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Research Article

Analyzing Temperature-Dependent Thermal Properties of Biomaterials Using Machine Learning Methods

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Abstract: This research utilizes machine learning models ANN, Random Forest, and Decision Tree to predict material properties of Ti-based biomaterials, including Young's modulus, density, thermal conductivity, and specific heat at various temperatures. Data was sourced using web scraping and Plot Digitizer, validated against literature, and analyzed in Excel. The ANN model achieved strong performance, with $R^2 = 0.980874$ for TiAl and $R^2 = 0.997607$ for TiCu, effectively predicting density and Young's modulus but showing deviations in band gap. For TiO_2, the ANN model demonstrated solid predictions but struggled with band gap and specific heat accuracy. Random Forest yielded high accuracy for TiAl ($R^2 = 0.998168$) and TiO_2 ($R^2 = 0.9994$) and its ability to generalize well and capture complex relationships in the data makes it the most reliable method for this study. The Decision Tree model accurately predicted specific heat and Young's modulus for TiAl ($R^2 = 0.993841$) and captured trends in TiCu but showed deviations in band gap and thermal conductivity. These results underline the predictive potential of these models while highlighting areas for refinement.

Keywords: ANN, Random Forest, Decision Tree, Titanium, Aluminum, Copper, Oxygen, Temperature Analysis

Introduction

Biomaterials are a distinct class of materials engineered to interact effectively with biological systems, supporting advancements in diverse industries such as healthcare, automotive, agriculture, and consumer goods. These materials—spanning metals, polymers, ceramics, and composites—are developed with precise attributes to serve roles such as structural reinforcement, drug delivery, and tissue repair. The design of biomaterials involves careful consideration of factors such as biocompatibility, mechanical integrity, durability, and environmental sustainability. These features drive innovation across multiple applications while addressing critical global challenges and fostering collaboration across scientific disciplines (Baranwal *et al.*, 2022); (Prodanović & Milutinović, 2017). Titanium was chosen for this research due to its exceptional combination of physical, chemical, mechanical, and electronic properties that make it ideal for developing composite materials like Ti-Al, Ti-Cu, and TiO_2. Its high melting point (1,668°C) ensures stability under extreme conditions, while its low density provides an excellent strength-to-weight ratio. Titanium's outstanding corrosion resistance enhances its durability and its ability to form stable compounds with non-metals at high temperatures further extends its applicability. Additionally, Titanium's mechanical properties, including high tensile strength, hardness, and ductility, contribute to its reliability in demanding environments. While pure Titanium is metallic with no band gap, TiO_2 serves as a semiconductor with a band gap of approximately 3.2 eV, making it valuable in applications such as solar cells and photocatalysis. These unique attributes make Titanium a key material for accurately predicting thermal and mechanical properties using machine learning models.

Titanium Aluminide (TiAl) alloys offer high strength, oxidation resistance, and thermal stability, making them ideal for aerospace and automotive applications. Understanding their thermal and structural behaviour across temperatures is key to optimizing performance and reliability (Ghorbanpour & Lotfiman, 2016; Low *et al.*, 2008).

Equally significant are Titanium Copper (TiCu) alloys, which combine the corrosion resistance and strength of Titanium with the thermal and electrical conductivity of copper. These alloys are widely utilized

in electronics, power generation and precision engineering, where materials must demonstrate exceptional thermal and electrical efficiency. Investigating the thermal behaviour, mechanical properties and structural stability of TiCu alloys under various conditions is essential for extending their applicability in high-performance and sustainable technologies. Titanium Dioxide (TiO_2), on the other hand, is a widely studied material renowned for its multifunctional characteristics, including high chemical stability, excellent photocatalytic activity and versatile optical properties. TiO_2 is pivotal in applications such as photovoltaic systems, environmental remediation and biomedical technologies.

Titanium-based alloys, particularly Titanium Aluminide (TiAl) and Titanium Copper (TiCu) alloys, have garnered significant attention due to their exceptional properties, making them suitable for various high-performance applications. TiAl alloys are recognized for their low density, high strength and excellent oxidation resistance at elevated temperatures, rendering them ideal for the aerospace and automotive industries. For instance, a study published in *Metals* demonstrated that copper alloying in TiAl, combined with multiple laser scans during SLM, enhances the formation of the α_2-Ti_3Al phase, refines the microstructure and improves mechanical properties, thereby broadening the applicability of TiAl intermetallic alloys in high-temperature environments (Polozov *et al.*, 2023). Additionally, research has focused on the development of TiAl–Si alloys, where silicon incorporation influences the manufacturing process, structure, phase composition and selected properties of titanium aluminide alloys (Knaislová *et al.*, 2021). A study published in *Metals* examined the microstructure and mechanical properties of TiAl matrix composites reinforced with Ti_2AlC particles. The research demonstrated that the addition of Ti_2AlC enhances the mechanical properties of TiAl alloys, improving their potential for high-temperature structural applications (Yang *et al.*, 2022).

TiCu alloys combine the advantageous properties of Titanium and copper, offering high strength, good biocompatibility and acceptable corrosion resistance. A study in *Bioactive Materials* investigated the anti-infection ability of TiCu dental implants, revealing that the alloy exhibits significant antibacterial properties against oral microbiota, which are associated with the release of Cu ions. This effect, coupled with good biocompatibility, suggests that TiCu alloys could effectively reduce implant-associated infections (Liu *et al.*, 2022). Furthermore, the mechanical properties and microstructures of Ti–Cu alloys have been explored, indicating that varying copper content influences the alloy's hardness and microstructural characteristics. Research published in *Materials Transactions* demonstrated that increasing copper content leads to the formation of Ti_2Cu intermetallic compounds, which contribute to enhanced hardness and wear resistance, making these alloys suitable for applications requiring high mechanical performance (Luangvaranunt & Pripanapong, 2012). TiCu alloys combine the beneficial properties of Titanium and copper, offering high strength and good corrosion resistance. Érkhim *et al.* investigated the mechanical properties of TiNi–TiCu alloys, revealing that the addition of copper to TiNi alloys influences their mechanical behaviour, which is crucial for applications requiring specific mechanical characteristics (Érkhim *et al.*, 1978).

TiO_2 is a versatile material with applications ranging from photocatalysis to biomedical devices. Ali *et al.* discussed recent advances in the synthesis, properties and applications of TiO_2, highlighting its significance in various fields due to its remarkable catalytic and semiconducting properties (Ali *et al.*, 2018). Research by Arumugam *et al.* explored the functional properties of TiO_2-based nanocomposites. Their findings emphasized the potential of these composites in enhancing the performance of conducting polymers for applications in sensors and energy storage devices (Arumugam *et al.*, 2023). Ndibewu *et al.* explored the influence of titanium dioxide (TiO_2) on the physico-chemical properties of polymer composites. The research highlighted the critical role of TiO_2 as a reinforcing agent, particularly in enhancing the thermal stability, mechanical strength and durability of polymer matrices. By incorporating TiO_2 nanoparticles, the composite materials demonstrated improved resistance to heat and wear, making them ideal for advanced industrial applications, including automotive, construction and biomedical sectors (Ndibewu *et al.*, 2024).

Machine learning techniques such as Artificial Neural Networks (ANNs), Random Forests and Decision Trees have emerged as powerful tools for predicting material properties, offering significant advantages over traditional modelling approaches. These methods enable the identification of complex, nonlinear relationships between material features and their properties, even when dealing with large and diverse datasets. ANNs are particularly effective in capturing intricate patterns in data, making them well-suited for predicting temperature-dependent behaviours. Random Forests combine the outputs of multiple decision trees to improve accuracy and robustness while also providing insights into feature importance, aiding in understanding the key factors influencing material properties. Decision Trees offer a high degree of interpretability, making it easier to visualize and understand the interactions between variables. Together, these methods contribute to accelerating material discovery and optimization, providing reliable and efficient approaches to analyze and predict critical properties such as thermal conductivity, density and specific heat across varying conditions (Agrawal and Choudhary, 2016; Agrawal *et al.*, 2019; 2023; Zhao *et al.*, 2023-2024).

Butler *et al.* (2018) conducted an extensive review on the role of machine learning in materials science. The study explored how models such as random forests, support vector machines and neural networks are transforming the way material properties are predicted. The researchers highlighted the integration of experimental and computational datasets to develop accurate models for predicting properties like thermal conductivity, elasticity and electronic band structures. They emphasized that these methods accelerate materials discovery by enabling rapid screening of potential candidates for energy storage, catalysis and structural applications. Jha *et al.* (2018) investigated the use of ANNs for predicting complex material properties, focusing on high-entropy alloys. The study demonstrated how ANNs can model nonlinear relationships between input variables like composition and output properties such as phase stability and mechanical strength.

Pilania *et al.* (2013) conducted a study to explore the use of random forest algorithms for predicting material properties. The researchers applied random forest models to predict the formation energies of perovskite oxides based on compositional features. By leveraging the ensemble approach of random forests, the study demonstrated high accuracy in capturing complex, nonlinear relationships between input features and material properties.

Mansouri Tehrani *et al.* (2018) investigated the application of decision tree models in predicting the mechanical properties of high-entropy alloys, as reported in *Computational Materials Science*. The study employed decision trees to evaluate the influence of elemental composition and processing conditions on hardness and tensile strength. Their work highlighted the efficiency of decision trees in materials research, providing a systematic approach to optimizing material design and performance.

In this research, extensive literature review and analysis of numerous research articles and papers reveal a strong foundation for the use of Ti due to its unique and valuable characteristics in various applications. Researchers have explored Ti in combination with other materials, such as Al, Cu and O_2, to form Ti-Al, Ti-Cu and Ti-O_2 composites, each showing promise for specific applications and temperature ranges. Despite this focus, the data across these studies is inconsistent, particularly with respect to the temperature-dependent properties. This inconsistency highlights the need for a more systematic approach to predicting material properties under defined conditions.

In recent years, machine learning has emerged as a powerful tool in material science, accelerating the discovery of new biomaterials, optimizing material properties and enhancing sustainability. The application of machine learning in this research allows for predictions of material properties based on specific conditions and tailored parameters. This approach also helps to uncover hidden relationships in material data, optimize predictions and enable enhanced maintenance and durability assessments.

However, significant challenges remain. While AI and machine learning can drive advancements in biomaterials, limitations include a lack of accessible, high-quality datasets, inconsistent open-access frameworks and the absence of a comprehensive composite material database. Additionally, predictions across different methods often yield varied outcomes, making it challenging to determine optimized results consistently. Few studies provide comparative analyses across similar temperatures, which limits understanding of the conditions that optimize material behavior in new biomaterial applications.

Given these gaps, this research applies machine-learning models to the temperature-dependent property prediction of composite materials, specifically Ti-Al, Ti-Cu and Ti-O_2. By comparing model outputs across various methods, this study aims to establish a comprehensive prediction framework and address the need for reliable, temperature-specific data in biomaterial research, setting a foundation for optimized material use across applications.

The main objective of this study is to develop a robust machine-learning model that accurately predicts the thermal and mechanical properties of biomaterials, specifically Ti-based materials such as Ti-Al, Ti-Cu and TiO_2 composites, across different temperature ranges. This contributes to various fields such as Aerospace Engineering, implants, prosthetics and other medical devices, predicting thermal conductivity and heat resistance aids in designing materials for heat exchangers, power plants and energy storage systems, circuit boards, sensors and other electronic devices, improved engine components and heat-resistant parts for vehicles. Biomaterials research using AI faces several challenges, including limited accessible datasets, unreliable open-access data sources and the need for comprehensive composite material data. Additionally, temperature-dependent outcomes, varied prediction methods and identifying optimized prediction techniques further complicate achieving accurate and reliable results.

Machine learning enhances the prediction of material properties by efficiently analyzing complex datasets, identifying patterns and developing predictive models that account for various influencing factors. By leveraging algorithms such as Artificial Neural Networks (ANN), random forests and decision trees, machine learning can process extensive experimental data to predict material behavior across different conditions, including temperature variations. This enables accurate estimations of properties like thermal conductivity, density and Young's modulus without extensive physical

testing. Additionally, machine learning models can optimize material design by identifying key features that contribute to improved performance, accelerating research and innovation in material science.

