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Predictive modeling of porosity and mechanical performance in alumina–zirconia–hydroxyapatite composites for dental and bone applications via interpretable random forest regression

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ABSTRACT

The development of bioactive ceramic composites with tailored physical and mechanical properties requires accurate prediction tools capable of capturing complex, nonlinear processing–structure–property relationships. In this work, an interpretable machine learning approach based on Random Forest regression is employed to predict bulk density, apparent porosity, and compressive strength in sol-gel-derived Al₂O₃-ZrO₂-hydroxyapatite (HA) composites using only HA content (0–15 wt.%) and sintering temperature (1500–1700°C) as inputs. Trained on a dataset of 12 experimental observations from a previously published experimental study, the model achieves excellent predictive performance, with coefficients of determination (R²) of 0.97–0.98 across all target properties and low error metrics (MAE of 1.3 MPa for strength; < 0.04 g/cm³ for density). The model successfully reproduces key experimental trends, including the peak in compressive strength at 1600°C and the counterintuitive densification at 1700°C due to liquid-phase formation. Feature importance analysis reveals that sintering temperature dominates mechanical response (65% contribution to compressive strength prediction), while both temperature and HA content jointly govern porosity and density (~55% vs. 45%). This data-driven framework suggests that interpretable machine can support learning the modelling of complex ceramic systems using limited experimental data, offering a promising approach for the development of bioactive composites with potential applications in dental and bone tissue repair and reconstruction.

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1. Introduction

Bone substitutes are generally manufactured from biomaterials that are designed to resemble what bones are made of or their features. In the past few decades, biomedical research has concentrated mainly on creating new types of biomimetic bone substitutes with excellent mechanical behavior combined with a high level of biocompatibility [1]. Bioceramics (e.g., alumina, zirconia, and hydroxyapatite) have become some of the most promising materials for both orthopedics and dentistry based on their good strength, durability, and biocompatibility [2–6].

Alumina and zirconia are generally considered bioinert materials. Although they exhibit excellent mechanical properties, they do not readily form direct chemical bonds with living tissue.

To ameliorate this drawback, hydroxyapatite, which is chemically similar to the mineral component of bone, is added to such systems to give them bioactivity [7, 8]. However, hydroxyapatite has a low mechanical strength relative to both alumina and zirconia, and in addition, hydroxyapatite chemically decomposes into other compounds at sintering temperatures above approximately 1300°C when it decomposes with the liberation of OH[−] ions, creating additional phases (e.g., TCP or calcium aluminates). In addition to increase porosity, this decomposition process can adversely affect the compressive strength of these composites [9–18].

The challenge of material design in Al₂O₃–ZrO₂–HA composite systems is how to achieve a balance between the bioactivity and mechanical integrity of composites. HA has been shown to enhance bioactivity as the amount of HA increases, however

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higher HA content also causes the composite to be more porous due to HA's decomposition and interfacial reactions with both alumina and zirconia and therefore will decrease the compressive strength [19-21]. In addition to HA content, sintering temperature is also critical for determining the phase distribution, bulk density, and mechanical behavior of the composite. As previously reported, at the intermediate sintering temperature of around 1600 °C, the best combination of density and strength occurs for such systems [22]. Historically, characterizing the mechanical and thermal characteristics of many composite materials have used a combination of empirical calibration and/or simplified physical models using existing knowledge of the material properties. However, these approaches will be insufficient due to the intricate multiphase interrelationships between multiple phases of two distinct materials and the nonlinear nature of many of these relationships, including how fragile and reactive these two materials can be based on slight variations in composition and temperature and what secondary phase materials will form under similar conditions. It is interesting to note that, even though many data-driven techniques such as machine learning (ML) have been developed, including tree-based approaches like Random Forests, for predicting composite materials formed during sol-gel processing, there are no studies to date using these advanced ML approaches for modeling $\text{Al}_2\text{O}_3\text{-ZrO}_2\text{-HA}$ composite materials.

