K - 2G}{2(3K + G)} \tag{2}$$

where K represents bulk modulus (GPa) and G is shear modulus (GPa).

Besides Poisson's ratio, variables related to heat treatment time (HT1: t, min and HT2: t, min) and temperatures (HT1: T, °C and HT2: T, °C) were found to increase the model accuracy.

3.2. Model for predicting tensile strength and yield strength

Evaluation of the Extra Trees Regression model for predicting tensile and yield strength provided significant results. For tensile strength prediction, the model achieved a relatively high correlation coefficient of 0.89 on the test set, with an MAE of 71.69 MPa (Table 2). Similarly, for yield strength prediction, the model showed a correlation coefficient of 0.87, with an MAE of 76.9 MPa (Table 3). These data are particularly significant as the average errors fall within the deviation range (around ±100 MPa) typically reported in the literature for experimental data. It should be noted here that in the database we used, the number of data that have information on tensile and yield strength was about 100. Achieving relatively good results with a small amount of data may be attributed to the elimination of data unsuitable for the model, a limitation that will be discussed later in this paper. Successful outcomes could also be credited to the reliable research results presented in these publications in our database.

Figure 4 (a) and (b) illustrate the discrepancies between predicted and actual values of tensile strength and yield strength in relation to the amount of test specimens. It can be concluded that a similar deviation trend is evident in both cases, especially evident in the same values of the test samples.

The influence of various variables on the target parameters, tensile strength and yield strength, was examined. Iron mass content, yield strength, and Mo

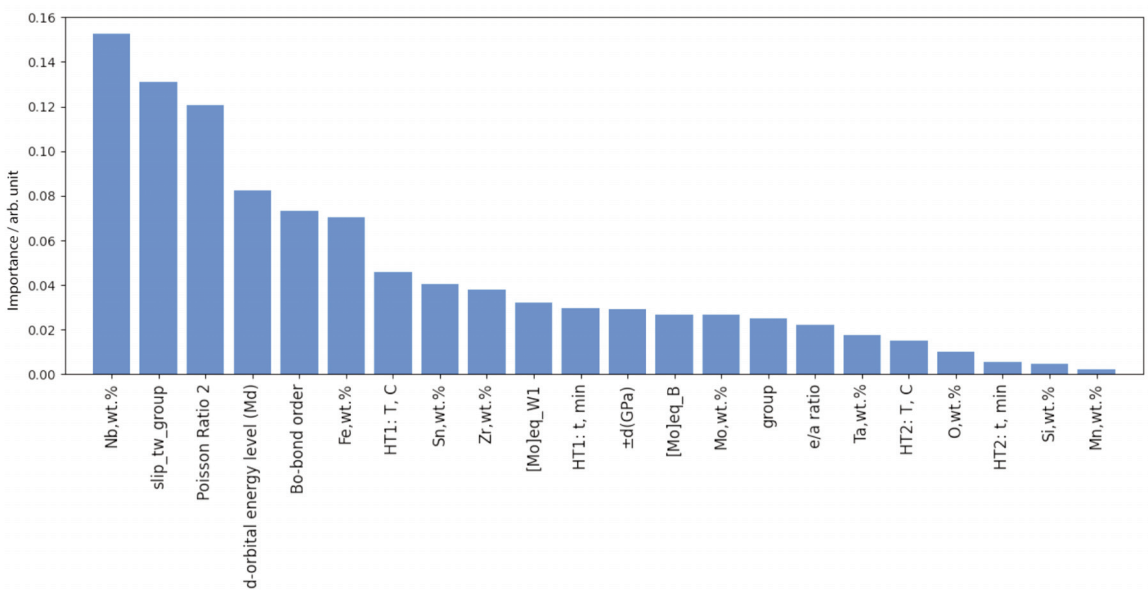

Figure 3. *Feature importance for experimental values of Young's modulus*

Table 2. *Metrics for train and test set in a model predicting tensile strength*

	MAE	R2	MSE	MAX	MAPE
Training set	0.0	1.0	0.0	0.0	0.0
Test set	71.692	0.893	9.697.006	274.670	0.086