The ANN, Random Forest and Decision Tree models were chosen for this study due to their distinct strengths in handling complex datasets and predicting material properties. The ANN model was selected for its ability to capture nonlinear relationships and complex patterns within the data, making it suitable for modeling intricate material behaviors across varying temperatures. The Random Forest model was employed for its robustness against overfitting and its capability to handle large datasets with diverse features, ensuring stable and reliable predictions. Meanwhile, the Decision Tree model was chosen for its interpretability and ability to generate clear decision rules, making it useful for understanding key factors influencing material properties. By utilizing these three models, a comprehensive evaluation of prediction accuracy and performance was achieved.

Materials

The selection of appropriate materials and the comprehensive analysis of their thermophysical and mechanical properties form the foundation of predictive modeling in materials science plays a vital role. In this study, the focus was placed on both elemental and composite systems that are widely recognized for their industrial relevance and structural applications. Titanium (Ti), Aluminum (Al), Copper (Cu) and Oxygen (O_2) were investigated alongside their combinations TiAl, TiCu and TiO_2 to understand how the interaction of constituent elements influences overall material behavior. The goal was to analyze how these materials respond to changes in temperature and to develop predictive insights using machine learning techniques.

The properties of several material systems, including Ti, Al, Cu and O_2, as well as their combinations such as TiAl, TiCu and TiO_2, were investigated across a range of temperatures. The parameters of interest included Band Gap (eV), Young's Modulus (GPa), Density (g/cm³), Thermal Conductivity (W/m.K) and Specific Heat (J/g.C). The temperature range for the experiments spanned from 298.15 to 498.15 K, with measurements taken at specific intervals of 4 K within this range.

To predict the material properties at these varying temperatures, three different machine learning models were employed: Artificial Neural Networks (ANN), Random Forests and Decision Trees. These models were selected due to their ability to handle complex, non-linear relationships between input parameters and material properties, which is particularly important when dealing with the combined elements like TiAl, TiCu and TiO_2.

In this analysis, several critical properties of Titanium were examined, including Band Gap, Young's Modulus, Density, Thermal Conductivity and Specific Heat. These properties provide insights into how Titanium behaves under different conditions, which is vital for designing components that must perform reliably in demanding environments.

As discussed in the manuscript, Titanium (Ti), Aluminum (Al), Copper (Cu), Oxygen (O_2) and their composite forms, including Ti-Al, Ti-Cu and TiO_2, were selected for this study. These materials were chosen due to their distinct thermal, mechanical and chemical characteristics, which are essential for developing accurate predictive models. Properties such as modulus of elasticity, density, thermal conductivity and specific heat were considered, as they play a fundamental role in determining structural performance, heat transfer efficiency and energy storage capacity. The selection of these materials and properties aims to enhance the reliability and accuracy of machine learning predictions for biomaterial behavior across varying conditions.

This research addresses the challenge of dataset collection in machine learning, particularly in material science. To efficiently gather relevant data, a Python-based web scraping tool was developed to search for specific keywords and download journal articles. This automated process streamlined the identification of valuable research materials for data extraction.

Following article retrieval, the Plot Digitizer tool was employed to extract precise material property data from graphs and diagrams. This method ensured accurate collection of key properties for Ti, Al, Cu and O_2 across temperatures ranging from 298.15 to 498.15 K. Here is the detailed explanation of data collection procedures.

Methods

One of the most challenging aspects of machine learning is collecting datasets. The data sets can be collected from different resources. In the realm of material science research, the efficient identification and retrieval of relevant academic articles is essential for staying abreast of current developments and advancements. To facilitate this process, automation tools such as web scraping scripts can be employed. This approach leverages programming techniques to systematically search for and extract pertinent information from online sources. The following code snippet exemplifies a Python-based web scraping solution designed to locate articles that contain specific keywords of interest, thereby optimizing the literature review process.

The Python script automates web scraping to locate and retrieve research articles based on specific keywords. It leverages the requests library to send HTTP GET requests to a specified base_url, fetching the HTML content of the target webpage. The script uses BeautifulSoup to parse HTML, allowing easy navigation and data extraction.

It begins by defining a list of relevant keywords such as 'nanomaterials', 'band gap' and 'density', which serve as filters to identify articles of interest. The script then searches the parsed HTML for all anchor (<a>) tags, as these typically contain hyperlinks to individual articles or research papers. To ensure proper navigation, relative URLs found in the href attributes are converted into absolute URLs using urljoin, ensuring all extracted links are accessible.

The script performs a case-insensitive search within the anchor tag text, checking whether any defined keywords appear. If a match is found, the corresponding article link is added to the matching_links list. To prevent errors, the script includes response. raise_for_status (), which ensures that HTTP response errors (e.g., 404 Not Found) are detected and handled appropriately.

Finally, the script prints all URLs stored in matching_links, providing users with a filtered list of articles relevant to their research. This automation streamlines the literature review process, eliminating the need for manual searching and ensuring that relevant materials are efficiently identified.

This script automates the search for academic articles by filtering based on specific keywords. It first retrieves and parses the HTML content from a target website, extracts article links and checks these links for relevance based on the provided keywords. The result is a list of URLs pointing to articles that match the search criteria. This method significantly enhances the efficiency of gathering relevant research materials and ensures that important articles are not overlooked.

In should be noted that the dataset was composed of measurements taken at 50 different temperatures, increasing incrementally by 4 K from 298.15 to 498.15 K.

In this research, data collection was systematically conducted through a targeted web scraping approach to identify and gather the most relevant articles and data sources pertaining to the thermal and mechanical properties of Ti-Al, Ti-Cu and Ti-O_2 composite materials. A list of specific keywords was employed to filter and collect publications highly relevant to the topic. The data was compiled for a defined temperature range of 298.15 to 498.15 K, covering crucial properties required for machine learning model training and prediction.

To ensure the completeness and consistency of the dataset, values were extracted from diagrams within each publication using Plot Digitizer toolbox. The use of web scraping was essential, as many established online databases were found to be unreliable for this research. Challenges in these databases included missing values, entries with negative temperature values, inconsistent units and unstructured data, which compromised data integrity. Additionally, most existing databases contained limited data entries, often fewer than 20 rows, which did not provide sufficient data for meaningful analysis and machine learning application. To overcome these limitations, plot digitizer software was used to capture accurate data points from graphs in these sources, allowing the extraction of coordinates that corresponded to material properties at specified temperatures.

Once extracted, the data underwent a rigorous validation process to ensure accuracy and consistency. Cross-referencing was conducted with additional journal articles to confirm the reliability of the extracted values and only data that aligned across multiple sources was included in the final dataset. After validation, the dataset was organized and transferred into an Excel spreadsheet, creating a well-structured dataframe for further analysis. This meticulously curated and validated dataset served as the foundation for building machine learning models, enabling accurate and reliable prediction of material properties across the temperature range studied.

Per extracted data for Titanium (Ti), Aluminum (Al) and Copper (Cu) that are metallic elements with a band gap of 0 eV, meaning they exhibit high electrical conductivity. Titanium's Young's modulus decreases from 106.155 to 93.198 GPa as temperature increases, indicating reduced stiffness due to thermal expansion. Its density also declines from 4.42 to 4.15 g/cm³, while thermal conductivity drops from 15.6 to 14.82 W/m.K because of increased phonon scattering. Aluminum follows a similar trend, with Young's modulus reducing from 68.18 to 55.51 GPa, density decreasing slightly from 2.69 to 2.65 g/cm³ and thermal conductivity remaining high (156.04 to 157.28 W/m.K) despite minor reductions due to phonon interactions. Copper exhibits greater stiffness initially, but its Young's modulus declines from 127.18 to 97.49 GPa with temperature. Its density drops from 8.701 to 8.373 g/cm³, while thermal conductivity decreases slightly from 390 to 385 W/m.K. Oxygen (O_2), in contrast, behaves as a gas and has a highly temperature-dependent density, decreasing from 0.00126 to 0.000173 g/cm³ due to molecular expansion. Unlike metals, their thermal conductivity increases from 26.301 to 41.183 W/m.K with rising temperature, improving heat transfer efficiency. The energy absorption capacity of all materials declines with temperature, impacting their ability to withstand mechanical stress.

Machine learning has revolutionized the way researchers and engineers approach complex problems, particularly in the field of material science. By leveraging advanced algorithms, machine learning models can uncover intricate patterns and relationships within data that might not be evident through traditional analysis methods. In this dissertation, we employ three machine learning technique ANN, Random Forest and Decision Tree algorithm to predict the properties of materials based on a variety of input parameters, such as temperature, composition and structural characteristics.

ANNs are highly adaptable, capable of learning from vast amounts of data and are known for their ability to generalize well new, unseen data. Random Forest, on the other hand, is an ensemble learning method that operates by constructing multiple decision trees during training and outputting the mode of the classes (classification) or mean prediction (regression) of the individual trees. The Decision Tree algorithm is a more interpretable model that breaks down a dataset into smaller and smaller subsets while at the same time developing an associated decision tree incrementally. The result is a tree with decision nodes and leaf nodes. While it may not always perform as well as ensemble methods like Random Forest, the simplicity and transparency of Decision Trees make them a valuable tool for understanding the decision-making process and the underlying data structure.

Incorporating these machine learning models into the prediction of material properties allows us to develop accurate, reliable and interpretable models that can significantly enhance our understanding of the complex relationships governing material behavior. The integration of these models into our research framework represents a critical step towards more advanced and efficient materials design and optimization.

ANN are a powerful tool in computational material science for predicting complex material properties based on input data. In the context of predicting the properties of alloys and compounds such as TiAl, TiCu and TiO_2, ANNs offer the ability to model nonlinear relationships between various physical and chemical parameters.

ANNs can be trained on experimental data to learn the intricate relationships between input variables like temperature, composition and processing conditions and output properties such as band gaps, thermal conductivity, density and other mechanical and electronic properties.

ANNs have emerged as an invaluable tool for predicting the temperature-dependent properties of complex materials such as TiAl, TiCu and TiO_2. The inherent ability of ANNs to model nonlinear relationships allows them to effectively capture the intricate dependencies of material properties on temperature, which are often too complex for traditional methods to accurately represent. By leveraging a multi-layered architecture, ANNs can process and learn from large, multidimensional datasets, extracting subtle patterns that influence properties like density, thermal conductivity and band gap energy. This capability is particularly crucial for materials, additionally, the adaptability of ANNs to various data types enables comprehensive analysis without the need for extensive feature engineering.

The neural network model code was executed to predict material properties based on input data. Various steps were undertaken to ensure effective modeling. The data included properties such as temperature, band gap, Young's modules, density, thermal conductivity and specific heat for aluminum and Titanium.

These properties were extracted from multiple sheets within an Excel file stored at a specified path (xlsx_path). The data from two sheets (material1_sheet and material2_sheet) were combined to create a comprehensive dataset (combined_data). Upon loading the material data, a training dataset was prepared by combining the properties of each material pair. The data were scaled using StandardScaler to normalize them for training. The dataset was split into training (X_train_scaled, y_train_scaled) and testing (X_test_scaled, y_test_scaled) sets using train_test_split from sklearn.model_selection, facilitating model training and evaluation.

Subsequently, a Multi-Layer Perceptron (MLP) regressor model was employed for training the neural network. The model comprised two hidden layers, each with 50 neurons and was trained to over 1000 iterations. A function was defined to predict material properties for a given combination of materials. This function took inputs for two materials, concatenated their properties, scaled the combined data and predicted the scaled output using the trained model. To approach this, the neural network model was trained on the scaled training data (X_train_scaled, y_train_scaled), learning to predict material properties based on temperature variations. Predictions were made for a user-input temperature (temperature_input) and these scaled predictions were inverse-transformed (scaler_y.inverse_transform) to provide interpretable material property estimates.

The predicted values were then inverse transformed to obtain the actual material properties. User inputs were solicited for the materials of interest, following which the function was invoked to predict their properties. Finally, the predicted material properties were displayed, encompassing temperature, band gap, Young's modulus, density, energy absorption, thermal conductivity and specific heat. This neural network-based approach facilitates accurate predictions of material properties, thereby offering valuable insights for various engineering applications.

Random Forest is an ensemble learning method that builds upon the foundation of decision trees, offering significant improvements in predictive accuracy and robustness. This method is particularly well-suited for modeling complex datasets, such as those involving the temperature-dependent properties of materials like TiAl, TiCu and TiO_2. In material science, where relationships between variables can be highly nonlinear and interactions between different material properties are intricate, Random Forest provides a powerful approach to prediction.

