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Investigation of the Effect of Alloying Elements on the Density of Titanium-Based Biomedical Materials Using Explainable Artificial Intelligence

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ABSTRACT Titanium alloys are widely preferred in the healthcare sector as biocompatible materials due to their superior properties such as low density and exceptional mechanical strength. Their low density provides lightweight solutions, and their density is closer to that of human bone compared to other metallic alloys with similar strength. This similarity facilitates a balanced load distribution between the bone and the implant, enhancing biomechanical compatibility. This study investigates the effects of alloying elements on the density of titanium-based biomedical materials using a computational materials science approach. A total of 72 different compositions of Ti-Al-V alloys were modeled using JMatPro software, and their densities were simulated at room temperature (25℃). The simulation produced a comprehensive dataset, which was utilized to train an explainable artificial intelligence (XAI) model. Advanced interpretability techniques, including SHAP (SHapley Additive exPlanations), LIME (Local Interpretable Model-agnostic Explanations), and Partial Dependence Plots (PDP), were employed to elucidate the influence of each alloying element on the density. The dataset was analyzed using an XAI-based regression model implemented with the Artificial Neural Network (ANN) algorithm. The interpretability graphs provided insights into the individual contributions of the alloying elements, revealing their positive or negative effects on the density. The findings offer a deeper understanding of the role of alloying elements in optimizing the performance of titanium-based biomedical materials, particularly in achieving lightweight designs. This study highlights the potential of integrating computational material modeling with explainable AI to advance the design and development of high-performance lightweight materials for biomedical applications.

KEYWORDS
Explainable artificial intelligence
Computational materials science
Biomedical materials
Titanium alloys

INTRODUCTION

Titanium and its alloys are widely recognized for their superior properties, such as low density, excellent mechanical strength, high corrosion resistance, and outstanding biocompatibility, which make them ideal candidates for biomedical applications. Among metallic materials, titanium's similarity in density to human bone allows for better load distribution, significantly enhancing its biomechanical compatibility as an implant material (Niinomi 2008). Over the years, extensive research has been conducted to improve the performance of titanium alloys by modifying their chemical compositions with alloying elements, focusing on achieving optimized mechanical properties and enhanced biological compatibility (Madalina Simona *et al.* 2019; Ikedaa *et al.* 2020).

Alloying elements such as niobium (Nb), tantalum (Ta), and zirconium (Zr) have been shown to positively influence the properties of titanium alloys. These elements not only reduce the elastic modulus, which minimizes the stress shielding effect, but also improve the alloys' strength, wear resistance, and corrosion resistance. This is particularly important in biomedical contexts where the implant material must integrate effectively with surrounding tissues while maintaining structural integrity under physiological loads (Zhou *et al.* 2007; Hayyawi *et al.* 2022). For instance, beta-titanium alloys incorporating Nb and Ta exhibit low Young's modulus and excellent biocompatibility, making them ideal for orthopedic and dental applications (Phume *et al.* 2012; Ivanov *et al.* 2018).

The development of titanium-based biomedical materials also addresses concerns regarding the cytotoxicity of conventional alloys such as Ti-6Al-4V, where the presence of vanadium and aluminum may pose health risks. Research has shifted towards creating non-toxic titanium alloys by incorporating elements such as niobium and zirconium, which maintain high mechanical performance while eliminating adverse biological effects (Manojlović and Marković 2023; Li *et al.* 2011). Furthermore, advanced manufacturing techniques like additive manufacturing enable the production of patient-specific implants, providing opportunities to tailor the properties of titanium alloys to meet specific clinical needs (Alqattan *et al.* 2020; Niinomi *et al.* 2016).

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Recently, computational materials science and machine learning approaches have emerged as powerful tools for exploring the effects of alloying elements on the performance of titanium alloys. Explainable Artificial Intelligence (XAI) methods, such as SHAP and LIME, provide valuable insights into how each alloying element contributes to key properties, guiding the development of lightweight and biocompatible titanium materials (Bărbînţă *et al.* 2013; Toğaçar *et al.* 2022, 2021). By integrating experimental and computational findings, researchers are now better equipped to design high-performance titanium alloys for biomedical applications, further advancing the field of implant materials science.

MATERIALS AND METHODS

This study investigates the effects of alloying elements on the density of titanium-based biomedical materials through a computational and data-driven approach. A total of 72 different compositions of Ti-Al-V alloys were modeled using JMatPro software, enabling accurate simulation of material densities at room temperature (25°C). The simulation results formed a comprehensive dataset, which was subsequently used to train an Artificial Neural Network (ANN)-based explainable AI (XAI) model. Advanced interpretability techniques, including SHAP (SHapley Additive exPlanations), LIME (Local Interpretable Model-agnostic Explanations), and Partial Dependence Plots (PDP), were applied to analyze the influence of individual alloying elements on density. This integrated methodology combines computational material science and machine learning to provide insights into the relationship between composition and material properties, guiding the optimization of lightweight titanium alloys for biomedical applications.