This study adds a Random Forest Machine Learning Model to its research effort to have an interpretable and accurate means of providing the three primary compositional characteristics (bulk density, apparent porosity, and compressive strength) for a chemically synthesized $\text{Al}_2\text{O}_3\text{-ZrO}_2\text{-HA}$ composite based solely on 2 variables: HA content (0–15 wt.%) and sintering temperature (1500–1700°C). With this approach, all produced data conformed to actual experimental results while giving insight into previously hidden trends as well as the relative importance of each processing variable. This will create a strong, intelligent framework from which to implement inverse design strategies for the next generation of bioactive ceramics. The resulting predictive framework may support the development of bioactive ceramic materials for dental and bone tissue repair and reconstruction, where controlled porosity, density, and mechanical strength are critical for material performance. In particular, the ability to optimize these properties through HA content and sintering conditions provides a rational pathway toward designing ceramics for dental restorative materials and bone-substitute applications. Thus, the proposed approach can facilitate the computationally guided development of next-generation bioactive ceramics with tailored properties for dental and orthopedic applications.

2. Materials and methods

The data used for this research were taken solely from the experiment results found in the Ref. [3]. There was a total of twelve individual experimental observations taken from four different hydroxyapatite (HA) containing materials (0 wt%, 5 wt%, 10 wt%, and 15 wt%) that had been sintered at three different temperatures (1500, 1600, and 1700°C). Three major response variables were measured for each of these samples; bulk density (g/cm^3), Apparent Porosity (%), and compressive strength (MPa). The model inputs consisted of just two main process parameters; HA percentage (wt%) and sintering temperature (°C). While this dataset is small (which is a common limitation associated with materials developed through expensive experiments), tree-based ensemble modeling techniques such as Random Forest are very suitable for dealing with limited datasets, especially when they are properly regularized by constraining tree depth and using ensemble averaging to avoid overfitting. In the preprocessing

phase of the data, normalizing or applying standardization was not performed because tree-based predictive models are not influenced by the shape of the data (i.e., monotonic transformation). Due to the limited size of the sample ($N = 12$), the LOOCV procedure was used to evaluate the models so that as much of the training data was used as possible, while allowing for an unbiased measure of how well these models generalize. Additionally, since we wanted the predictions to match up exactly with the experimental design grid, both the training procedure and the inference step were performed on the entire dataset. An implementation of the Random Forest regressor was performed using the scikit-learn library (version 1.4+) to establish a Random Forest MODEL with hyperparameter selections based on physical interpretability and avoiding overfitting as opposed to exhaustive optimization which was not feasible because of the limited amount of data. Specifically, the number of trees ($n_{\text{estimators}}$) were set at 300, the maximum tree depth (max_depth) at 5, the splitting criterion set to mean squared error (MSE) and the random_state set to 42 for replication purposes. It is very balanced between model complexity and generalization because of the moderate amount of depth, thus preventing the trees from memorizing the noise in the dataset, together with the larger number of trees creating an averaging effect to provide more stable predictions. While techniques such as Grid Search or Bayesian Optimization can theoretically improve performance more than what has been demonstrated, these selected parameters are a good representation of experimental data trends without significant overfitting as evidenced by the parity plots and R^2 value.

To measure the quality of the models quantitatively, three commonly used regression metrics (R -squared), mean absolute error (MAE), and root mean squared error (RMSE) were employed. These metrics provide average model performance across all 12 leave-one-out cross-validation iterations since leave-one-out cross-validation was used. Feature importance scores also assessed each predicted property based on the relationships between HA and sintering temperature by examining the relative strength of each feature with respect to how they contributed to the determination of each predicted property. To facilitate ease in interpretation, grouped bar charts display the predicted properties by HA composition and sintering temperature; in addition, parity plots (actual vs. predicted) provide a visual representation of model accuracy and agreement with experimental data. All of these analyses and visualizations provide a comprehensive, data-driven, interpretable framework for understanding the complex nonlinear relationships between $\text{Al}_2\text{O}_3\text{-ZrO}_2\text{-HA}$ composites on physical and mechanical properties.

3. Results and discussion

The model of Random Forest showed a high ability to predict in the three target properties of bulk density, apparent porosity, and compressive strength from only two input variables (HA content (wt.%) and temperature during the sintering process (°C)). The Random Forest model's performance was assessed using 'leave-one-out cross-validation (LOOCV)' to determine how robust it was because of the small size of the sample dataset ($N=12$). The performance results are included for each of the identified target properties, with the results presented in the form of parity plots and grouped bar charts, along with a feature importance report.