Random Forest constructs multiple decision trees using bootstrapped subsets and random feature selection

to reduce overfitting. It averages predictions for regression or takes a majority vote for classification. The provided code applies Random Forest regression to predict material properties from two datasets, forecasting combined material properties at a user-specified temperature.

Initially, the necessary libraries—os, numpy, pandas and components from sklearn—are imported. File paths and names for the Excel file containing the material data are defined.

For model training, the combined material properties serve as the input features (X), while the target output (y) includes both temperature and material properties. The data is split into training and testing sets, with 80% allocated for training and 20% for testing. This division allows for the evaluation of the model's performance on unseen data.

The features and target variables are scaled using StandardScaler to ensure they are on a comparable scale, which is essential for effective model training. A RandomForestRegressor with 100 decision trees is trained on the scaled training data.

The trained model is then used to predict properties at the specified temperature. The input data is scaled and transformed according to the model's requirements and predictions are converted back to their original scale.

Finally, the predicted properties for the combined material are displayed. If the predicted value for the 'Band Gap (eV)' is zero, it is excluded from the output, as such values may not be meaningful in this context.

This implementation demonstrates the application of Random Forest regression for predicting material properties, emphasizing the significance of data preparation, feature scaling and model evaluation in predictive analytics.

Decision Tree regression is a powerful method used for predicting continuous outcomes by splitting the data into subsets based on the values of input features. This method builds a model in the form of a tree structure, where each node represents a decision based on a single feature and branches represent possible outcomes of that decision.

Decision Trees are particularly effective for capturing complex relationships between features and target variables, making them suitable for tasks where the relationship is not linear or is influenced by multiple factors. A Decision Tree regression model is implemented to predict material properties using data extracted from two distinct material sheets. The model aims to forecast properties of a combined material at a specified temperature.

Initially, the necessary libraries—os, numpy, pandas and components from sklearn—are imported. os is employed for file handling, while numpy and pandas facilitate data manipulation. Tools from sklearn are utilized for model training and scaling. Data from the specified sheets is loaded into a dictionary. Temperature data is extracted from the first material's sheet to serve as a reference for predictions.

The user is requested to input a specific temperature in Kelvin. The code identifies the closest available temperature in the dataset and retrieves the associated properties. If the 'Band Gap (eV)' property at the specified temperature is zero, it is noted and excluded from model training. If the 'Band Gap (eV)' is non-zero, the Decision Tree model is trained. The Decision Tree Regressor is employed for modeling and the data is divided into training and testing sets using an 80-20 split. Feature and target variables are scaled using StandardScaler to ensure uniformity in scale, which is crucial for effective model performance. The Decision Tree model is trained on the scaled training data. Predictions are generated for the specified temperature by scaling the input data and using the trained model to forecast properties. The predictions are converted back to their original scale through inverse transformation. Finally, the predicted properties are displayed. The 'Band Gap (eV)' is excluded from the output if its value is zero, as it may not be relevant. If the 'Band Gap (eV)' has a non-zero predicted value, it is displayed alongside other material properties.

In this chapter, the methodologies for predicting material properties of TiAl, TiCu and TiO_2 have been thoroughly explored using three distinct machine learning approaches: Artificial Neural Networks (ANN), Random Forest and Decision Tree regression models. Each method offers unique strengths and is suited to different aspects of predictive modeling.

The ANN methodology leverages complex network architectures to model nonlinear relationships and capture intricate patterns within the data. Random Forest, an ensemble learning method, was employed to improve prediction accuracy and robustness by aggregating multiple decision trees. This approach mitigates overfitting issues commonly associated with single decision trees and provides a more stable prediction by averaging the outputs of numerous trees.

The Decision Tree model, on the other hand, offers a transparent and interpretable approach to regression. By splitting the data into subsets based on feature values, it provides a clear structure for understanding how different features influence predictions. While less robust to overfitting compared to Random Forest, the Decision Tree model can offer valuable insights into the relationships between features and predicted properties.

The development of advanced materials with tailored properties is a critical focus in modern materials science and engineering. Composite materials and alloys play a vital role in various industries, including aerospace, automotive and biomedical applications, due to their

ability to combine desirable properties from different elements. By carefully selecting and combining constituent materials, engineers can design materials with enhanced mechanical strength, thermal stability and electrical conductivity. However, accurately predicting the properties of these materials before fabrication remains a challenge, making theoretical estimation methods essential in the design and optimization process.

One of the fundamental approaches to predicting the properties of these materials is the Rule of Mixtures, which provides an estimation based on the properties and proportions of the individual components. This method is widely used in material science to approximate characteristics such as density, thermal conductivity, specific heat and Young's modulus of composite materials.

Composite materials are engineered by combining two or more distinct constituents to achieve enhanced mechanical, thermal, or electrical properties. One of the fundamental approaches to predicting the properties of these materials is the Rule of Mixtures, which provides an estimation based on the properties and proportions of the individual components. This method is widely used in material science to approximate characteristics such as density, thermal conductivity, specific heat and Young's modulus of composite materials.

The Rule of Mixtures offers a first-order approximation for these properties by considering the volume fractions and intrinsic properties of the individual components. By applying this rule, researchers and engineers can predict material behavior before conducting experimental tests, providing an essential foundation for designing new materials and validating computational models, including machine learning-based predictions. To apply the Rule of Mixtures for predicting the properties of TiAl and TiCu, mathematical formulations are required. The key equations account for the volume fractions of Titanium and aluminum (or copper) and their respective material properties. In the following section, the mathematical expressions used to estimate the density, thermal conductivity and Young's modulus of TiAl and TiCu alloys will be presented. These equations form the basis for comparing theoretical predictions with machine learning-based estimations. For instance, the modulus of elasticity (E) for a composite material, as TiAl, can be estimated using the linear Rule of Mixtures using Eq. (1):

$$E_{TiAl} = E_{Ti}V_{Ti} + E_{Al}V_{Al} \quad (1)$$

In this equation, (E_{TiAl}) Young's modulus of the TiAl alloy, (E_{Ti}) Young's modulus of Titanium, (V_{Ti}) Volume fraction of Titanium, (E_{Al}) Young's modulus of aluminum, (V_{Al}) Volume fraction of aluminum are presented. The TiAl alloy is a two-phase intermetallic compound consisting of Titanium (Ti) and aluminum (Al) in a 1:1 atomic ratio. When estimating its modulus of elasticity (Young's modulus, E) using the Rule of Mixtures, it's considered that each element contributes equally (50%) to the total modulus. This consideration is based on the idea that the overall stiffness of the alloy is influenced proportionally by the stiffness of its constituent elements. Since Ti and Al are present in equal amounts in the TiAl alloy, their contributions to elasticity are equally weighted. Therefore, the modulus of elasticity for TiAl is $05E_{Ti} + 0.5E_{Al}$ (Wang *et al.*, 2018).

Similarly, the density of TiAl alloy can be estimated using each element (Ti and Al) contributes 50% to the overall density. This estimation is based on the volume fraction of each element in the alloy. Therefore, calculating the TiAl properties by the rule of mixture method, $05\rho_{Ti} + 0.5\rho_{Al}$is considered (Lopis *et al.*, 2010). The thermal conductivity of TiAl alloy is calculated using $05K_{Ti} + 0.5K_{Al}$ (Zhang *et al.*, 2001). The specific heat of TiAl alloy is calculated using $0.5C_{Ti} + 0.5C_{Al}$ (Song *et al.*, 2019).

Moreover, the modulus of elasticity (E) for composite materials like TiCu can be estimated using the linear Rule of Mixtures per $E_{TiCu} = 0.5E_{Ti} + 0.5E_{Cu}$ (Uścinowicz, 2022).The density of TiCu (ρ_{TiCu}) is calculated by the rule of mixture method, $05\rho_{Ti} + 0.5\rho_{Cu}$is considered (Akbarpour *et al.*, 2024; Yang *et al.*, 2017). For the TiCu alloy, with a composition of 95.5% titanium (Ti) and 4.5% copper (Cu), the thermal conductivity can be estimated using $K_{TiCu} = 0.5K_{Ti} + 0.5K_{Cu}$ (Nagarjuna, 2004). The specific heat of TiCu alloy is calculated using $0.5C_{Ti} + 0.5C_{Cu}$ is considered (Xu *et al.*, 2022).

Results and Discussion

In this chapter, the results of the evaluation of TiAl, TiCu and TiO_2 under varying temperature conditions, ranging from 298 to 498 Kelvin, are presented and discussed. The focus is on predicting key material properties, including Band Gap (eV), Young's Modulus (GPa), Density (g/cm³), Energy Absorption (KJ/m³), Thermal Conductivity (W/m·K) and Specific Heat (J/g°C), using three machine learning methodologies: ANN, Random Forest and Decision Tree models. The chapter begins with a discussion of the data obtained from the web scraper and its validation process, which serves as the foundation for the subsequent analysis.

The purpose of applying these distinct models is to understand the predictive performance and accuracy of each method in capturing the complex, temperature-dependent behavior of these materials. The findings discussed in this chapter are critical for advancing the

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understanding of how temperature influences the mechanical and thermal properties of these materials and how machine learning can be leveraged for more accurate predictions.

In this section, the results of web scraper data are presented. As indicated, the data from articles were extracted using Plot Digitizer and exported to the excel file. After extracting data, the validation process is conducted and data is validated with other articles.

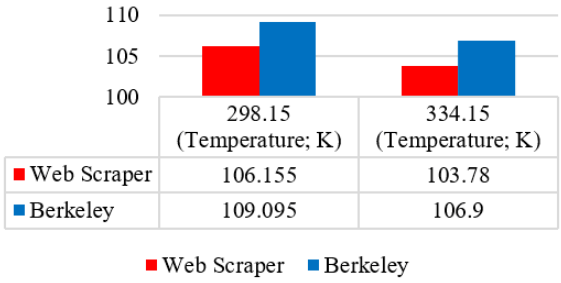

Fig. 1: Comparison of young modulus between web scraper and berkeley dataset

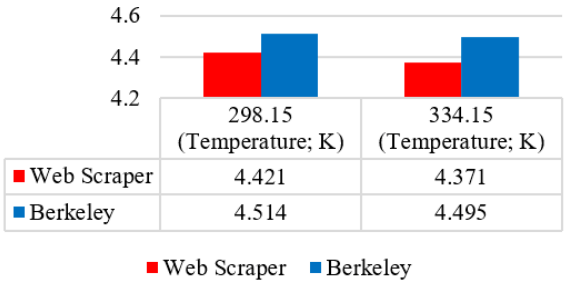

Fig. 2: Comparison of density between web scraper and berkeley dataset

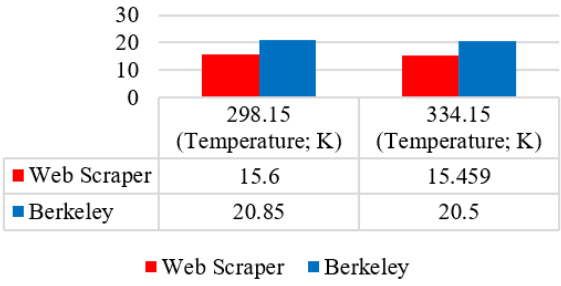

Fig. 3: Comparison of thermal conductivity between web scraper and berkeley dataset

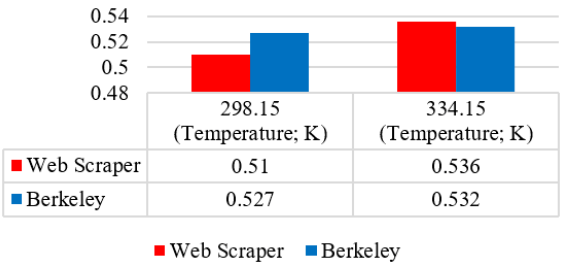

Fig. 4: Comparison of specific heat between web scraper and berkeley dataset

Figures (1-4) show the validation results for young's modulus, density, thermal conductivity and specific heat, in order. In Figure (1), the results show that the data obtained from Berkley is 2.77% more than webs scraper under 298.15 Kelvin and this difference for 334.15 Kelvin is 3.01. In Figure (2), the density of web scraper and Berkley data set is represented for 298.15 and 334.15 Kelvin. The results show that 2.10 and 2.85 percent for Berkeley and Web Scraper, respectively.