Dataset Preparation

The dataset utilized in this study comprises 72 different Ti-Al-V-based alloy compositions, which were modeled within the compositional ranges provided in Table 1. The titanium content ranged from 77% to 94%, while aluminum (Al) and vanadium (V) varied between 3–7% and 2.5–5.4%, respectively. Trace elements such as tin (Sn), zirconium (Zr), and molybdenum (Mo) were included within limited ranges (0–2%, 0–4%, and 0–4%). These specific composition ranges were selected based on their prominence in biomedical alloy design, particularly to achieve optimal density and mechanical properties (Brusewitz Lindahl *et al.* 2015). Each of the 72 alloy compositions was modeled using JMatPro software, and the density values at room temperature (25°C) were calculated and recorded for each entry.

The choice of these composition ranges stems from the widespread use of titanium-based alloys, particularly Ti-Al-V combinations, in biomedical applications such as orthopedic and dental implants (Kartamyshev *et al.* 2020). Titanium, as the base material, offers excellent biocompatibility, corrosion resistance, and a density closer to that of human bone (Li *et al.* 2024). Aluminum is included to stabilize the α-phase, providing strength and reducing weight, while vanadium contributes to the β-phase, improving the alloy's flexibility and toughness (Luan *et al.* 2017). However, excessive amounts of V and Al may lead to biocompatibility concerns, prompting exploration of their optimal content (Bodunrin *et al.* 2020). Elements like Zr, Sn, and Mo were introduced to further enhance specific properties, such as strength, corrosion resistance, and stability, without compromising biocompatibility (Sun and Mi 2023). The simulation of density values at room temperature was essential to evaluate the lightweight nature of the modeled alloys. Room temperature properties are particularly relevant for biomedical applications where implants must retain consistent structural and mechanical integrity under physiological conditions (Alipour *et al.* 2022). By systematically analyzing 72 alloy compositions, this study provided a comprehensive dataset for training an explainable AI model to elucidate the contributions of individual elements to the density of titanium-based materials. Such insights are critical for advancing the design of lightweight, high-performance biomedical materials optimized for biomechanical compatibility (Wan *et al.* 2020).

Development of the Explainable Artificial Intelligence Model In this study, an Artificial Neural Network (ANN)-based regression model was employed to predict the density of titanium-based biomedical materials, replacing conventional machine learning algorithms such as XGBoost. ANNs are widely recognized for their capability to model complex, non-linear relationships in high-dimensional datasets, making them ideal for applications in material science where properties depend on intricate compositional interactions (Valipoorsalimi 2023). The use of ANN ensures robust predictions by simulating material density for the 72 compositions of titanium alloys. This approach was particularly advantageous given the non-linear and multivariable nature of the relationship between alloying elements and material properties (Maitra *et al.* 2024).

The ANN regression model was trained on a comprehensive dataset generated through simulations using JMatPro software, where the density values of titanium-based alloys were computed at room temperature (25°C). The network architecture was optimized by fine-tuning hyperparameters such as the number of hidden layers, neurons per layer, activation functions, and learning rates to minimize errors and improve generalization capability (Hagan *et al.* 2014). To prevent overfitting, regularization techniques such as dropout and L2 weight penalties were incorporated, ensuring that the ANN model remained robust across the dataset. The high predictive accuracy achieved by the ANN highlights its suitability for capturing complex relationships within the data (Goodfellow *et al.* 2016).

To ensure the transparency and interpretability of the developed ANN model, Explainable Artificial Intelligence (XAI) methods, including SHAP (SHapley Additive exPlanations), LIME (Local Interpretable Model-agnostic Explanations), and Partial Dependence Plots (PDP), were integrated into the analysis. XAI techniques address the "black-box" nature of neural networks, providing insights into how the input features (alloying elements) influence the model's predictions (Lundberg and Lee 2017). This step is particularly crucial in material design and biomedical applications, where understanding the effect of alloying elements on density can guide the development of lightweight, high-performance materials (Ribeiro *et al.* 2016).

SHAP was utilized to quantify the contribution of each alloying element to the predicted density. By leveraging Shapley values from cooperative game theory, SHAP ensures fair attribution of feature importance to the model's predictions (Scavuzzo *et al.* 2022). This method offers both local (individual predictions) and global (model-wide) interpretability, enabling a detailed analysis of how elements like aluminum, vanadium, zirconium, and tin influence the material density. For example, it was observed that increasing the vanadium content consistently reduced density, while aluminum showed a more complex interaction, stabilizing density within a specific range (Sun and Mi 2023).

