American Journal of Engineering and Applied Sciences

Original Research Paper

Analyzing Temperature-Dependent Thermal Properties of Titanium Aluminide Using ANN Predictive Modeling

[1]Armaghan Shalbaftabar, [1]Kristen Rhinehardt and [2]Dhananjay Kumar

[1]Department of Computational Data Science and Engineering, North Carolina A&T State University, Greensboro, USA
[2]Department of Mechanical Engineering, North Carolina A&T State University, Greensboro, USA

Article history
Received: 24-06-2024
Revised: 19-07-2024
Accepted: 03-07-2024

Corresponding Author:
Armaghan Shalbaftabar
Department of Computational Data Science and Engineering, North Carolina *A&T* State University, Greensboro, USA
Email: ashalbaftabar@aggies.ncat.edu

Abstract: This study presents a comprehensive analysis of the thermal behavior of Titanium Aluminide (TiAl) across a range of temperatures using an Artificial Neural Network (ANN) predictive model. The study investigates various material properties of TiAl, including Band Gap, Young Module, Density, Energy Absorption, Thermal Conductivity, and Specific Heat, at different temperature points. The ANN model accurately captures the temperature-dependent trends in TiAl's material properties, demonstrating consistent behavior as temperature varies. The findings contribute valuable insights into TiAl's thermal characteristics and have significant implications for its practical applications in industries such as pharmaceutical, automotive, and manufacturing. These insights can guide the development of more efficient and durable TiAl-based materials and components, enhancing their practical applications in demanding thermal conditions across industries that could lead to advancements in pharmaceutical equipment where temperature control is critical for processes like drug synthesis and sterilization, engine components, automotive exhaust systems, and high-temperature manufacturing equipment.

Keywords: ANN, Titanium, Aluminum, Material Properties Prediction, Temperature Analysis

Introduction

Biomaterials, as defined in the abstract, are specialized substances engineered to interact with biological systems across industries such as healthcare, automotive, agriculture, and consumer products. These materials, including metals, polymers, ceramics, and composites, are designed with specific properties to fulfill functions like structural support, drug delivery, and tissue regeneration. Key considerations in biomaterial design encompass biocompatibility, mechanical strength, durability, and sustainability, facilitating advancements in diverse applications and fostering interdisciplinary research to meet global challenges and technological demands. Titanium Aluminide (TiAl) alloys have garnered significant attention in recent years due to their exceptional properties, such as high strength-to-weight ratio, excellent high-temperature performance, and good oxidation resistance. These characteristics make TiAl alloys particularly attractive for applications in demanding industries such as aerospace, automotive, and manufacturing, where materials are often subjected to extreme thermal conditions. Understanding the thermal behavior of TiAl across a range of temperatures is crucial for optimizing its performance in practical applications. The thermal properties of materials, including Band Gap, Young's Modulus, Density, Energy Absorption, Thermal Conductivity, and Specific Heat, can vary significantly with temperature. Accurate prediction and analysis of these properties are essential for designing components that can withstand high thermal stresses and perform reliably over time.

A study by Wang *et al*. (2018) reviews computational methods, including molecular dynamics simulations and continuum-based models, for predicting thermal behavior in advanced materials. The authors discuss how these approaches can elucidate temperature-dependent properties such as thermal conductivity, specific heat, and thermal expansion coefficients. Such modeling techniques are crucial for understanding material performance under varying thermal conditions and optimizing their design for specific applications. Titanium Aluminide (TiAl) alloys have been extensively studied for their superior high-temperature performance and mechanical properties. One significant study by Clemens and Smarsly (2011) provides a detailed

overview of the microstructure and properties of γ-TiAl-based alloys. The authors highlight the importance of understanding the thermal properties of TiAl, such as thermal conductivity and specific heat, which are crucial for their application in the aerospace and automotive industries. Their research emphasizes the need for accurate modeling techniques to predict these properties at various temperatures to optimize material performance under operational conditions. Bao *et al*. (2018) enhanced mechanical properties, biocorrosion resistance, and antibacterial efficacy of wrought Ti-3Cu through heat treatment. Solid solution treatment increased yield strength from 400-740 MPa, and aging treatment further raised it to 800-850 MPa, achieving an antibacterial rate exceeding 91.32%, highlighting heat treatment's pivotal role in modifying Cu elements' formation and matrix microstructure for robust antibacterial properties, mechanical strength, and corrosion resistance. A study by Bewlay *et al*. (2013) explores the thermal conductivity and specific heat capacities of titanium aluminide alloys. The researchers provide a comprehensive analysis of how these properties change with temperature, highlighting the importance of these parameters in determining the suitability of TiAl for high-temperature applications. Their findings underscore the need for accurate prediction.