Table 3. *Metrics for train and test set in a model predicting yield strength*

	MAE	R2	MSE	MAX	MAPE
Training set	0.0	1.0	0.0	0.0	0.0
Test set	76.904	0.868	12.924.185	317.540	0.099

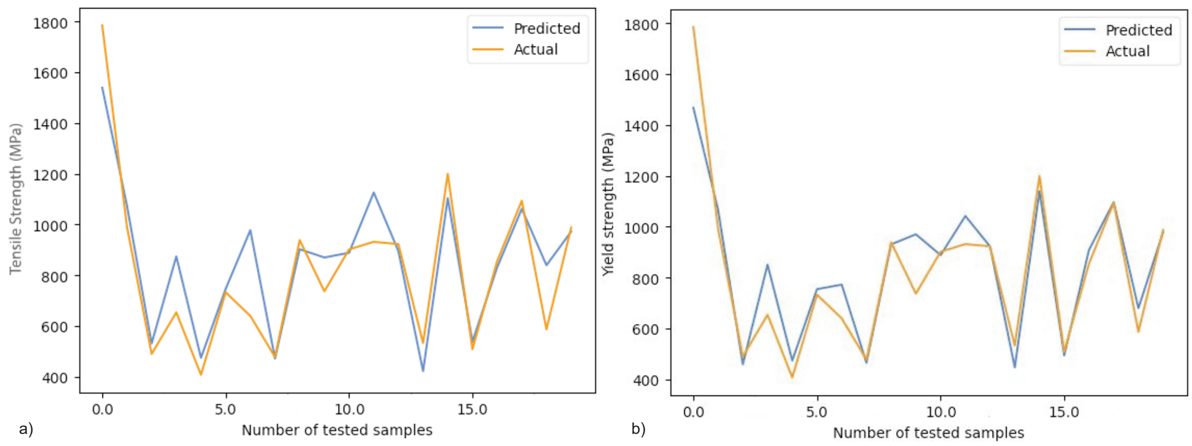

Figure 4. *Comparison of predicted and actual values by the number of tested samples for (a) tensile strength and (b) yield strength*

equivalent emerged as the three most influential variables affecting tensile strength (Figure 5). A direct correlation was observed between the tensile strength and the increase in the mass content of Fe in alloys of the Ti_x-Fe_x-1 type, which indicates a uniform increase in tensile strength with higher concentrations of Fe The enhancement in this mechanical property was primarily ascribed to the forceful hybridization between the Ti-3d and Fe-3d orbitals [37]. The relationship between tensile strength and yield strength has long been established, and some of the expressions that connect these two concepts refer to the Hollomon, Swift and Voce equations [38]. Mo equivalent is a parameter that indicates the stability of certain phases in titanium alloys, defined by the presence of various alloying elements. There is no direct relationship between Mo eq and tensile strength, but obviously the presence of the alloying element affects the microstructure, and thus the mechanical properties. The influence of individual elements, which includes the Mo equivalent, in multicomponent alloys is complex, which is why machine learning models are good for such analyses.

The two most influential parameters for yield strength were tensile strength and Sn, wt.% (Figure 6). The influence of tensile strength is obvious from the reasons for the mechanics of metal deformation. The influence of the Sn content on the yield strength was investigated (Figure 5). In the Ti-17Nb-6Ta alloy, the addition of Sn up to 1.5 wt.% increased the yield strength [39]. Similarly, in the Ti–7.5Nb–4Mo–xSn alloys (x=1–4), a change in the deformation mechanism