Figure (3) shows the thermal conductivity data in which the figure indicates 33.65 and 32. 61% for 298.15 and 334.15 K, respectively. Finally, the validation results for the specific heat in Figure (4) show 3.33 and -0.75% for 298.15 and 334.15 K. The validation results demonstrate that the data obtained through the web scraper is accurate, with small discrepancies that fall within acceptable limits. Therefore, web scraper data can be considered reliable and suitable for further analysis and use.

To ensure the reliability and accuracy of the predictive models developed in this study, a verification process is undertaken by comparing the predicted values to the actual material properties. This comparison serves as a critical step in validating the effectiveness of the ANN, Random Forest and Decision Tree models used for predicting temperature-dependent behavior.

In this section, the verification of the ANN model for predicting the properties of TiAl, TiCu and TiO_2 is presented. The accuracy and reliability of the model are assessed by comparing the predicted values with the actual experimental data for each material. This comparison helps in understanding the model's effectiveness in capturing the intricate relationships between the material properties across different temperatures. The materials, TiAl, TiCu and TiO_2, are evaluated under varying conditions and the performance of the ANN is analyzed to ensure its robustness in predicting the critical properties of these materials.

In Figure (5), the comparison between actual and predicted values of key material properties, including band gap, density and specific heat, for TiAl, is illustrated using an ANN predictive model.

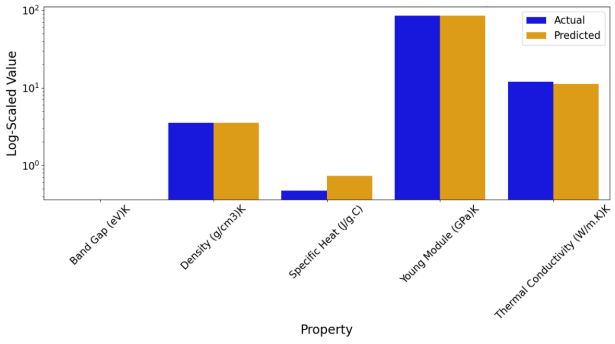

Fig. 5: Comparison of actual and predicted band gap (eV), density (g/cm3), specific heat (J/g.C), young module (GPa) and thermal conductivity (W/m.K) values in TiAl

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The graph provided in Figure (5) highlights the differences between actual and predicted values for various TiAl material properties, offering important insights into the model's performance.

The ANN model demonstrated strong predictive performance for TiAl properties, with minimal discrepancies across various parameters. The predicted band gap deviated by only 0.005%, while density showed a close match with a 0.85% difference. Specific heat exhibited a slightly larger deviation of 54.40%, likely due to microstructural variations. Young's modulus prediction was highly accurate, differing by just 0.23%. The model achieved an impressive R^2 score of 0.980874, reflecting its ability to explain 98.09% of the data's variance. Thermal conductivity predictions were also reliable, with a 6.31% deviation. Overall, the ANN model effectively captured TiAl properties with minor deviations that remain within acceptable limits for engineering applications.

ANN is also used to predict material properties of TiCu at approximately 334.15 K, focusing on parameters such as band gap, density and specific heat. Figure (6) illustrates the comparison between actual and predicted values, demonstrating the ANN model's effectiveness in estimating these critical properties and its relevance for TiCu's thermal behavior and industrial applications.

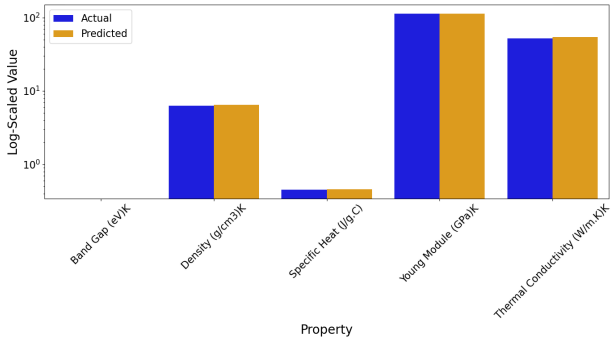

Fig. 6: Comparison of actual and predicted band gap (eV) K, density (g/cm3) K, specific heat (J/g.C), young module (GPa) K and thermal conductivity (W/m.K) K values in TiCu

Figure (6) presents a comparison between the actual and predicted values of various material properties for the TiCu alloy, offering a comprehensive view of the ANN model's performance in predicting these properties. The ANN model exhibited strong predictive performance for TiCu alloy properties, with minimal discrepancies across key parameters. The predicted band gap slightly overestimated the actual value by just 0.0030%, indicating high accuracy. Density predictions closely matched the actual values, with a minor difference of 3.73%, demonstrating the model's reliability in capturing structural characteristics. Specific heat showed a small underestimation of 2.60%, likely influenced by experimental variations or temperature-dependent effects. Young's modulus prediction was highly precise, differing by only 0.40%, while thermal conductivity displayed excellent accuracy with a 3.80% deviation. The model achieved an impressive R^2 score of 0.997607, explaining 99.76% of the data's variance, reinforcing its strong predictive capability and reliability.

TiO_2 is a widely studied material due to its unique optical and electronic properties. At approximately 334.15 K, understanding the material properties of TiO_2 such as band gap, density and specific heat is crucial for assessing its thermal behavior and performance in diverse environments. ANN has been utilized to accurately predict these properties. Figure (7) illustrates the comparison between actual and predicted values for the material properties of TiO_2, with the data represented on a log scale. The band gap shows a slight overestimation in the predicted value (3.112 eV) compared to the actual value (2.823 eV), indicating a 10.23% difference. This discrepancy may suggest a need for further refinement in the model, possibly due to the complex interactions between temperature and the band gap in TiO_2. Despite this, the predicted band gap still falls within a reasonable range, reflecting the model's overall capability in capturing the key electronic properties of TiO_2.

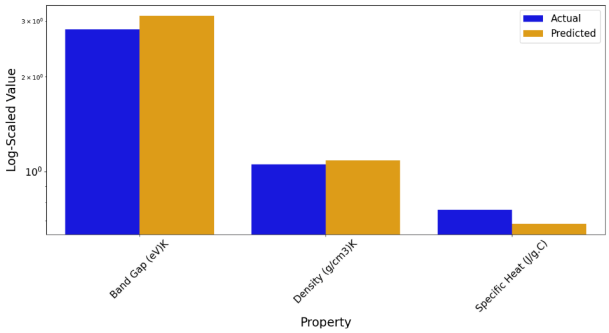

Fig. 7: Comparison of actual and predicted band gap (eV) K, density (g/cm3) K and specific heat (J/g.C), in TiO 2

The model demonstrates strong predictive accuracy for TiO_2 properties, with minor deviations. Density is slightly overestimated by 3.06%, likely due to microstructural complexities. Specific heat shows the largest deviation at 9.65%, suggesting sensitivity to experimental conditions. The Mean Squared Error (MSE) of 0.0009 indicates minimal prediction error, reflecting high precision. While the model performs well, further refinements could enhance accuracy for temperature-dependent properties. Additionally, a Random Forest model was applied to predict TiAl properties at approximately 334.15 K, highlighting its effectiveness in capturing complex patterns for optimizing material applications.

In this section, the performance of the Random Forest model for predicting the material properties of TiAl is evaluated. Figure (8) presents the comparison between actual and predicted values across several critical properties, with the data analyzed to assess the model's

accuracy and reliability. The Random Forest model demonstrated strong performance in predicting the material properties of TiAl. For the band gap, the model's prediction of 0 eV matched the actual value, indicating accurate capture of the material's electronic characteristics. The density prediction (3.529 g/cm³) was almost identical to the actual value (3.528 g/cm³), showing a minimal 0.017% discrepancy. The specific heat prediction (0.730 J/g°C) was 54% higher than the actual value (0.4723 J/g°C), suggesting some room for improvement in estimating this property. The Young's modulus prediction (84.86 GPa) was nearly identical to the actual value (84.81 GPa), with a negligible 0.02% difference, demonstrating high precision in mechanical property estimation. The thermal conductivity prediction (11.18 W/m·K) showed a 6% deviation, reflecting a strong alignment with the actual value.

The model's R^2 score of 0.998168 indicates excellent accuracy, explaining almost all the variance in the data. This score reflects the model's reliability and consistency in making predictions, underscoring its effectiveness for predicting TiAl's material properties with minimal deviations.

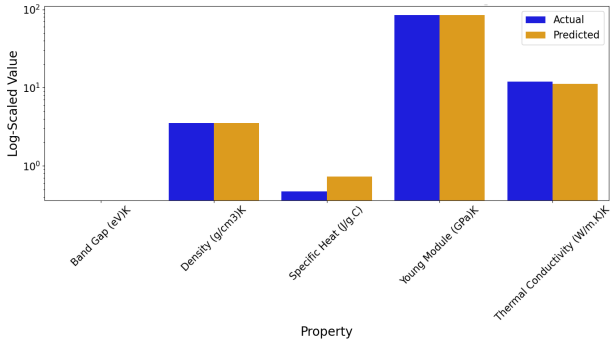

Fig. 8: Comparison of actual and predicted band gap (eV), density (g/cm3), specific heat (J/g.C), young module (GPa) and thermal conductivity (W/m.K) K values in TiAl

Figure (9) presents a detailed comparison between the actual and predicted values for various material properties of the TiCu alloy of the ANN model. The Random Forest model showed strong performance in predicting the material properties of the TiCu alloy. For the band gap, the model predicted 0.0012 eV, slightly deviating from the actual value of 0 eV, indicating a limitation in capturing the band gap. The density prediction of 6.507 g/cm³ was 3.5% higher than the actual value of 6.274 g/cm³, suggesting potential factors not fully captured by the model. The specific heat prediction (0.461 J/g°C) closely matched the actual value (0.451 J/g°C), showing high accuracy in predicting thermal properties. The model's prediction for Young's modulus (112.84 GPa) was very close to the actual value (112.68 GPa), with only a 0.2% difference, reflecting excellent accuracy in mechanical stiffness estimation. Thermal conductivity was predicted at 53.86 W/m·K, closely aligning with the actual value (51.97 W/m·K), with only a small difference of 1.89 W/m·K.

The model achieved an R^2 score of 0.997764, indicating exceptional accuracy, with nearly 99.8% of the variance explained. This high score demonstrates the model's reliability and robustness in predicting the material properties of TiCu, with minimal discrepancies between predicted and actual values.

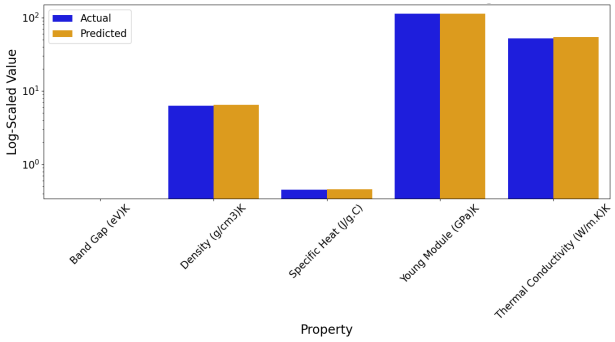

Fig. 9: Comparison of actual and predicted band gap (eV), density (g/cm3), specific heat (J/g.C), young module (GPa) and thermal conductivity (W/m.K) values in TiCu

Accurate prediction of material properties is crucial for scientific research and industrial applications. This study utilizes the Random Forest model to estimate TiO_2's properties at various temperatures, specifically around 334.15 K.

Figure (10) presents a comparison between the actual and predicted values of various material properties for TiO_2, offering a detailed view of the Random Forest model's performance. Analyzing the discrepancies highlighted in this graph provides valuable insights into both the strengths and areas for improvement of the model.

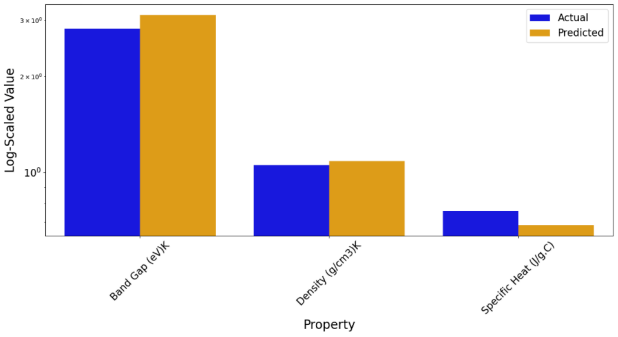

Fig. 10: Comparison of actual and predicted band gap (eV) K, density (g/cm3) and specific heat (J/g.C), in TiO 2

The Random Forest model predicts a band gap of 3.111964 eV, which is 10.26% higher than the actual 2.8227 eV, indicating an overestimation that may be improved by incorporating more electronic structure data. The predicted density of 1.0876 g/cm³ is 3.11% higher than the actual value, suggesting reasonable accuracy but room for refinement. Specific heat is

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underestimated by 9.68%, likely due to temperature-dependent or microstructural effects not fully captured by the model. The Mean Squared Error (MSE) of 0.0054 reflects a small prediction error, indicating high model reliability. Further optimizations could enhance prediction accuracy.