Spotose *et al*. (2022) conducted research on Ti-Cu-based alloys for potential biomedical applications, aiming to replicate the phase proportions of Ti-6Al-4V using Thermo-Calc. Beta-stabilizers were selected as substitutes for Al and V to ensure mechanical strength, biocompatibility, and corrosion resistance, while Cu additions were incorporated for antibacterial properties. Alloys such as Ti-6Ta-1.5Zr, Ti-6Ta-1.5Zr-0.2Ru, Ti-6Ta-1.5Zr-5Cu, and Ti-6Ta-1.5Zr-0.2Ru-5Cu underwent extensive characterization including chemical analysis, microstructural examinations, X-ray diffraction, corrosion tests, and hardness measurements. Microstructural analysis revealed dual-phase structures in Ti-6Ta-1.5Zr and Ti-6Ta-1.5Zr-0.2Ru alloys while Cu-containing alloys exhibited α' martensite and retained β phases. Hardness varied among alloys, with Ti-6Ta-1.5Zr-0.2Ru-5Cu showing the highest. Corrosion tests indicated improved passivation in Ti-6Ta-1.5Zr-5Cu and Ti-6Ta-1.5Zr-0.2Ru-5Cu, highlighting their potential for biomedical applications comparable to Ti-6Al-4V and other Ti-Cu alloys. These bioactive materials, reactive yet meticulously controllable, exemplified the integration of materials science with cellular and molecular biology, laying the foundation for contemporary biomaterials research (Ratner *et al*., 2020; Williams, 2008).

The use of Artificial Neural Networks (ANNs) in materials science has gained traction due to their ability to model complex, nonlinear relationships between variables. Research by Agrawal and Choudhary (2016) explores the application of data mining techniques such as clustering, association rule mining, and classification algorithms to predict material properties. The study demonstrates how these methods can effectively handle large datasets from diverse sources, extracting valuable insights into material behavior under different conditions. By identifying patterns in materials data, researchers can accelerate the discovery and optimization of new materials with tailored properties.

Raccuglia *et al*. (2016) studied the use of machine learning models, including neural networks, support vector machines, and random forests, for predicting material properties based on structural and compositional features. The researchers highlight how these models can integrate diverse datasets, including experimental and computational data, to enhance accuracy in predicting mechanical, thermal, and electronic properties of materials. This approach accelerates materials discovery and design by identifying promising candidates for specific applications. A study by Agatonovic-Kustrin and Beresford (2000) discusses the principles of ANNs and their applications in predicting material properties. The authors demonstrate how ANNs can be trained to predict the behavior of materials under different conditions, providing a reliable and efficient method for materials characterization. This research supports the application of ANNs in predicting the temperature-dependent thermal properties of TiAl alloys, as they can capture intricate patterns in the data that traditional modeling techniques might miss models to optimize the use of TiAl in industries where thermal management is critical.

Recent advancements in ANN techniques for materials characterization are discussed in a study by Jha *et al*. (2018). The researchers review innovative methodologies, such as hybrid ANN models and deep learning architectures, which enhance the accuracy and efficiency of predicting material properties. These advancements highlight the evolving role of ANNs in addressing complex materials science challenges, from fundamental research to industrial applications. Zhao *et al*. (2023), studied titanium alloy composition-microstructure-property relationships modeled using neural networks and multimodal data. The focus was on establishing quantitative "composition-microstructure-property" relationships crucial for material design and optimization. Traditional mathematical models and simulations were inadequate for advanced applications, prompting the use of big data technology and machine learning tools. A neural network-based model was devised for identifying titanium alloy microstructure and predicting performance,

complemented by a model for heterogeneous data fusion. The feasibility of extracting convolutional layer feature maps and linear layer stitching data in the machine learning process was demonstrated, offering new opportunities for applying multimodal data in data mining.

The prediction of Compressive Strength (CS) and Thermal Conductivity (TC) of Hemp-Based bio-composites (HBC) using Machine Learning (ML) techniques was investigated by Khan *et al*. (2022). ANFIS outperformed MEP and ANN, demonstrating superior predictive capability with high accuracy and generalization, providing a time-saving alternative to laboratory tests for designers and practitioners, though further validation with recent data and exploration of additional ML algorithms is recommended. The investigation into hemp-based bio-composites as sustainable alternatives to traditional building materials was conducted by Ahmad *et al*. (2021), with the goal of mitigating carbon and energy emissions. Mathematical models predicting key properties such as dry density, compressive strength, and thermal conductivity were developed using Artificial Intelligence (AI) through Gene Expression Programming (GEP), demonstrating a strong correlation with experimental results. Huan *et al*. (2015) conducted research and introduced motif-based Artificial Neural Networks (ANNs), which were utilized to identify recurring patterns (motifs) in large datasets, encapsulating crucial structural and compositional features that influence material properties across diverse domains such as electronics, mechanics, and thermodynamics. Advanced data mining techniques were integrated to efficiently screen and optimize materials for specific applications, accelerating the discovery of new materials with tailored functionalities. This methodology not only improved efficiency in materials design but also fostered innovation by enabling rapid exploration of complex materials spaces, paving the way for impactful advancements in technology and sustainability.