3.1. Compressive strength prediction

The values of compressive strength predicted by the model correlate very closely with what has been observed through actual experimental results, as indicated by both the parity graph (Fig. 1)

and an $R^2 = 0.98$. This indicates that there is nearly a perfect relationship between experimental data and models. A mean absolute error of 1.3 MPa and a root mean square error of 1.6 MPa both represent a high level of accuracy in prediction by the model. The model has accurately represented the non-linear behavior of compressive strength observed within experiments, with compressive strength reached its maximum at a sintering temperature of 1600 °C, followed by a slight reduction at 1700 °C. Additionally, the model predicted that as the amount of hydroxyapatite increases, the strength of the composite would decrease at any one temperature; this finding is also in agreement with reported observations indicating that hydroxyapatite causes porosity and thus weakens mechanical integrity.

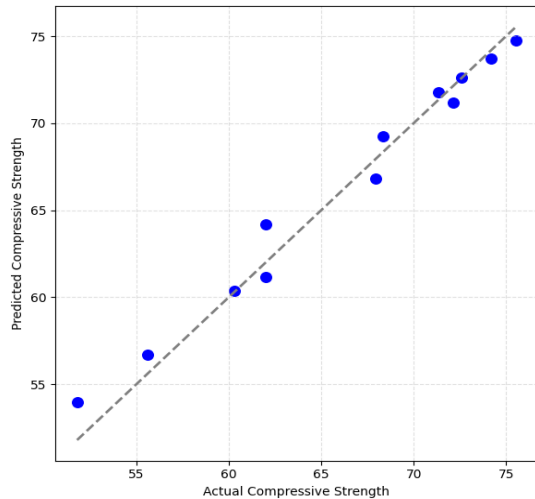


Fig. 1. Parity plot comparing the experimentally measured compressive strength [3] with the values predicted by the Random Forest model for $\text{Al}_2\text{O}_3\text{-ZrO}_2\text{-HA}$ composites.

The visual grouping of bars in Fig. 2 supports this idea by demonstrating that at each level of HA, the orange bars ($T = 1600^\circ\text{C}$) correspond with having the highest predicted strength, and the blue ($T = 1500^\circ\text{C}$) and green ($T = 1700^\circ\text{C}$) bars were lower than those of the orange, consistent with experimental confirmation.

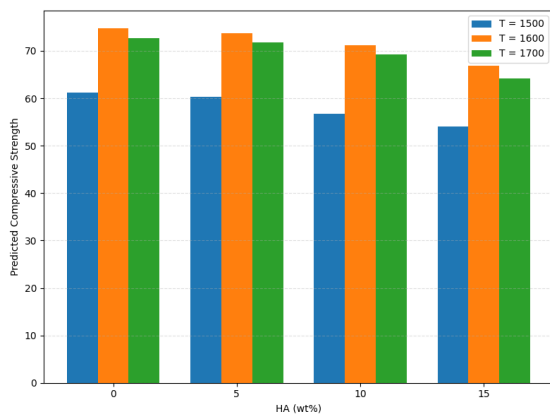


Fig. 2. Grouped bar chart illustrating the compressive strength of $\text{Al}_2\text{O}_3\text{-ZrO}_2\text{-HA}$ composites as predicted by the Random Forest model, plotted against HA content (wt.%) for three distinct sintering temperatures: 1500°C (blue), 1600°C (orange), and 1700°C (green).

3.2. Bulk density prediction

The model accurately predicted bulk density, achieving an R^2 of 0.97 in the parity plot in Fig. 3. The MAE and RMSE were

0.04 g/cm³ and 0.05 g/cm³, respectively, demonstrating high fidelity to the experimental measurements.