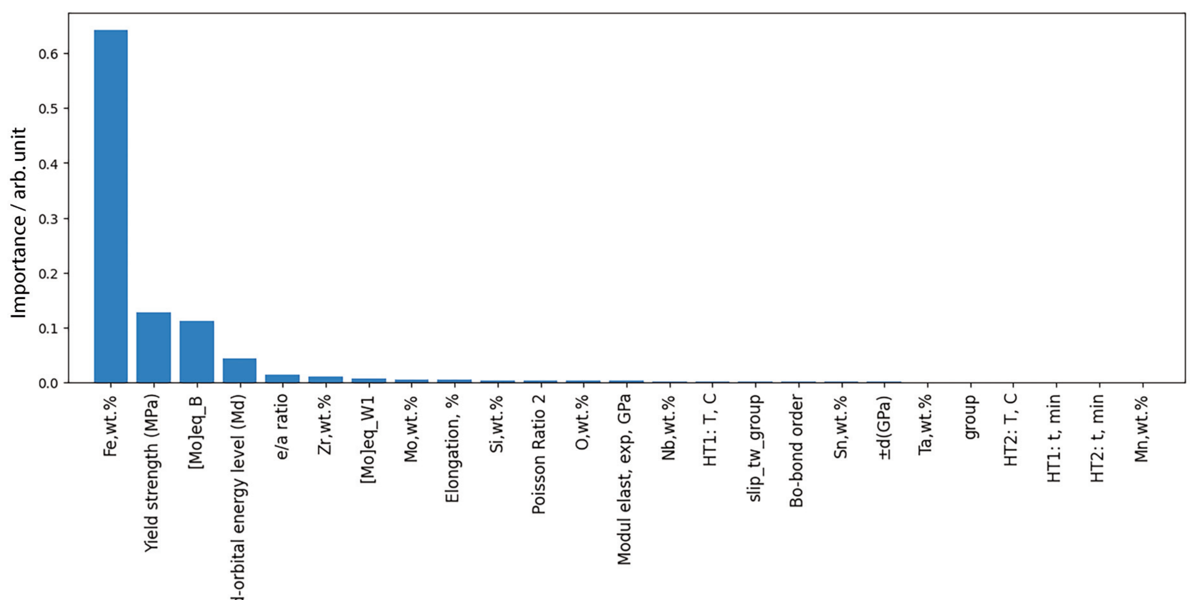

Figure 5. *Feature importance for tensile strength showing the content of iron as the most influential parameter*

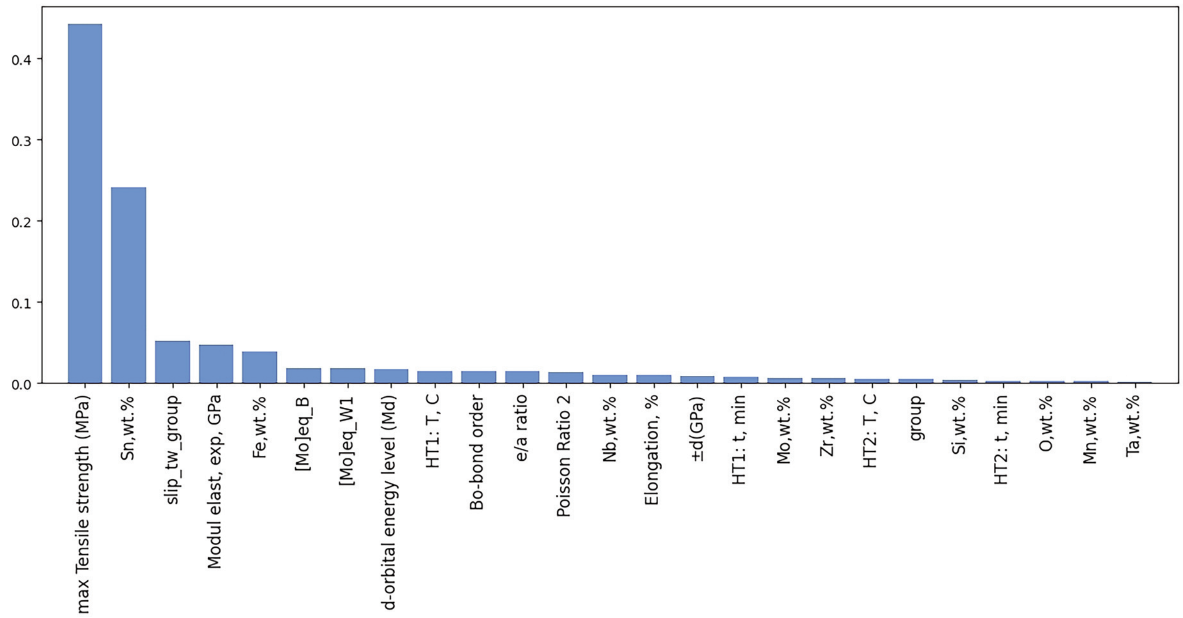

Figure 6. *Feature importance for yield strength showing the content of tin as the most influential parameter, beside Tensile strength*

from twisting to the transformation and then to sliding was observed, resulting in a higher yield stress [40].