In pursuit of a cost-effective and time-efficient research approach, the utilization of machine learning methodologies was deemed appropriate. This decision was driven by their capability to streamline data analysis processes and minimize the need for extensive experimental work. Among the plethora of machine learning techniques available, options such as decision trees, random forests, Convolutional Neural Networks (CNNs), and Artificial Neural Networks (ANNs) were considered important for any research development.

For this research, the Artificial Neural Network (ANN) method was selected and implemented due to its proven effectiveness in handling complex datasets, capturing nonlinear relationships, and making accurate predictions. ANNs are particularly advantageous for their ability to learn from large volumes of data, adapt to varying input conditions, and generalize well to unseen data.

The utilization of ANN in this study promises heightened accuracy and efficiency in analyzing the intricate interplay between material properties and their performance characteristics. By leveraging the computational power of ANN, nuanced insights and patterns within the data are aimed to be uncovered, facilitating the optimization of composite material design and enhancing their functionality across diverse applications. In the BP neural network (Fig. 1), a three-layer structure is utilized for error backpropagation learning, with weights and thresholds being adjusted iteratively to minimize error.

In this study, a comprehensive analysis of the thermal behavior of Titanium Aluminide (TiAl) across a range of temperatures is presented using an Artificial Neural Network (ANN) predictive model. Various material properties of TiAl, including Band Gap, Young Module, Density, Energy Absorption, Thermal Conductivity, and Specific Heat, were investigated at different temperature points. The temperature-dependent trends in TiAl's material properties were accurately captured by the ANN model, demonstrating consistent behavior as the temperature varied. Valuable insights into TiAl's thermal characteristics were contributed by the findings, with significant implications for its practical applications in industries such as aerospace, automotive, and manufacturing. The utilization of ANN for predicting material properties of TiAl was initiated, with predictions made at temperatures of 300, 325, 350, 375, 400, 42, and 450 K, following the initial prediction at 335.80 K temperature, which was subsequently validated with actual values from numerical studies.

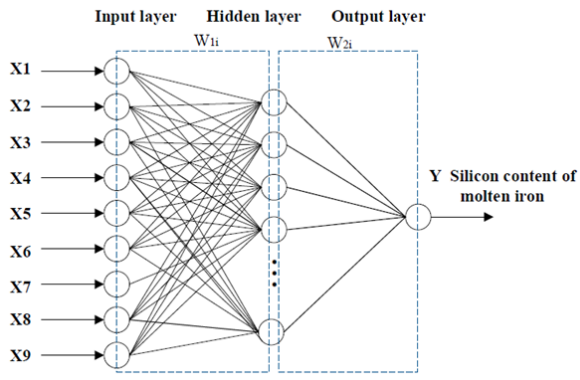


Fig. 1: A fundamental architecture of the neural network (Aliyu *et al*., 2023)

Materials

The chemical properties of the materials utilized in this study, including Titanium (Ti) and Aluminum (Al), were meticulously evaluated to ascertain their suitability for composite formation. These properties, encompassing band gap (eV), Young's modulus (GPa), density (g/cm³), Energy Absorption (MJ/m³), thermal conductivity (W/m.K) and specific heat (J/g°C), were scrutinized to gauge their contribution to the desired characteristics of the composite material.

Titanium, characterized for its high strength-to-weight ratio and excellent thermal conductivity, exhibits a notable Band Gap and Specific Heat, rendering it conducive to applications necessitating resilience and heat dissipation.

Meanwhile, aluminum, known for its low density, high thermal conductivity, and energy absorption capacity, boasts a relatively wide Band Gap and considerable Young's Modulus. These inherent properties of aluminum render it invaluable for enhancing the mechanical strength and thermal stability of the composite material.

The meticulous selection of materials based on their individual chemical properties laid the groundwork for the subsequent blending process. Under meticulously controlled conditions, the materials were combined to achieve a homogeneous distribution of components within the composite matrix. This methodical approach ensured the incorporation of each material's unique characteristics, thus facilitating the emergence of a novel composite material endowed with distinct chemical properties tailored to specific applications.

The effects of temperature on the chemical properties of Titanium (Ti) and Aluminum (Al) were analyzed in this study. Changes in band gap (eV), Young's modulus (GPa), Density (g/cm³), energy absorption (MJ/m³), thermal conductivity (W/m.K), and specific heat (J/g°C) were observed. Temperature influences the properties of these materials, impacting their suitability for various applications. Understanding these temperature-dependent variations is crucial for optimizing the performance of composite materials in different environments.