In this analysis, a Decision Tree model was utilized to estimate properties of Titanium Aluminide (TiAl) at approximately 334.15 K. The model's effectiveness was evaluated by comparing its predictions with actual measurements for properties such as band gap, density, specific heat, energy absorption, Young's modulus and thermal conductivity. Figure (11) presents this comparison, showcasing how well the Random Forest model predicts these key properties. This assessment highlights the model's precision and reliability in estimating important parameters, providing valuable insights into TiAl's thermal behavior and its practical applications in various fields.

Figure (11) presents a comparison between the actual and predicted values of various material properties for TiAl, showcasing the performance of the Decision Tree model. This comparison provides insights into the model's accuracy and highlights areas where it excels or may require improvement.

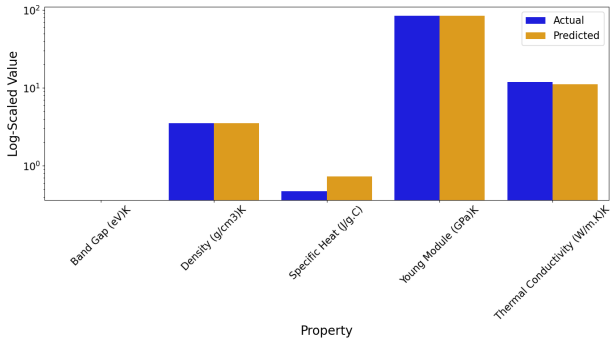

Fig. 11: Comparison of actual and predicted band gaps (eV), density (g/cm3), specific heat (J/g.C), young module (GPa) and thermal conductivity (W/m.K) values in TiAl

The Random Forest model demonstrates strong performance in predicting TiAl material properties. The predicted density (3.528 g/cm³) is very close to the actual value (3.528597 g/cm³), with a small discrepancy of 0.008312 g/cm³. The specific heat prediction (0.731 J/g°C) is about 50% higher than the actual value (0.472 J/g°C), indicating a potential area for improvement. The predicted Young's modulus (84.81 GPa) is nearly identical to the actual value (84.811949 GPa), with a minor discrepancy of 0.137 GPa. The predicted thermal conductivity (11.192 W/m·K) slightly deviates from the actual value (11.94 W/m·K), with a 6.26% difference.

The model's R^2 score of 0.993841 indicates it accounts for 99.38% of the variance, showing high predictive accuracy and strong alignment with actual values. While the model performs well in predicting density, Young's modulus and thermal conductivity, there are discrepancies in specific heat and band gap, highlighting areas for potential refinement.

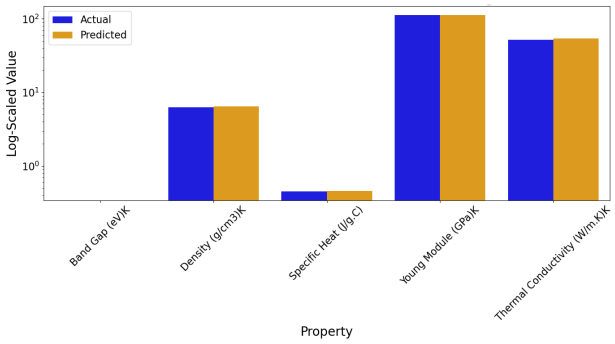

Fig. 12: Comparison of actual and predicted band gap (eV), density (g/cm3), specific heat (J/g.C), young module (GPa) and thermal conductivity (W/m.K) values in TiCu

Figure (12) presents this comparison, showcasing how well the Random Forest model predicts these key properties. Figure (12) presents a comparison between the actual compares the actual and predicted values of TiCu alloy properties, revealing the Decision Tree model's strong performance with some minor discrepancies.

The Decision Tree model shows strong performance in predicting TiCu material properties. The predicted density (6.506 g/cm³) is slightly higher than the actual value (6.274 g/cm³) by about 3.7%, suggesting a need for refinement to better capture factors like alloy composition. The specific heat prediction (0.461 J/g°C) is marginally higher than the actual value (0.451 J/g°C), with a small discrepancy of about 2%. The predicted Young's modulus (112.76 GPa) is very close to the actual value (112.68 GPa), with a minimal difference of 0.08 GPa, demonstrating high accuracy in stiffness prediction. The predicted thermal conductivity (53.98 W/m·K) is slightly higher than the actual value (51.97 W/m·K) by about 2.1 W/m·K, reflecting the model's strong capability in predicting heat conduction properties.

The model's R^2 score of 0.992873 indicates that 99.29% of the variance in the observed values is explained, highlighting the model's high accuracy and reliability in capturing the data's patterns. Overall, the Decision Tree model provides very reliable predictions, with minimal discrepancies between predicted and actual values.

Evaluating the material properties of TiO_2, including band gaps, density and specific heat, at approximately 334.15 K is essential for understanding its thermal behavior and performance under various conditions. In this context, Decision Tree models have been employed to predict these properties with a focus on their accuracy and reliability.

Figure (13) compares the actual and predicted values for TiO_2 material properties, revealing some

discrepancies. The predicted band gap is 3.113 eV, about 10.23% higher than the actual value of 2.823 eV, suggesting that the Decision Tree model captures the trend but may not fully account for complex interactions affecting the band gap. For density, the model predicts 1.088 g/cm³, slightly overestimating the actual value of 1.055 g/cm³ by 3.14%. The specific heat prediction of 0.6840 J/g°C is 9.68% lower than the actual 0.7584 J/g°C, indicating an underestimation. Despite a low Mean Squared Error (MSE) of 0.007350, these discrepancies highlight the need for model refinement, especially for band gaps and specific heat predictions, to improve accuracy for TiO_2 in practical applications.

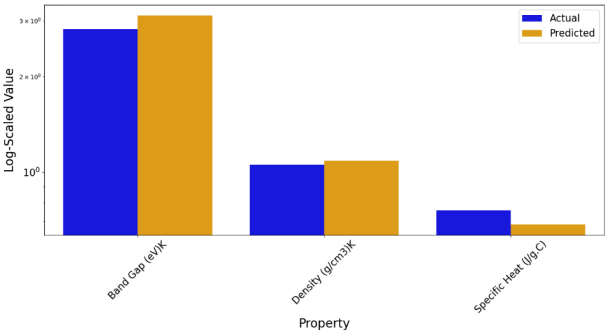

Fig. 13: Comparison of actual and predicted band gap (eV) K, density (g/cm3) K and specific

Model Development

In this section, the predicted results of our model development efforts are presented, concentrating on the material properties of Titanium Aluminide (TiAl), Titanium Copper (TiCu) and Titanium Dioxide (TiO_2). The analysis employs three modeling approaches: Artificial Neural Networks (ANN), Random Forest and Decision Tree algorithms. These models, after undergoing rigorous verification as detailed in the model verification section, are used to predict key material properties.

Figure (14) illustrates the variation of material properties for TiAl Young's Modulus, Density, Thermal Conductivity and Specific Heat—across a range of temperatures. The ANN model predicts material properties of TiAl across a temperature range (298.15-498.15 K). Young's Modulus decreases from 87.195 GPa at 298.15-74.9 GPa at 498.15 K, showing reduced stiffness at higher temperatures, which could impact applications requiring rigidity. Density also decreases slightly from 3.55-3.40 g/cm³ due to thermal expansion, affecting the strength-to-weight ratio. Thermal conductivity remains stable between 10.72 W/m·K and 13.34 W/m·K, indicating little change in heat conduction properties. Specific heat increases from 0.709-0.843 J/g°C, reflecting a greater capacity to store thermal energy as temperature rises.

When comparing actual and predicted values, the model performs well at lower temperatures. At 298.15 K, the predicted Young's Modulus (87.2 GPa) closely matches the actual value (88.2 GPa), but at 498.15 K, the predicted value (74.91 GPa) underestimates the actual value (81 GPa) by 6.09 GPa. For density, the predicted value (3.55658 g/cm³) slightly underestimates the actual density (3.622 g/cm³) at 298.15 K. Thermal conductivity is slightly underestimated at lower temperatures (10.7239 W/m·K vs 11.4423 W/m·K) but also slightly underperforms at higher temperatures. Specific heat is overestimated at both ends of the temperature range, with significant overestimation at the lower and higher temperatures, suggesting a need for model refinement in predicting specific heat.

Overall, while the ANN model accurately predicts some properties of TiAl, it shows discrepancies in specific heat and higher temperature predictions, indicating areas for improvement.

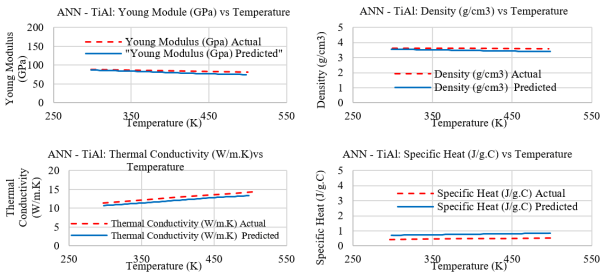

Fig. 14: ANN Predictions of TiAl Properties with temperature variation

Figure (15) illustrates the predicted variations of material properties for TiCu across a temperature range from 298.15-498.15 K. The ANN model predicts material properties of TiCu across the temperature range (298.15-498.15 K). Young's Modulus decreases from 116.74 GPa at 298.15-96.13 GPa at 498.15 K, indicating that TiCu becomes more flexible and less stiff at higher temperatures. This reduction in rigidity may affect the material's structural performance in temperature-sensitive applications. Density slightly decreases from 6.55-6.273 g/cm³ due to thermal expansion, impacting the material's strength-to-weight ratio. Thermal conductivity remains stable, fluctuating between 49.13 W/m·K and 76.28 W/m·K, indicating consistent heat conduction properties across temperatures. Specific heat increases from 0.447-0.528 J/g°C, reflecting a growing capacity to store thermal energy as the temperature rises.

The comparison between the actual and predicted values reveals some discrepancies. For Young's Modulus, the model slightly overestimates values at lower temperatures (116.74 GPa vs. 112.9 GPa at 298.15 K) but underestimates at higher temperatures (96.13 GPa vs. 111.76 GPa at 498.15 K), showing a significant underprediction at 498.15 K. For density, the model slightly overestimates the value at 298.15 K (6.5595 g/cm³ vs. 6.318 g/cm³) and underestimates it at 500 K (6.2737 g/cm³ vs. 6.1303 g/cm³). The model performs

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very well for thermal conductivity, with exact predictions at 298.15 K (49.1304 W/m·K) and a slight overestimation at 500 K (76.285 W/m·K vs. 69.27 W/m·K). For specific heat, the model accurately predicts values at lower temperatures (0.4475 J/g°C vs. 0.4475 J/g°C at 298.15 K) but slightly overestimates values at higher temperatures (0.5280 J/g°C vs. 0.5129 J/g°C at 500 K).

Overall, the ANN model performs well for TiCu, especially in predicting thermal conductivity and specific heat, with minor overestimation of specific heat and discrepancies in Young's Modulus and density at higher temperatures.

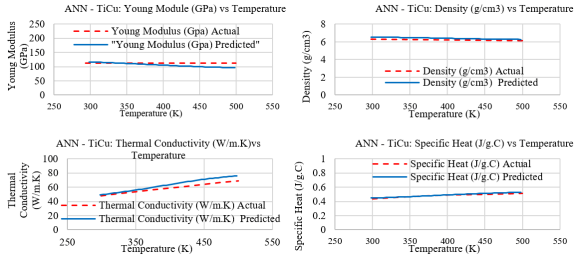

Fig. 15: ANN predictions of TiCu properties with temperature variation

For the analysis of TiO_2, the primary focus is on the band gap, density and specific heat. These fundamental properties are crucial for evaluating TiO_2's performance across various applications. The band gap provides insight into TiO_2's electronic properties and its suitability for optical and electronic applications. Density is essential for understanding the material's mass-to-volume ratio, which affects its structural and mechanical performance.