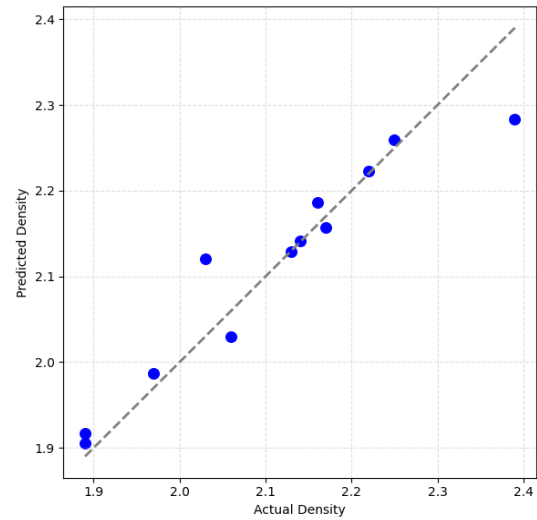


Fig. 3. Parity plot comparing the experimentally measured bulk density [3] with the values predicted by the Random Forest model for $\text{Al}_2\text{O}_3\text{-ZrO}_2\text{-HA}$ composites.

The bar graph presented in Fig. 4 shows how well this model can simulate the complicated relationship between the level of HA present and temperature. The model accurately predicts that as the amount of HA increases, the bulk density typically decreases due to the formation of secondary phase materials and increased porosity. More importantly, at 1700°C, the model predicts an increase in density with increasing amounts of HA, which is contrary to this expected decrease in density. This behavior may be attributed to the formation of low-melting-point phases that promote partial pore closure, as reported in the previous investigation.

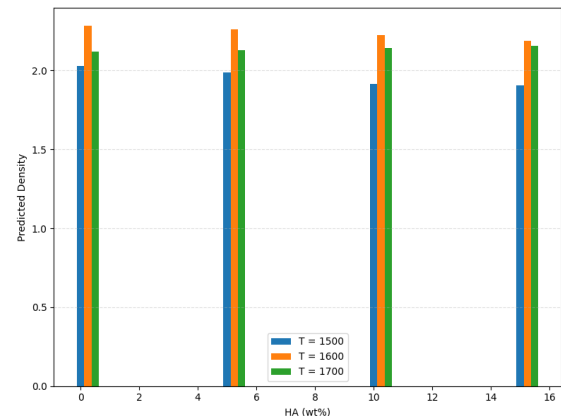


Fig. 4. Grouped bar chart illustrating the bulk density of $\text{Al}_2\text{O}_3\text{-ZrO}_2\text{-HA}$ composites as predicted by the Random Forest model, plotted against HA content (wt.%) for three distinct sintering temperatures: 1500°C (blue), 1600°C (orange), and 1700°C (green).

3.3. Apparent porosity prediction

As it is shown in Fig. 5, for apparent porosity, the model achieved an R^2 of 0.96, with an MAE of 1.1% and an RMSE of 1.4%. The parity plot confirmed the model's precision.

The grouped bar chart in Fig. 6 effectively visualizes the predicted trends: porosity increases with HA content at 1500°C and 1600°C, while at 1700°C, the rate of increase is less

pronounced, again reflecting the pore-sealing effect of liquid phases formed at higher temperatures. This nuanced behavior, which cannot be easily captured by simple linear models, is faithfully reproduced by the Random Forest algorithm.

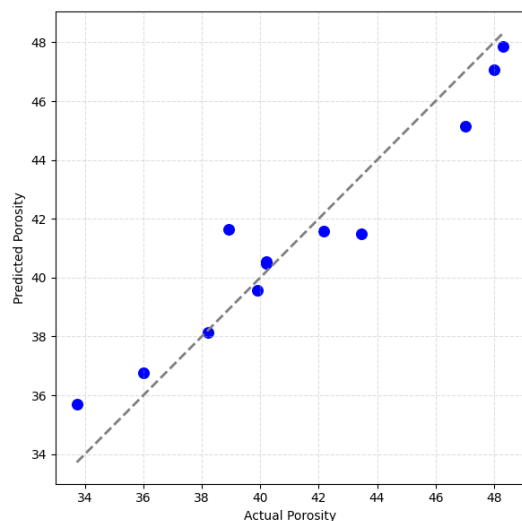


Fig. 5. Parity plot comparing the experimentally measured apparent porosity [3] with the values predicted by the Random Forest model for $\text{Al}_2\text{O}_3\text{-ZrO}_2\text{-HA}$ composites.