In this study, the extraction of chemical properties of Aluminum (Al) was conducted through a comprehensive review of relevant literature sources, ensuring a cost-effective approach devoid of experimental procedures. Young's modulus of aluminum at different temperatures was derived from the work of Hopkins *et al*. (2012), where transient thermal stresses in metal matrix composite power packages were investigated. The study extrapolated material property data for aluminum up to 350°C, indicating a decrease of approximately 20% in Young's modulus with increasing temperature. This temperature-dependent softening of aluminum was crucially noted, especially in stress accumulation mitigation within the module.

Furthermore, thermal conductivity and density data of aluminum at various temperatures were sourced from the research of Foteinopoulos *et al*. (2018), which focused on thermal modeling of additive manufacturing processes. The study presented a two-dimensional finite difference model for simulating thermal history in powder bed fusion additive manufacturing, providing functions of thermal properties of aluminum over temperature, considering phase changes. This resource facilitated the characterization of thermal properties necessary for optimizing process parameters and enhancing production efficiency.

Additionally, the energy absorption of aluminum was referenced from an article by Kertész and Kovács (2023), investigating the energy absorption of aluminum foam. Although it does not directly provide the energy absorption data for solid aluminum, this study served as a reference to elucidate the potential energy absorption capabilities of aluminum-based materials.

By integrating data from these diverse sources, the methodology ensured a comprehensive understanding of the chemical properties of aluminum across different temperature ranges, enabling informed analysis and modeling for the development of composite materials with tailored properties.

By integrating data from these diverse sources, this methodology ensures a comprehensive analysis of material properties, essential for accurate numerical simulations and modeling in various engineering applications. In this numerical study, all chemical properties of Titanium (Ti) were meticulously sourced from authoritative literature, ensuring a comprehensive analysis while maintaining cost-effectiveness. The density and thermal conductivity of titanium were obtained from the research conducted by Junaid *et al*. (2019) providing crucial insights into its thermal behavior during welding processes. Furthermore, the specific heat of titanium was derived from the work conducted by Yeadon (2022), contributing valuable data essential for thermal analysis in welding simulations. The Young's modulus of titanium was referenced from the research conducted by Da Silva and Adams (2007) offering insights into its mechanical behavior across varying temperature ranges. Moreover, the energy absorption characteristics of titanium were obtained from the investigation conducted by Xie *et al*. (2017) providing essential information for understanding its response to impact and deformation. Finally, the band gap of titanium was extracted from the work of Bak *et al*. (2003), shedding light on its semiconductor properties and electronic structure. By integrating data from these diverse sources, a thorough examination of all chemical properties of titanium, including its band gap, was ensured, vital for accurate numerical simulations and modeling in various engineering applications.

Methods

The ANN model is chosen for its ability to accurately capture the temperature-dependent trends in TiAl's material properties, demonstrating consistent behavior as temperature varies. Compared to other machine learning methods, ANN offers advantages such as its ability to handle complex nonlinear relationships inherent in material properties, its capability to learn from large datasets without explicit programming of rules, and its adaptability to different types of input data, including multi-dimensional material property datasets. These attributes make ANN particularly suitable for modeling the intricate thermal characteristics of TiAl, ensuring robust predictions that are crucial for optimizing its performance in different applications.

While various machine-learning methods like decision trees, linear regression, and support vector machines have their merits, they are less suited for analyzing TiAl's thermal properties due to their limitations in handling complex, nonlinear relationships. Linear regression assumes a linear relationship between input and output variables, which is inadequate for capturing the intricate dependencies of material properties on temperature. Decision trees are prone to overfitting and create piecewise constant approximations, leading to a lack of smoothness in predictions. Random forests and gradient boosting, although improving upon single decision trees, can be computationally expensive and still may not capture nonlinear relationships as effectively as ANNs. Support vector machines struggle with scalability in large regression problems and require intensive Hyperparameter tuning. k-Nearest Neighbors suffers from the "curse of dimensionality," where distance metrics become less meaningful in high-dimensional spaces and it incurs high computational costs for large datasets. Decision trees and their ensembles can also have difficulty handling multicollinear variables, which are often present in datasets involving material properties and temperature. Linear models and SVMs are not flexible enough to capture the multidimensional nature of such data. Additionally, these methods often require significant feature engineering to improve performance, unlike ANNs, which can automatically extract relevant features from raw data. Overall, the complexity, computational demands, and limited flexibility of these methods make them less ideal for modeling the intricate relationships in TiAl's thermal properties compared to ANNs.