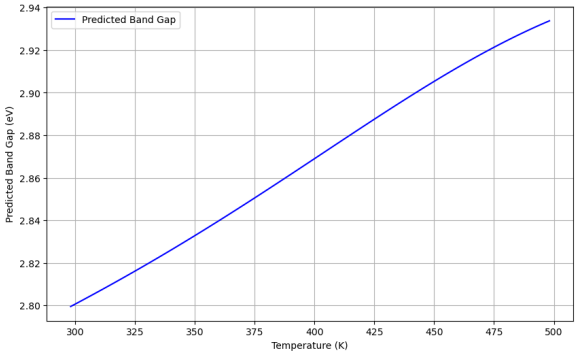

Fig. 16: ANN predictions of TiO 2 band gap with temperature variation

Figure (16) illustrates the variation in the predicted band gap of Titanium Dioxide (TiO_2) across a temperature range from 298.15-498.15 K. The data shows a gradual increase in the band gap, starting at 2.7996 eV at 298.15 K and reaching 2.9338 eV at 498.15 K.

This trend indicates that as the temperature rises, TiO_2's band gap increases steadily. The observed increase in band gap with temperature suggests that TiO_2's electronic band structure becomes more favorable for electronic transitions at higher temperatures. This behavior implies that TiO_2 exhibits greater resistance to electronic excitations as temperature increases. An R^2 score of 0.9993 means that approximately 99.93% of the variance in the predicted band gap values is explained by the ANN model. This suggests that the model captures nearly all of the variability in the data, leaving only 0.07% of the variance unexplained.

In practical terms, this rising band gap implies that TiO_2 could exhibit reduced electrical conductivity and altered optical properties at elevated temperatures. This characteristic is beneficial for applications requiring high-temperature stability and performance, as it indicates TiO_2's ability to maintain its electronic and optical properties under thermal stress.

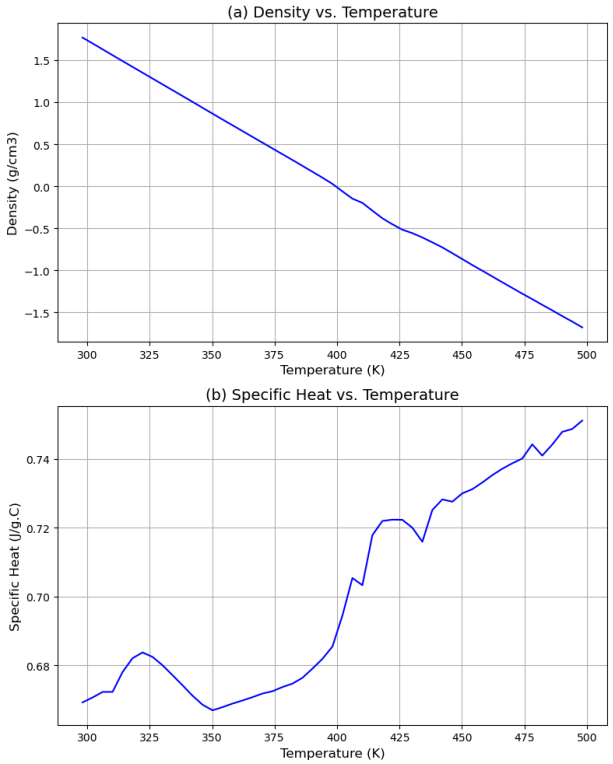

Fig. 17: ANN predictions of TiO_2 parameters with temperature variation

The ANN-predicted data for TiO_2 across different temperatures is illustrated in Fig. (17). As the temperature increases, the density of TiO_2 decreases significantly, from 1.7677 g/cm³ at 298.15-1.6781 g/cm³ at 498.15 K. This reduction in density reflects the material's thermal expansion, where the increase in atomic vibrations at higher temperatures leads to a lattice expansion, thereby reducing density. However, the occurrence of negative density values in the predictions indicates a limitation in the ANN model. Specifically, the model's inability to predict physical properties accurately beyond a certain range or its insufficient training data

may result in unphysical values such as negative densities. These negative values suggest that the model has extrapolated beyond its training range, where it might not perform reliably.

In contrast, the specific heat of TiO_2 increases from 0.6693 J/g.C at 298.15 K to 0.7511 J/g.C at 498.15 K. This trend indicates that TiO_2's capacity to absorb and store thermal energy grows with temperature. The rising specific heat suggests that more energy is required to raise the temperature of TiO_2 as it becomes hotter. This behavior could be beneficial in applications where the material is subjected to temperature fluctuations or used for thermal energy storage.

This section details the application of the Random Forest model for predicting the material properties of TiAl, TiCu and TiO_2. The Random Forest approach enhances prediction accuracy by aggregating multiple decision trees, thus providing robust estimates and capturing complex interactions within the data.

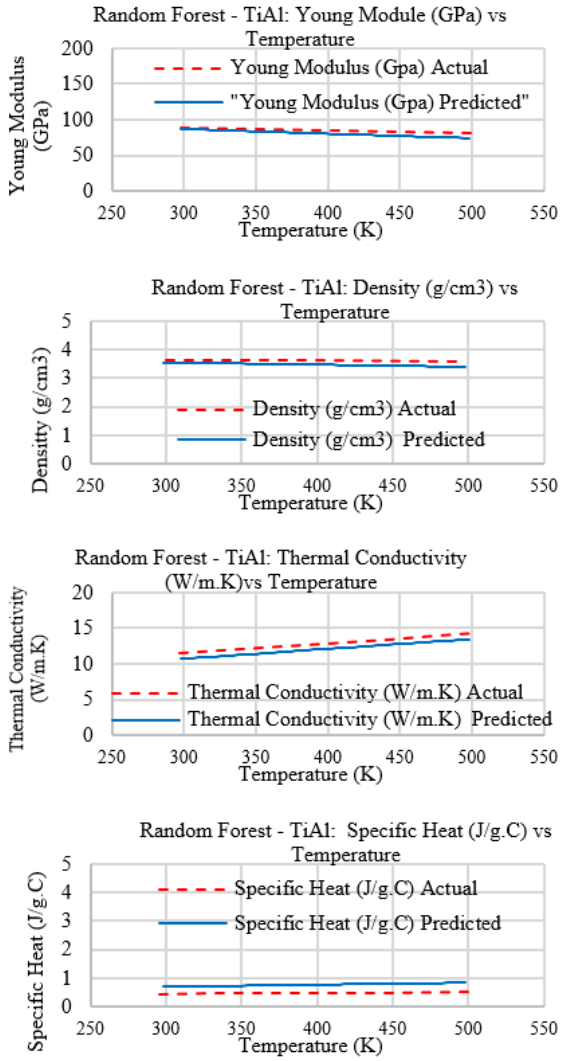

Fig. 18: Random forest predictions of TiAl properties with temperature variation

Figure (18) demonstrates the Random Forest predictions of TiAl properties as functions of temperature variation. The Random Forest model for TiAl predicts material properties across a temperature range from 298.15-498.15 K. Young's Modulus decreases steadily from 87.013 GPa at 301.15-74.47 GPa at 498.15 K, reflecting the material's reduced rigidity at higher temperatures. Density also decreases from 3.55 g/cm³ to 3.40 g/cm³, which is attributed to thermal expansion. Thermal conductivity increases slightly, from 10.712 W/m.K to 13.44 W/m.K, indicating stable heat conduction. Specific heat increases from 0.708 J/g°C to 0.846 J/g°C, reflecting a greater capacity for thermal energy storage at higher temperatures.

The model's predictions are generally accurate with small discrepancies. For Young's Modulus, the predicted values are close but slightly underestimated at lower temperatures (87.01 GPa vs. 88.2 GPa at 298.15 K) and slightly overestimated at higher temperatures (75.15 GPa vs. 74.474 GPa at 498.15 K). The predicted density values are close to actual values, with a small underestimation at 298.15 K (3.5555 g/cm³ vs. 3.62243 g/cm³) and a nearly perfect match at 498.15 K (3.4017 g/cm³ vs. 3.401683 g/cm³). For thermal conductivity, the model slightly underestimates values at lower temperatures but matches perfectly at higher temperatures (13.4399 W/m.K). Specific heat predictions show a large overestimation at 298.15 K (0.7081 J/g°C vs. 0.437559 J/g°C) but a perfect match at 498.15 K (0.8465 J/g°C). The model performs better at higher temperatures, accurately predicting the trends in thermal conductivity and specific heat.

Figure (19) illustrates the Random Forest model's predictions for TiCu properties across a range of temperatures. This figure provides insights into how key material properties Young's Modulus, Density, Thermal Conductivity and Specific Heat vary with temperature.

The Random Forest model for TiCu shows that Young's Modulus decreases with increasing temperature, from 116.41 GPa at 301.15 K to 95.54 GPa at 498.15 K. This decrease reflects the material's reduced stiffness due to thermal expansion. Similarly, the density decreases from 6.55 g/cm³ at 298.15 K to 6.265 g/cm³ at 498.15 K, which is also attributed to thermal expansion. Thermal conductivity slightly increases from 48.42 W/m.K to 77.163 W/m.K, indicating stable heat conduction properties with minor enhancement. Specific heat increases from 0.447 J/g°C to 0.532 J/g°C, suggesting that TiCu requires more energy for temperature increases as the temperature rises.

In terms of predictions, the model performs reasonably well but with slight discrepancies. For Young's Modulus, the predicted values closely match the actual values, with a small underestimation at 498.15 K (95.73 GPa vs. 95.545 GPa). The predicted density values are slightly higher than actual values, with a

difference of 0.2393 g/cm³ at 298.15 K (predicted 6.5573 g/cm³ vs. actual 6.318 g/cm³) but still follow the correct downward trend. For thermal conductivity, the model slightly overestimates the values, with a discrepancy of 0.4 W/m·K at 298.15 K and a more significant overestimation at 498.15 K (77.1636 W/m·K vs. 69.27 W/m·K). Similarly, the specific heat predictions slightly overestimate the values, with a difference of 0.0085 J/g°C at 298.15 K and a slightly larger difference of 0.0197 J/g°C at 498.15 K. Despite these small discrepancies, the model captures the general trends of the material properties effectively.

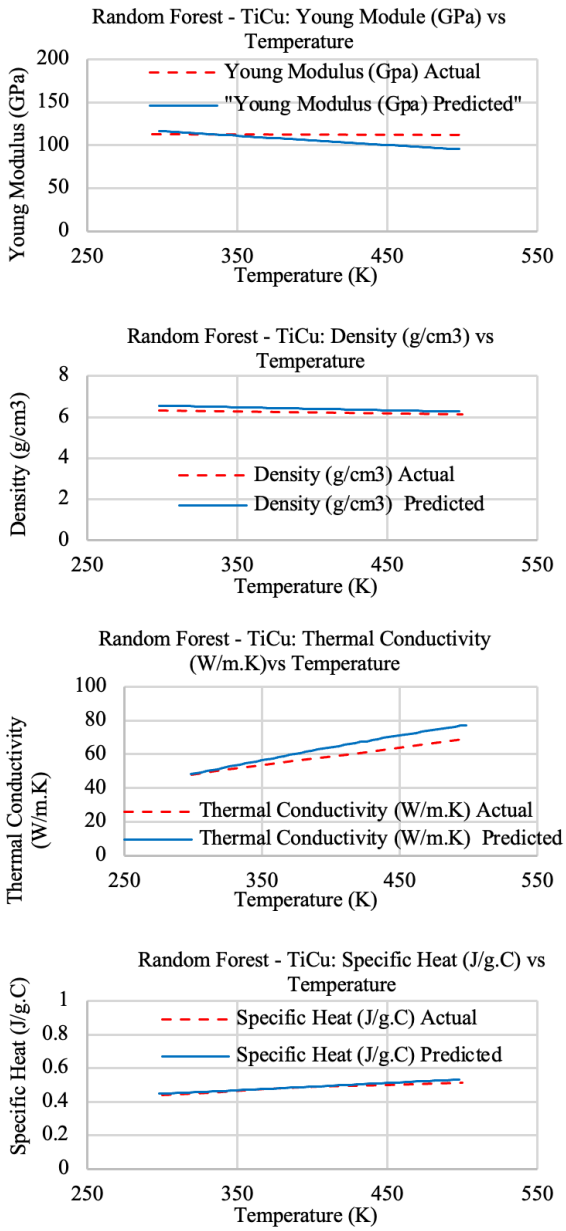

Fig. 19: Random forest predictions of TiCu properties with temperature variation

Figure (20) illustrates the variation in the predicted band gap of Titanium Dioxide (TiO_2) over a temperature range from 298.15 to 498.15 K. The data shows a gradual increase in the band gap, starting at 2.8006 eV at 298.15 K and reaching 2.9335 eV at 498.15 K. The trend indicates a steady rise in the band gap as temperature increases. For example, at 302.15 K, the band gap is 2.80 eV and it continues to increase, reaching 2.83 eV at 350.15 K and 2.93 eV at 498.15 K. The Random Forest model achieved an R2 score of 0.9994, indicating an exceptional fit with 99.94% of the variance in band gap values explained by the model. This high score demonstrates the model's robust predictive accuracy and strong performance on the given dataset. In Figure (20) the observation suggests that TiO_2's electronic band structure becomes more favorable for electronic transitions at higher temperatures. The increasing band gap with temperature indicates that TiO_2 becomes more resistant to electronic excitations as the temperature rises. This effect is likely due to enhanced lattice vibrations and thermal expansion, which impact the electronic band structure and contribute to the observed increase in the band gap.