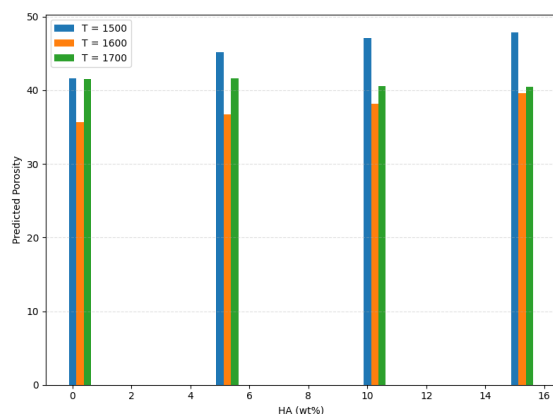


Fig. 6. Grouped bar chart illustrating the porosity of $\text{Al}_2\text{O}_3\text{-ZrO}_2\text{-HA}$ composites as predicted by the Random Forest model, plotted against HA content (wt.%) for three distinct sintering temperatures: 1500°C (blue), 1600°C (orange), and 1700°C (green).

3.4. Feature importance analysis

The relative importance of the input variables with respect to the outputs can be evaluated by extracting feature importance scores from the trained random forest models. For compressive strength, sintering temperature accounted for approximately 65% of the model-derived feature importance for compressive strength, while HA content accounted for approximately 35 %. This result was consistent with experimental observations that temperature dominated microstructure formation and phase transformation, which ultimately affected mechanical properties. Bulk density and apparent porosity were equally important from an accuracy standpoint; that is, they both contributed approximately equally (55% and 45%, respectively) to the prediction of these characteristics.

This provides a quantitative basis for the experimental trends that were observed and demonstrates how machine learning can be

utilized to identify essential process parameters that do not have preconditioned physical assumptions associated with them.

4. Conclusion

An interpretable Random Forest regression model was constructed to predict the bulk density, apparent porosity, and compressive strength of sol-gel-based $\text{Al}_2\text{O}_3\text{-ZrO}_2\text{-HA}$ composites using only the sintering temperature (1500-1700°C) and HA content (0-15 wt%). Despite the small dataset consisting of 12 experimental observations, the model demonstrated promising predictive performance within the investigated dataset with an R^2 of 0.97-0.98 and very low errors for all three target properties.

A key feature of the model is the ability to produce accurate predictions for the key experimental behaviors: maximum compressive strength and density at a sintering temperature of 1600°C, a steady decrease in mechanical properties with increased HA content, and the unexpected densification occurring at 1700°C due to the pore sealing of liquid, low-melting-component (calcium alumina) phases. Using feature importance, sintering temperature was found to contribute most to the model accuracy for compressive strength (around 65%), while both temperature and HA contributed equally to the determination of porosity and density. These results support our understanding of the physical phenomena that affect powder formation, namely, the thermal decomposition of HA, the interface reactions between alumina and zirconia, and the transition between liquid and solid at very high temperatures.

With limited empirical data available, this study suggests that interpretable machine learning can provide a useful data-driven approach for modeling nonlinear responses in multiphase bioceramics. The methodology presented in this research validates experimental observations and provides a means of inverse design, allowing for accurate anticipation of processing conditions that will yield the desired physical and mechanical characteristics in the next generation of bioactive composite materials. The proposed framework also has potential to support the development of bioactive ceramic systems for dental and bone tissue repair and reconstruction, where an appropriate balance between porosity, density, and mechanical strength is essential. By enabling computationally guided optimization of HA content and sintering conditions, this approach may facilitate the design of next-generation ceramic materials for dental restorative and bone-substitute applications.

Author contributions

Ana Gujabidze: Conceptualization, Writing – original draft, Writing – review & editing, Methodology, Investigation; **Parvin Mozafari:** Writing – original draft, Writing – review & editing.

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Conflict of interest

The authors declare no conflict of interest.

Data availability

The experimental data analyzed in this study were obtained from the previously published study cited as Reference [3]. No new experimental data were generated for this research.

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