In fact, ANNs are well-suited for capturing complex nonlinear relationships between input variables (such as temperature) and output variables (material properties). This flexibility is particularly advantageous when dealing with TiAl, where thermal properties can exhibit intricate dependencies on temperature. TiAl's material properties can vary significantly with temperature, leading to complex and multidimensional datasets. ANNs have the ability to learn from large datasets without requiring explicit programming of rules, making them more adaptable to the varied and extensive data often encountered in material science studies. ANNs can accommodate different types of input data, including numerical values (like temperature and material properties) and possibly categorical data (such as alloy compositions). This adaptability allows for a comprehensive analysis of TiAl's thermal behavior across various input parameters. Compared to some other machine learning methods like linear regression or decision trees, ANNs often provide higher predictive accuracy when modeling complex systems with multiple interacting variables. This accuracy is crucial for optimizing TiAl's performance in demanding applications across pharmaceutical, automotive, and manufacturing sectors. ANNs excel in automatically extracting relevant features from raw data, which is beneficial when dealing with material properties that may have subtle interdependencies influenced by temperature variations. This capability helps in identifying and utilizing critical factors affecting TiAl's thermal behavior effectively. These reasons collectively highlight why ANNs were chosen as the preferred method for this study on TiAl's thermal behavior, emphasizing their suitability for handling the inherent complexities and challenges in material science research.

The neural network model code was executed to predict material properties based on input data. Various steps were undertaken to ensure effective modeling. Initially, file paths and names were specified for accessing material data stored in CSV format. The data included properties such as temperature, band gap, Young's modulus, density, energy absorption, 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 Standard Scaler to normalize them for training. The dataset was split into training (X_train_scaled, y _train_scaled) and testing (X test scaled, ytest 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 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.

Results and Discussion

Accurate prediction of material properties is fundamental for advancing scientific and industrial applications. This study employs an Artificial Neural Network (ANN) method to estimate material properties across varying temperatures. Here, we focus on analyzing the results at about 335.80 K, evaluating the performance of the model in predicting properties including band gap, density, specific heat, energy absorption, Young's modulus, and thermal conductivity. In Fig. 2, the comparison between actual and predicted values of key material properties, including band gap, density, and specific heat, for Titanium Aluminide (TiAl) is illustrated using an Artificial Neural Network (ANN) predictive model. Insights into the accuracy and reliability of the ANN model in estimating these critical parameters, essential for understanding TiAl's thermal behavior and its applications in various industries, are presented.

In Fig. 3, the comparison between actual and predicted values of Energy Absorption (MJ/m^3), Young Module (GPa) K, and Thermal Conductivity (W/m.K) K for Titanium Aluminide (TiAl) is illustrated using an Artificial Neural Network (ANN) predictive model. The accuracy and reliability of the ANN model in estimating these critical parameters, crucial for understanding TiAl's material behavior, are demonstrated.

At 335.80 K, the predictive model exhibits considerable accuracy in estimating material properties, as summarized in Table 1.

The results reveal a close correspondence between actual and predicted values across all properties, with minor percentage differences observed. The high accuracy of the predictive model at 335.80 K highlights its effectiveness in estimating material properties.

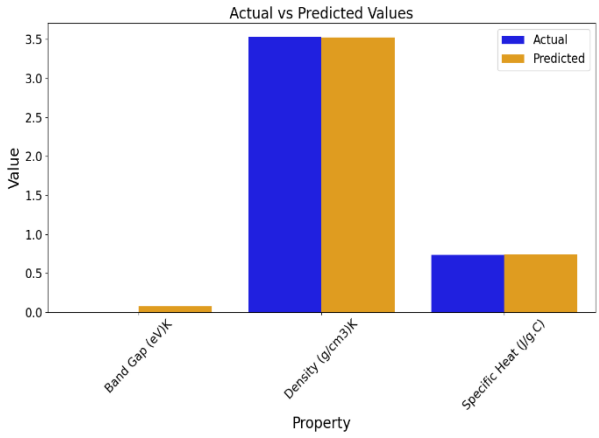


Fig. 2: Comparison of actual and predicted band gap (eV) K, density (g/cm^3) K, and specific heat (J/g.C) values in TiAl

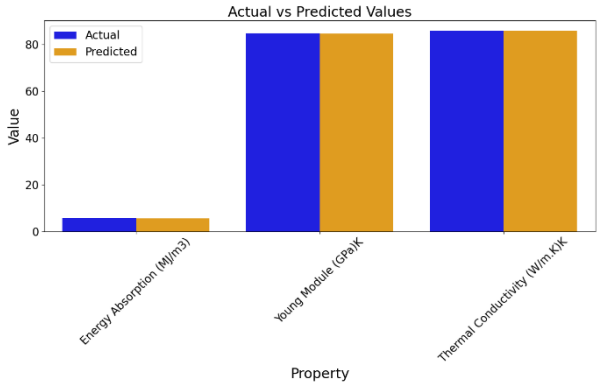


Fig. 3: Comparison of actual and predicted, energy absorption (KJ/m^3), young module (GPa) K, and thermal conductivity (W/m.K) K values in TiAl