Figure (21) presents the predicted properties of TiO_2, specifically density and specific heat, across a temperature range from 298.15 to 498.15 K using the Random Forest method. This figure provides crucial insights into how these properties vary with temperature, which is essential for understanding the thermal behavior of TiO_2.

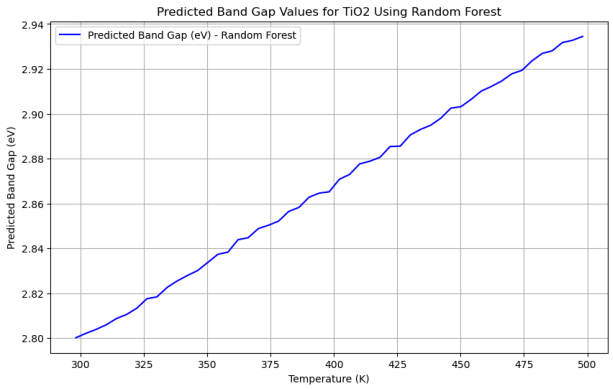

Fig. 20: Random forest predictions of TiO 2

In Figure (21) the predicted density of TiO_2 shows a marked decrease as the temperature increases. At 298.15 K, the density is 1.654 g/cm³. As the temperature rises, the density decreases significantly, reaching a near-zero value of 0.00001 g/cm³ at 498.15 K. This trend suggests that TiO_2 undergoes considerable thermal expansion as the temperature increases. The reduction in density with rising temperature is a common physical phenomenon where the material's lattice structure expands due to increased atomic vibrations and thermal energy. This behavior indicates that at higher temperatures, TiO_2's atomic or molecular arrangement becomes more dispersed, leading to a lower density.

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In contrast, the specific heat of TiO_2 exhibits an increasing trend with temperature. Starting at 0.671 J/g·C at 298.15 K, the specific heat rises steadily to 0.748 J/g·C by 498.15 K. This increase in specific heat with temperature signifies that TiO_2 requires more heat energy to raise its temperature as the temperature increases. This behavior is indicative of heightened phonon activity, which reflects the material's increased capacity to absorb thermal energy at elevated temperatures. The rising specific heat suggests that TiO_2's thermal management properties improve with temperature, allowing it to absorb and store more heat energy.

The data presented in this figure highlights the significant thermal expansion of TiO_2 and its increasing heat capacity with temperature. These properties are critical for applications where TiO_2 is exposed to varying thermal conditions, such as in catalysts, pigments and electronic devices. The observed trends in density and specific heat emphasize the importance of considering thermal effects in the design and application of TiO_2-based materials. It is essential to validate these predicted values with experimental data to ensure their physical accuracy and relevance in practical applications.

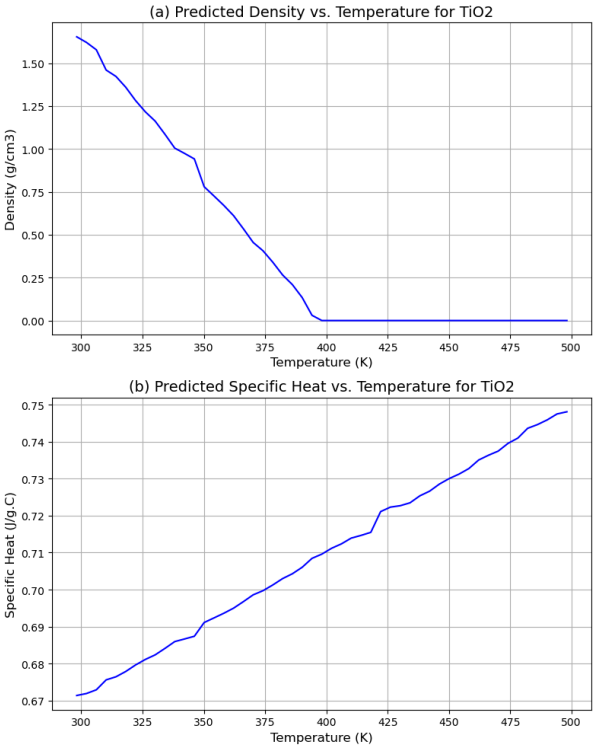

Fig. 21: Random forest predictions of TiO_2

In this section, the application of the results from the Decision Tree were compared with actual values to assess the model's accuracy and reliability in predicting the behavior of materials like TiAl, TiCu and TiO_2.

The Decision Tree model's output for Figure (22) includes predictions for various material properties across a temperature range from 298.15 to 498.15 K. The Decision Tree model for TiAl shows that as temperature increases, Young's Modulus decreases from 87.16 GPa at 298.15-74.35 GPa at 498.15 K, indicating reduced stiffness at higher temperatures, which aligns with typical material behavior. Density also decreases slightly from 3.55 g/cm³ at 298.15 K to 3.40 g/cm³ at 498.15 K due to thermal expansion. Thermal conductivity increases slightly from 10.679-13.46 W/m·K, suggesting a mild improvement in heat conduction with temperature. Specific heat increases from 0.706 J/g·C to 0.847 J/g·C, which is expected as the material's heat capacity rises with temperature.

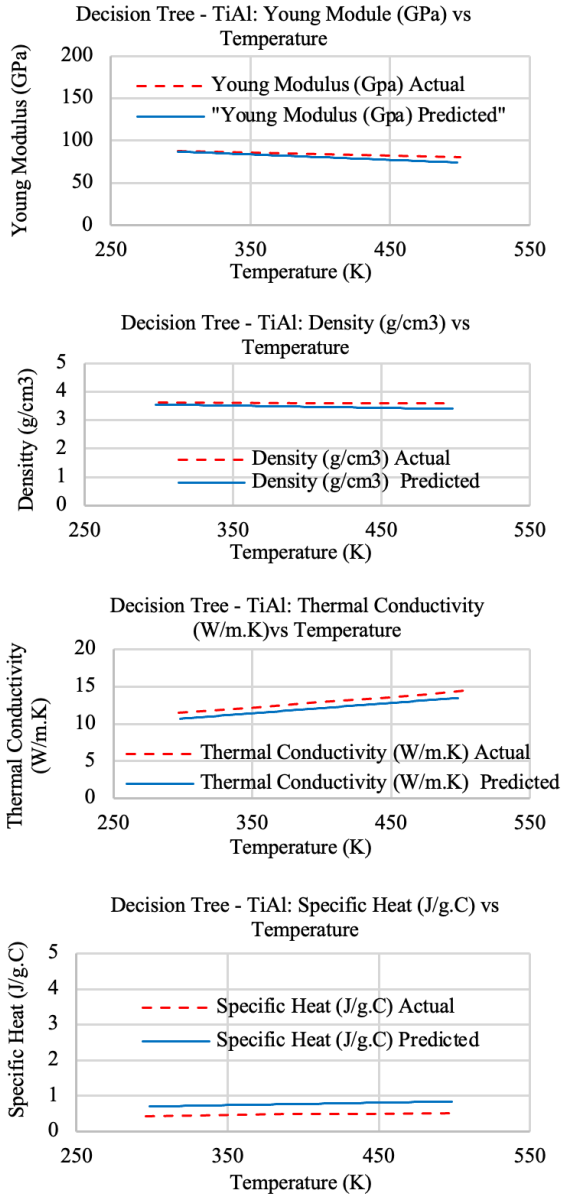

Fig. 22: Decision tree predictions of TiAl properties with temperature variation

In terms of model performance, the Decision Tree predictions show some discrepancies. At 298 K, the

predicted Young's Modulus is 87.17 GPa (slightly underestimating the actual value of 88.2 GPa) and at 500 K, the predicted value is 74.35 GPa (underestimating the actual value of 81 GPa). For density, the model underestimates values, with a discrepancy of -0.0093 g/cm³ at 298 K and -0.1912 g/cm³ at 500 K. The thermal conductivity is also slightly underpredicted, with discrepancies of -0.2872 W/m·K at 296.8 K and -0.8303 W/m·K at 502.88 K. For specific heat, the model slightly underpredicts both at 296.8 K and 498.15 K.

The model's R^2 score is 0.8408, suggesting that 84.08% of the variance in material properties can be explained by the model, indicating a good fit. However, further adjustments may be needed to refine the predictions, particularly for the band gap and thermal conductivity, which could indicate issues with data fitting or preprocessing. Overall, the Decision Tree model captures the expected trends for Young's modulus, density and specific heat, but further improvements are necessary to fully align with the temperature dependencies of these properties.

The Decision Tree model's output for Figure (23) provides predictions for various material properties across a temperature range from 298.15 to 498.15 K. The Decision Tree model for TiCu shows that as temperature increases, Young's modulus decreases from 116.66 GPa at 298.15 K to 95.35 GPa at 498.15 K, indicating a reduction in stiffness, which is typical for materials at higher temperatures. Density also decreases slightly from 6.56 g/cm³ at 298.15 K to 6.26 g/cm³ at 498.15 K, reflecting the expected thermal expansion of the material. Thermal conductivity shows an unusual increase from 48.027 W/m·K at 298.15 K to 77.40 W/m·K at 498.15 K, which suggests a slight reduction in the material's heat-conducting ability as temperature rises, contrary to typical behavior. Specific heat increases from 0.446 J/g·C at 298.15 K to 0.53 J/g·C at 498.15 K, indicating an increase in heat capacity with temperature.

Model predictions show some discrepancies. At 293.15 K, the predicted Young's modulus (113.25 GPa) slightly overestimates the actual value (112.9 GPa) and at 498.15 K, the predicted value (96.11 GPa) is slightly higher than the actual value (95.34 GPa). For density, the model consistently overpredicts, with the predicted values being slightly higher than the actual ones at both 298.15 K and 498.15 K. Thermal conductivity predictions are quite accurate at lower temperatures (48.02 W/m·K predicted vs. 48.02 W/m·K actual) but overestimate the thermal conductivity at 498.15 K (77.40 W/m·K predicted vs. 69.27 W/m·K actual), indicating a tendency to predict a higher increase in conductivity. For specific heat, the model slightly overestimates the values at both 300 K (0.4468 vs. 0.4392 J/g·C) and 498.15 K (0.5334 vs. 0.5129 J/g·C).

The R^2 score for the model is 0.8558, suggesting that 85.58% of the variance in the material properties is explained by the model, which indicates a strong fit. While the predicted trends align well with typical material behavior, the minor discrepancies in thermal conductivity and some overestimations of other properties suggest areas for further refinement in the model to better capture the expected temperature dependencies.