LIME was implemented to further enhance local interpretability by generating simplified surrogate models for individual predic-

Table 1 Elemental Composition Ranges of Alloys in the Dataset (values represent wt%)

Ti (%)	Al (%)	V (%)	Sn (%)	Zr (%)	Mo (%)	Fe (%)	N (%)	C (%)	H (%)	O (%)
77–94	3–5–7	2.5–3.5–4.5	0 and 2	0 and 4	0 and 4	0.3	0.05	0.08	0.015	0.2

tions. LIME creates perturbations around specific alloy compositions and fits an interpretable model, such as linear regression, to approximate the behavior of the ANN model locally (Ferdib-Al-Islam *et al.* 2023). This approach allowed for a clearer understanding of the decision-making process for specific alloy compositions, ensuring that model predictions aligned with physical and chemical principles. The combination of SHAP and LIME provided a multi-faceted view of model behavior, improving confidence in the ANN predictions.

Finally, Partial Dependence Plots (PDPs) were employed to visualize the global effects of individual features on the predicted density. PDPs reveal the average influence of an alloying element while holding other elements constant, enabling the identification of critical compositional ranges for density optimization (Friedman 2001). By integrating PDPs into the analysis, it was possible to uncover non-linear dependencies and interactions, offering valuable insights into the optimal ranges for alloying elements. For example, Zr and Sn demonstrated significant effects on density only within specific intervals, highlighting their potential for fine-tuning material properties.

RESULTS AND DISCUSSION

In this study, the influence of alloying elements on the density of titanium-based biomedical materials was analyzed using an explainable artificial intelligence (XAI) approach. The ANN-based regression model demonstrated high predictive accuracy for density values, supported by advanced interpretability techniques such as SHAP, LIME, and Partial Dependence Plots (PDP). These methods provided comprehensive insights into the individual and combined effects of alloying elements, enabling the identification of critical ranges and interactions. The results revealed that certain alloying elements, such as zirconium (Zr) and tin (Sn), play a significant role in enhancing the density, while others, such as molybdenum (Mo) and vanadium (V), contribute to reducing the density. These findings underline the potential of integrating computational materials science with XAI to optimize the design of lightweight titanium alloys for biomedical applications.

The results of the XAI analysis are illustrated in Figure 1, which presents the predicted density value and the contribution of each alloying element. The predicted density of the alloy composition is approximately 4.60 g/cm³, as shown on the horizontal bar. The SHAP plot highlights the positive (orange) and negative (blue) contributions of individual elements. Notably, Zr ($0.98 \leq Zr \leq 1.02$ wt%) and Sn ($-0.95 \leq Sn \leq 1.05$ wt%) exhibit the most significant positive effects on density, while Mo and Al negatively impact the overall density. This visualization underscores the critical role of individual alloying elements and their optimized compositions in achieving the desired material properties for biomedical applications.

Figure 2 highlights the contributions of key alloying elements to the density of titanium-based biomedical materials. The analysis reveals that zirconium (Zr), tin (Sn), and aluminum (Al) have the most significant positive impacts, with feature values of 1.02, 1.05,

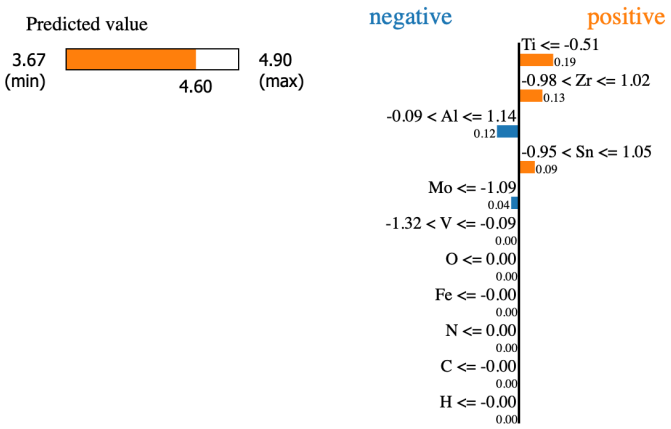

Figure 1 Predicted density and SHAP-based contributions of alloying elements in titanium-based biomedical materials

and 1.14, respectively. These elements play a vital role in optimizing the density while maintaining the mechanical properties of the alloy. Conversely, molybdenum (Mo) and vanadium (V) exhibit slight negative contributions (-1.09 and -0.09), reflecting their density-reducing characteristics. Titanium (Ti), as the base element, demonstrates a moderate negative impact (-0.80), consistent with its lightweight nature. The negligible contributions of other elements (O, Fe, N, C, H) suggest their minimal influence on the alloy's density within the studied composition. These insights provide a comprehensive understanding of how specific elements contribute to achieving desired material properties for biomedical applications.