Despite all the mentioned achievements and benefits of the applied models, there are also limitations, especially concerning the data related to the mass concentrations of oxygen, nitrogen and hydrogen as impurities in the alloys. Currently, only the mass fraction of oxygen content is considered in the predictions, depending on availability. In addition, the lack of information on the porosity of the alloy is a significant limitation. In certain studies, the precise dimensional changes after mechanical treatments remain undetected, with only the final dimensions of the product. However, a complicating factor arises from the scarcity of new alloys' characterization reported data. All these aforementioned issues can greatly impact the predictive models under discussion, therefore requiring consideration in future research work.

4. Conclusion

Using the Extra Trees Regressor model has provided valuable insight into predicting the mechanical properties of titanium alloys critical for biomedical applications. We found that integrating Poisson's ratio and heat treatment parameters made the prediction of Young's modulus more accurate, achieving an R^2 value of approximately 0.793 in the test set and reducing the MAE from 7,402 to 7,160 GPa.

In addition, our models showed strong predictive performance for both yield strength and tensile strength, despite a not particularly-large database. Moreover, the mass content of iron that affects the tensile strength, and the mass content of tin that affects the yield stress were identified, and the correlation coefficient was 0.893 and 0.868, respectively.

Although the built model showed significant reliability in predicting the target properties, it is necessary to point out the limitations arising from the incomplete data on the impurity concentrations (oxygen, nitrogen, hydrogen), the porosity of the alloys, as well as the changes resulting from mechanical treatment.

Looking ahead, further research should investigate additional variables such as the impurity mass content, the alloy porosity, and the strain values after mechanical processing to refine the prediction models for titanium alloys, improving their accuracy and suitability for biomedical applications.

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Author Contributions

Conceptualization, investigation, supervision, V. M.; investigation, formal analysis, data curation, *G.M. And D. M.; investigation, formal analysis, G.M.; software, methodology, validation, V.M., G.M. and M.S.; conceptualization, data curation, writing—original draft preparation, supervision, G.M. and J. R. All authors have read and agreed to the final version of the manuscript.*

Data Availability Statement

The data presented in this study are available on request from the corresponding author.

Conflicts of Interest

The authors declare no conflicts of interest.

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PREDVIĐANJE MODULA ELASTIČNOSTI, GRANICE RAZVLAČENJA I ZATEZNE ČVRSTOĆE U BIOKOMPATIBILNIM LEGURAMA TITANIJUMA

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Apstrakt

Biokompatibilne legure titanijuma imaju uravnoteženu kombinaciju poboljšanih mehaničkih svojstava i dobre biokompatibilnosti, što ih čini važnim materijalima u biomedicinskom inženjeringu. Postoji sve veća potražnja za ovim novim legurama sa superiornim svojstvima. Pored toga, postoji potreba za razumevanjem odnosa između parametara i svojstava, a mašinsko učenje se koristi kako bi ceo proces bio jeftiniji i efikasniji. Cilj ove studije je razvijanje preciznih modela mašinskog učenja za predviđanje mehaničkih svojstava: modula elastičnosti, zatezne čvrstoće i granice razvlačenja, specifično korišćenjem modela „Extra Trees Regressor“. U poređenju sa prethodnim rezultatima, uočeno je poboljšanje modela za predviđanje modula elastičnosti nakon uključivanja podataka o parametrima termičke obrade i Poasonovog odnosa. Ovo se odrazilo na smanjenje MAE sa 7,402 na 7,160 GPa. Kreirani su modeli za predviđanje vrednosti zatezne čvrstoće i granice razvlačenja, pri čemu su gvožđe i kalaj bili najznačajnije karakteristike, dok su koeficijenti korelacije za testni set bili 0,893 i 0,868.

Ključne reči: *Modul elastičnosti; Zatezna čvrstoća; Granica razvlačenja; Biokompatibilnost; Mašinsko učenje*