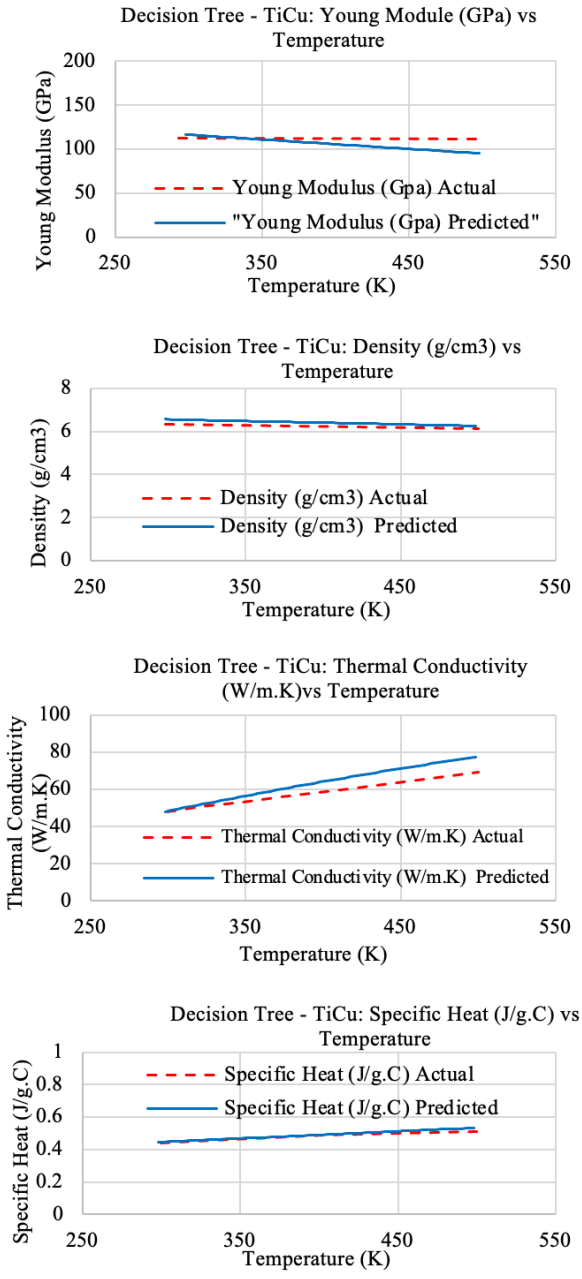

Fig. 23: Decision tree predictions of TiCu properties with temperature variation

Figure (24) depicts the variation in the predicted band gap of Titanium Dioxide (TiO_2) over a specified temperature range. The data shows a general trend of increase in the band gap, with values starting at 2.7959 eV and reaching up to 2.9344 eV. The band gap increases

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progressively with temperature. For example, starting at 2.7959 eV, it rises to 2.8046 eV, then fluctuates slightly but generally increases, reaching 2.8691 eV and eventually peaks at 2.9344 eV. Specific values include 2.8323 eV at one point and 2.8860 eV at another, reflecting a steady increase in band gap values. This trend indicates that TiO_2's electronic band structure becomes more favorable for electronic transitions at higher temperatures. The gradual increase in band gap suggests that TiO_2 becomes more resistant to electronic excitations as the temperature rises. This behavior is likely due to enhanced lattice vibrations and thermal expansion, which affect the electronic band structure and contribute to the observed increase in the band gap. An R2 score of 0.9946 of the models signifies that approximately 99.46% of the variance in the predicted band gap values can be explained by the model.

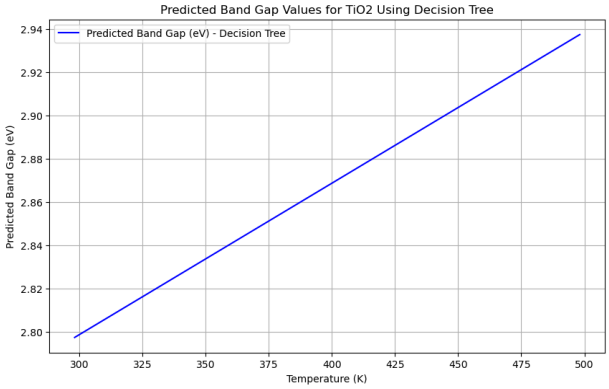

Fig. 24: Decision tree predictions of TiO_2

In Figure (25), which illustrates the outputs from the Decision Tree model for predicting density and specific heat of TiO_2, several key observations can be made. The predicted density shows an initial decrease from 1.705 g/cm³ at 298.15 K to a minimum around 0.745 g/cm³ at 350.15 K. This decrease aligns with the general trend that materials expand with increasing temperature, leading to lower density. However, beyond 350.15 K, the density values drop dramatically to near zero, indicating a potential issue with the model. Such extreme values are unusual and suggest that the Decision Tree might be overfitting or extrapolating inaccurately at higher temperatures. In contrast, the specific heat shows a consistent and realistic increase with temperature, rising from 0.670 J/g.C at 298.15 K to 0.749 J/g.C at 498.15 K. This increase is consistent with the expected behavior of materials, which generally require more energy to raise their temperature as they become hotter. The decision tree's prediction of specific heat appears reasonable, reflecting the typical trend for thermal properties.

Random Forest often performs better than ANN and Decision Trees due to its ensemble nature, where multiple decision trees work together to make predictions. By averaging the outputs of many trees, it reduces the risk of overfitting, which is common in individual Decision Trees. This ensemble approach improves accuracy and robustness, as the model can generalize better to unseen data. Unlike individual Decision Trees, which may overfit due to their complexity, Random Forest uses random subsets of data and features for each tree, preventing any single tree from having too much influence on the final prediction. It is also more robust to noise and outliers, as the combined predictions of many trees tend to smooth out the impact of anomalous data. Furthermore, Random Forest does not require as much hyperparameter tuning as ANN models, which need careful adjustments to layers and learning rates, making it easier to use with minimal tuning. Its ability to handle both linear and nonlinear relationships in the data and provide more accurate predictions, especially with complex or noisy data, makes it a superior choice in many cases. Additionally, while ANN models are often seen as "black boxes," Random Forest offers more interpretability, as each tree can be visualized and understood, which helps in diagnosing model performance. Overall, Random Forest's flexibility, accuracy and ability to manage complex data relationships contribute to its superior performance compared to both Decision Trees and ANN models.

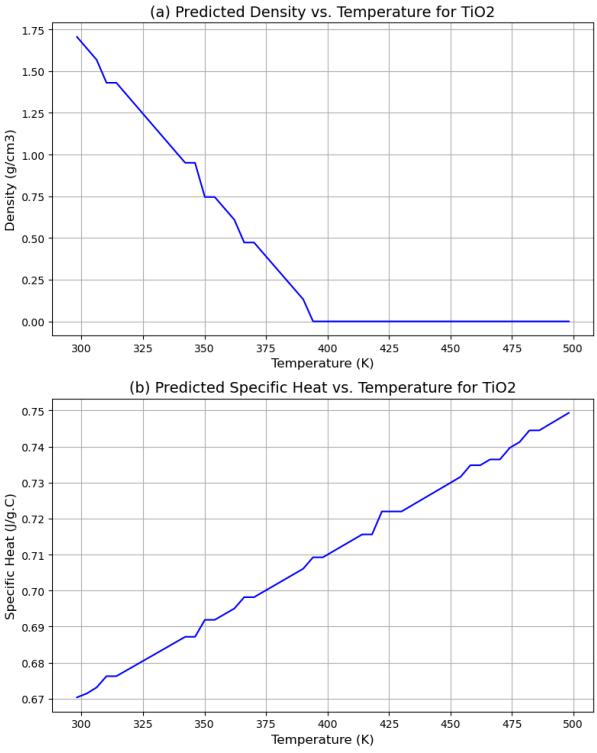

Fig. 25: Decision tree predictions of TiCu properties with temperature variation

For future research, developing a model that automatically collects data through a web scraper could significantly enhance the efficiency of gathering material property data. By integrating real-time data collection from scientific publications, databases, or online

resources, such a model would streamline the data acquisition process for training predictive models. Automating data retrieval through web scraping would not only save time but also allow for the continuous update of material property datasets, ensuring that models stay relevant with the latest available information. This approach could be particularly beneficial for materials science research, where new findings and experimental data are frequently published.

Machine learning models, particularly Random Forest, have demonstrated strong capabilities in predicting material properties such as Young's modulus, density, thermal conductivity and specific heat across various temperatures. These models outperformed other methods, including Artificial Neural Networks (ANN) and Decision Trees, in terms of accuracy and consistency. The ability of Random Forest to handle complex, nonlinear relationships in material property data without overfitting makes it an ideal choice for predicting the behavior of materials under different conditions. This approach can significantly reduce the time and cost associated with traditional experimental methods, allowing for faster development and optimization of materials. The predictive accuracy of machine learning models, especially for materials like TiAl, TiCu and TiO_2, holds significant promise in fields such as aerospace, automotive, biomedical and energy sectors. For instance, in the aerospace industry, these models can be used to design lightweight, high-strength alloys by predicting material properties under varying temperatures and stress conditions. In the biomedical field, machine-learning models could assist in the development of biomaterials for implants or prosthetics by predicting their mechanical properties and biocompatibility under different physiological conditions. Additionally, these models can support the design of more efficient energy materials by predicting thermal properties essential for energy storage or heat exchange applications.

Conclusion

In conclusion, the application of machine learning methods, including ANNs, Random Forests and Decision Trees, demonstrates their effectiveness in accurately predicting material properties across varying conditions:

- ANN Model for TiAl: Achieved an R^2 score of 0.980874, accurately predicting density, Young's modulus and thermal conductivity, with minor deviations in band gap
- ANN Model for TiCu: Achieved an R^2 score of 0.997607, demonstrating high precision in predicting density, Young's modulus and thermal conductivity, with minor deviations in band gap and specific heat
- ANN Model for TiO_2: Showed a low MSE of 0.0009, accurately predicting density and specific heat, but overestimated the band gap and had slight deviations in density
- Random Forest Model for TiAl: R^2 score of 0.998168, accurately predicted density, specific heat and thermal conductivity, with minimal deviations, though further refinement is necessary for band gap predictions
- Random Forest Model for TiCu: Achieved an R^2 score of 0.997764, providing reliable predictions for specific heat and Young's modulus, but showed significant deviations in density and band gap
- Random Forest Model for TiO_2: Excellent R^2 score of 0.9994 for band gap predictions; however, density predictions approached zero at high temperatures, indicating model issues needing further validation
- Decision Tree Model for TiAl, TiCu and TiO_2: Demonstrated strong predictive capabilities with high R^2 scores (TiAl: 0.993841, TiCu: 0.992873, TiO_2: 0.9946)
- ANN model provides valuable insights into how the material properties of TiAl, TiCu and TiO_2 change with temperature. While the model is robust for most properties, addressing issues such as density for TiO_2 values is crucial for ensuring reliable predictions. Understanding these trends is essential for optimizing material performance in temperature-sensitive applications
- Random Forest model offers valuable insights into how TiAl, TiCu and TiO_2 properties change with temperature. Its strong predictive capabilities make it a robust tool for analyzing material behavior in temperature-sensitive applications. Therefore, the Random Forest method can accurately predict the alloy material properties and their behavior in different temperatures range
- Decision Tree model provides valuable insights into the temperature-dependent behavior of TiAl, TiCu and TiO_2. While the predictions for Young's Modulus, Density and Specific Heat align with expected trends, issues
- Improved Material Performance in Biomedical Applications: The precise prediction of specific heat, thermal conductivity and density facilitates the development of advanced biomedical solutions, including orthopedic implants, surgical tools and antimicrobial coatings, ensuring improved durability, stability and performance in clinical environments
- Contribution to Thermal Management Strategies: The research provides valuable insights for industries requiring effective thermal regulation, such as aerospace, automotive and electronics. By understanding the thermal behavior of these materials, engineers can optimize designs for improved heat dissipation and enhanced system efficiency
- Machine learning models, particularly Random Forest, excel in predicting material properties like Young's modulus, density and thermal conductivity, outperforming ANN and Decision Trees. These

models offer faster, cost-effective material design, particularly in aerospace, automotive, biomedical and energy sectors. They enable the optimization of materials for applications such as high-strength alloys, biomedical implants and energy-efficient materials

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Author's Contributions

Armaghan Shalbaftabar: Conducted research development, performed data cleaning, data manipulation and machine learning analysis and conducted research development on statistical analysis and participated in writing the manuscript.

Kristen Rhinehardt: Provided the research topic, guided research development and participated in writing the manuscript.

Dhananjay Kumar: Provided the research topic and participated in writing the manuscript.

Ethics

This article is an original research paper. There are no ethical issues that may arise after the publication of this manuscript.

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