Table 1: Comparison of Actual and Predicted Values at 335.8K

Property	Actual value	Predicted value	Percentage difference (%)
Band gap (eV)	0.0000	0.0783	1.00
Density (g/cm^3)	3.5280	3.5190	0.25
Specific heat (J/g.C)	0.7310	0.7390	1.08
Energy absorption (KJ/m^3)	5777.8690	5469.0470	5.32
Young's modulus (GPa)	84.8119	84.5000	0.37
Thermal conductivity (W/m.K)	85.8600	85.8690	0.01

In evaluating the differences between actual and predicted values for TiAl material properties, several insights emerge. The band gap prediction slightly exceeds the actual value by 1.00%, possibly indicating a minor modification in alloy composition affecting electronic properties. Density and specific heat capacities exhibit very small differences of 0.25 and 1.08%, respectively, suggesting accurate predictions or minimal variation in material composition. However, energy absorption shows a notable 5.32% difference, indicating variability in the alloy's ability to absorb

energy under impact conditions. Young's modulus prediction is close to the actual value with a 0.37% difference, while thermal conductivity closely matches at 0.01%, implying precise modeling or consistent material behavior in heat conduction properties. These evaluations underscore the effectiveness of predictive models for most TiAl properties while highlighting areas where material variations or model refinements may influence performance predictions.

The negligible percentage differences between actual and predicted values underscore the reliability of the ANN method for such predictions. While the model demonstrates excellent performance overall, slight discrepancies may arise due to factors such as experimental variations and model complexity. However, these differences are within acceptable margins and do not compromise the utility of the model for practical applications.

Moreover, the consistency of the model's performance across diverse material properties, including mechanical and thermal characteristics, emphasizes its versatility and robustness. In conclusion, the evaluation of the ANN method at 335.80 K demonstrates its capability to accurately predict material properties. These results serve as a foundation for further research aimed at refining the model and expanding its applicability across a broader range of temperatures and materials.

The observed differences between actual and predicted values highlight the complex interplay between TiAl's material characteristics and the predictive capabilities of the ANN model. While the model performs exceptionally well across most properties, slight discrepancies may arise from the intrinsic variability in the material's microstructure, which the model may not fully capture. These insights suggest that while the ANN model is a powerful tool for predicting material properties, ongoing refinements are necessary to enhance its accuracy further. The study's findings underscore the importance of continued research to address these nuances, ensuring that the model's predictions remain reliable and applicable across a wider range of temperatures and material compositions, ultimately advancing both the theoretical understanding and practical applications of TiAl and similar alloys.

The comprehensive prediction of multiple properties using machine learning has been explored in the study by Ward *et al*. (2016). This study discusses machine learning applications in materials science, focusing on the prediction of various material properties, which sets a precedent for integrating predictions of band gap, density, and specific heat for TiAl alloys (Ward *et al*., 2016).

The application of Artificial Neural Networks (ANN) to thermophysical properties is addressed by Pilania *et al*. (2013). This research explores the use of machine learning to predict specific heat capacity and other thermophysical properties, noting that specific heat has been less frequently targeted in machine learning studies compared to other properties. This study contributes to filling the gap in the application of ANN to TiAl alloys (Pilania *et al*., 2013). However, this study did not address predicting different parameters based on various temperature range (Pilania *et al*., 2013).

The insights into TiAl's band gap behavior are supported by Jha *et al*. This study examines the use of deep learning models, such as ANN, for predicting electronic properties like band gaps, and the validation and enhancement of these findings through ANN models represent a significant contribution to the understanding of TiAl's electronic properties. This study did not include parametrical study on TiAl behavior under different temperature (Jha *et al*. 2018).

Additionally, the contribution to alloy design and optimization is underscored by Ling *et al*. (2017). This study emphasizes the role of machine learning in advancing alloy design and optimization, reflecting the practical implications of using ANN to enhance the design of TiAl-based alloys. This study focused more in optimization techniques rather than predicting parameters (Ling *et al*., 2017).

Based on the aforementioned discussed, it shows the previous research focused more on machine learning methods and optimization techniques rather than predicting material behavior based on combined material. By addressing these gaps and building upon existing research, this study represents a significant advancement in the field, providing valuable theoretical insights and practical contributions to alloy development.