Feature	Value
Ti	-0.80
Zr	1.02
Al	1.14
Sn	1.05
Mo	-1.09
V	-0.09
O	0.00
Fe	-0.00
N	0.00
C	-0.00
H	-0.00

Figure 2 Contributions of Alloying Elements to Density

Figure 3 presents the LIME (Local Interpretable Model-Agnostic Explanations) analysis for the contributions of individual alloying elements to the density of a specific titanium-based composition. Positive contributions are shown in green, while negative ones are indicated in red. Tin (Sn) and aluminum (Al) are the most

significant positive contributors, with their effects observed within the ranges -0.95 < Sn $\leq$ 1.05 and -0.09 < Al $\leq$ 1.14, respectively. Titanium (Ti) also exhibits a moderate positive impact. Zirconium (Zr) shows a neutral to slightly positive influence, whereas molybdenum (Mo) and vanadium (V) contribute negatively, reducing the density. Elements such as oxygen (O), iron (Fe), nitrogen (N), carbon (C), and hydrogen (H) display negligible contributions, highlighting their limited role in this specific alloy composition. These results provide localized insights into the effects of alloying elements, enabling targeted optimizations for biomedical material design.

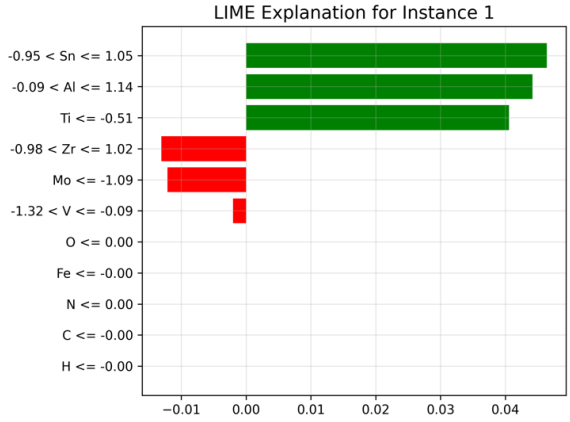

Figure 3 LIME Explanation of Alloying Element Contributions

Figure 4 presents the SHAP dependence plots for various alloying elements, providing insights into their individual contributions to the predicted density of titanium-based biomedical materials. The plots reveal that aluminum (Al) and tin (Sn) have strong positive effects on density, showing a direct relationship as their values increase. Zirconium (Zr) exhibits a nonlinear contribution, with its optimal effect occurring within a specific range. Conversely, vanadium (V) and molybdenum (Mo) contribute negatively, reducing density as their values increase. Elements like oxygen (O), nitrogen (N), carbon (C), and hydrogen (H) show negligible SHAP values, indicating minimal influence on density. These results highlight the importance of optimizing the composition of critical elements such as Al, Sn, and Zr to achieve desired density properties in biomedical applications.

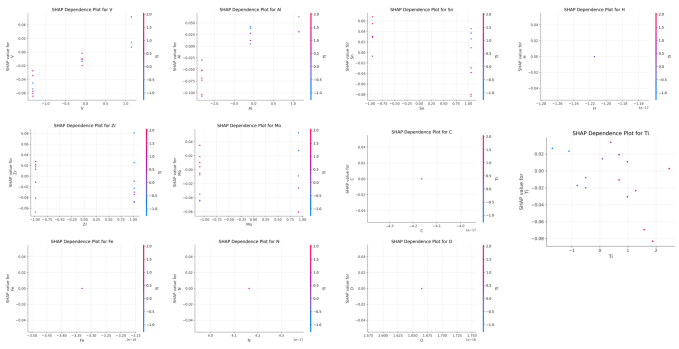

Figure 4 SHAP Dependence Plots for Alloying Elements

CONCLUSION

This study investigated the effects of alloying elements on the density of titanium-based biomedical materials using a computational materials science approach integrated with explainable artificial intelligence (XAI). The findings demonstrated that specific elements, such as aluminum (Al), tin (Sn), and zirconium (Zr), play a critical role in enhancing density, while others like molybdenum (Mo) and vanadium (V) reduce it. SHAP and LIME analysis provided valuable insights into the contributions of individual elements, revealing their importance in achieving optimal density for lightweight and biocompatible materials. The integration of computational modeling with XAI enables precise evaluation of complex relationships between alloy compositions and material properties, offering a systematic approach to improving implant designs.

Future studies should explore a broader range of alloying elements and their interactions to optimize additional properties such as mechanical strength, corrosion resistance, and biocompatibility. Advanced machine learning techniques combined with experimental validation can further enhance the reliability of predictions and provide a more comprehensive understanding of material performance under physiological conditions. The adoption of such data-driven methodologies holds significant potential for advancing the development of high-performance titanium alloys tailored for specific biomedical applications.

Availability of data and material

Not applicable.

Conflicts of interest

The authors declare that there is no conflict of interest regarding the publication of this paper.

Ethical standard

The authors have no relevant financial or non-financial interests to disclose.

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