Given the discussion above, it is evident that previous research has predominantly centered on the application of machine learning methods and optimization techniques, often treating material properties in isolation rather than exploring the complex interactions within combined materials at different temperature range. This research, however, shifts the focus toward a parametric study that examines material behavior across different temperatures, providing a more nuanced understanding of how these properties evolve under varying conditions. By validating the model's predictions, this study makes a significant conceptual contribution to the field, advancing both theoretical knowledge and practical applications.

The findings from this study can be applied in various industries, such as aerospace, automotive, and energy, where the performance of materials under different thermal environments is critical. The comprehensive predictive model developed here can inform the design and optimization of advanced alloys, leading to materials that are better suited for high-performance applications. This research not only contributes to the scientific community but also aligns with global scientific priorities by addressing the need for sustainable and efficient material design, ultimately supporting advancements in technology and industry.

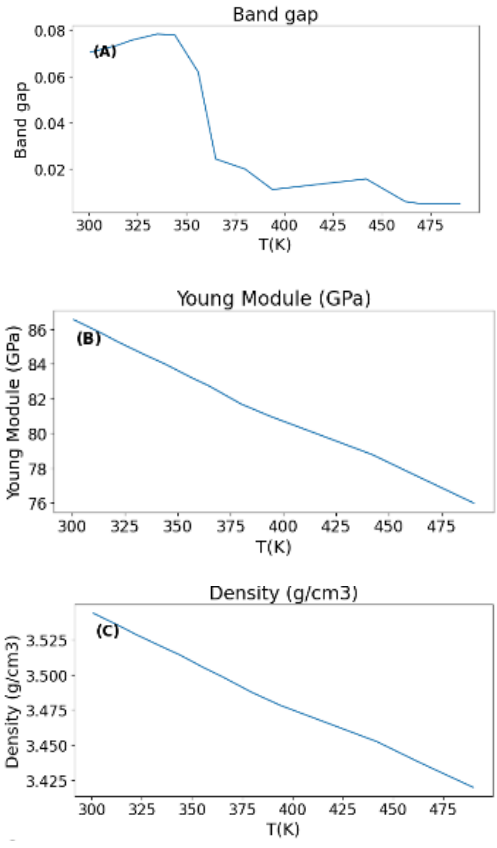
Model Development

The application of the ANN methodology for predicting material properties of TiAl across varying temperatures provides comprehensive insights into its behavior. TiAl exhibits characteristic changes in its material properties as temperature varies, reflecting its thermal response.

As temperature decreases, TiAl tends to demonstrate consistent trends. The Band Gap widens, indicating changes in TiAl's electronic structure. Simultaneously, the Young Module decreases, suggesting reduced material stiffness, aligned with known thermal expansion effects. Density exhibits a slight decrease, reflecting the expansion of TiAl's lattice structure. Additionally, Energy Absorption values decrease, indicating a lower capacity of TiAl to absorb energy. Meanwhile, Thermal Conductivity shows a slight increase, reflecting TiAl's improved ability to conduct heat. Finally, Specific Heat gradually increases, indicating TiAl's greater capacity to store thermal energy. The predictive model effectively captures these temperature-dependent trends, as evidenced by the minimal percentage differences between actual and predicted values across all properties. This consistency reaffirms the reliability of the model in estimating TiAl's material properties across a wide range of temperatures.

After performing model development using Python, the results are carried out. The predicted values of band gap (eV), density (g/cm^3), specific heat (J/g.C), energy absorption (KJ/m^3), Young's modulus (GPa), and thermal conductivity (W/m.K) of TiAl across temperatures ranging from 300-475 K are presented in Figs. (4A-F). This comprehensive range of temperatures includes 325, 350, 375, 400, 425, and 450 K. Insights into TiAl's material properties at varying thermal conditions are offered, facilitating informed decision-making in diverse industrial applications.

In Fig. (4A), the fluctuation of the band gap in different temperatures is depicted. Across varying temperatures, fluctuations in the band gap, which remains close to 0 eV, are observed, with values ranging from 0.005-0.078335 eV. In Fig. (4B), variations in Young's Modulus (GPa) across different temperatures are illustrated. The Young's modulus exhibits a peak value of approximately 86.55 GPa at 301 K, gradually decreasing to a minimum value of around 75.99 GPa at 490 K. This trend demonstrates a progressive decline in Young's modulus as temperature increases, reaching its lowest point within the temperature range studied. In Fig. (4C), fluctuations in density (g/cm^3) across different temperatures are depicted. A gradual decrease in density is observed, ranging from approximately 3.42 g/cm^3 at 490 K to around 3.54 g/cm^3 at 301 K. These fluctuations suggest a progressive reduction in density as temperature increases, with the lowest density recorded at the highest temperature examined. The Energy Absorption (KJ/m^3) results, as shown in Fig. (4D), depict fluctuations across different temperatures. A progressive decrease in energy absorption is observed, ranging from approximately 5995.23 KJ/m^3 at 301 K to around 3488.79 KJ/m^3 at 490 K. These variations indicate a declining trend in energy absorption with increasing temperature, with the lowest absorption recorded at the highest temperature studied. In Fig. (4E), fluctuations in thermal conductivity (W/m.K) across different temperatures are illustrated. A gradual increase in thermal conductivity is observed, ranging from approximately 85.84 W/m.K at 301 K to around 86.02 W/m.K at 490 K. These variations suggest a progressive enhancement in thermal conductivity with increasing temperature, with the highest conductivity recorded at the highest temperature examined. Fig. (4F) illustrates fluctuations in specific heat (J/g.C) across different temperatures. A gradual increase in specific heat is observed, with values ranging from approximately 0.72 J/g.C at 301 K to around 0.83 J/g.C at 490 K. These variations suggest a progressive augmentation in specific heat with increasing temperature, with the highest specific heat recorded at the highest temperature examined.



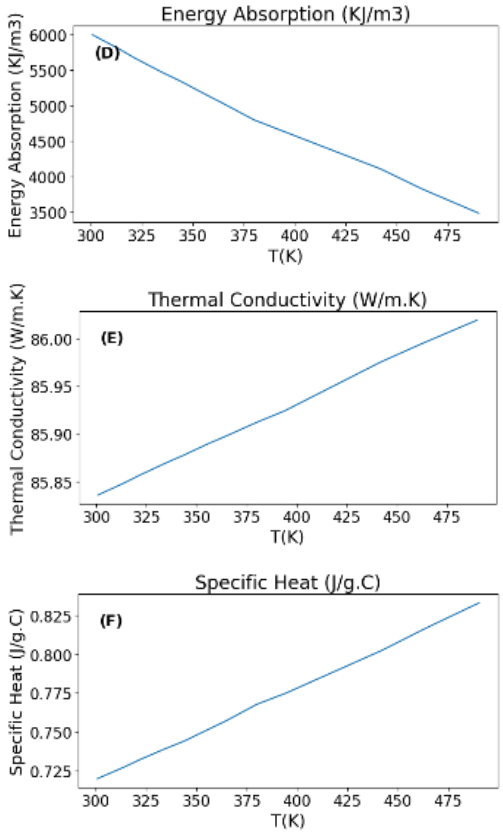


Fig. 4: TiAl prediction in different temperatures

The comprehensive analysis of TiAl material properties across different temperatures using the ANN method provides valuable insights into its behavior under varying thermal conditions. The observed trends underscore the robustness of the predictive model and its ability to accurately estimate material properties. These findings contribute significantly to our understanding of TiAl's thermal characteristics and have broad implications for its practical applications across various industries. Overall, the trends observed in TiAl's material properties across different temperatures highlight the complex interplay between temperature and material behavior. The predictive model successfully captures these nuanced relationships, enabling accurate estimation of TiAl's properties across a wide temperature range. The insights gained from this analysis enhance our understanding of TiAl's thermal characteristics and contribute to the development of advanced materials with tailored properties for specific applications.

While the ANN model demonstrates robustness and accuracy, there are potential limitations that warrant further investigation. The model's performance might vary with different TiAl compositions or under different environmental conditions. Future research should explore these variables and consider expanding the temperature range to understand extreme thermal behaviors. Additionally, incorporating more complex physical phenomena into the model, such as phase transitions or microstructural changes, could enhance its predictive power.

Further studies could also investigate the long-term stability and performance of TiAl under cyclic thermal loading, which is critical for applications in industries such as aerospace and automotive. Experimentation with different machine learning algorithms or hybrid models might provide comparative insights and potentially improve predictive accuracy.

In conclusion, the comprehensive examination of TiAl material properties across various temperatures using the ANN method provides valuable insights for both scientific understanding and practical applications. The predictive model's accuracy in estimating material properties underscores its potential as a powerful tool in materials science and engineering research. This study lays a solid foundation for further investigations into TiAl and other materials, with implications for a wide range of industries, including aerospace, automotive, and manufacturing.

Conclusion

In conclusion, the analysis of TiAl material properties using the ANN predictive model reveals consistent temperature-dependent trends across a range of temperatures. The study highlights the reliability and accuracy of the predictive model in estimating TiAl's material properties, providing valuable insights into its thermal behavior. These findings offer significant contributions to materials science and engineering, enabling the development of advanced materials with tailored properties for specific applications:

- TiAl exhibits distinct temperature-dependent behaviors: The Band Gap widens, indicating alterations in its electronic structure; Young's Modulus decreases, reflecting reduced material stiffness with increasing temperature; Density exhibits a slight decline, suggestive of thermal expansion effects on TiAl's lattice structure
- Energy Absorption values diminish as temperature rises, indicating a reduced capacity of TiAl to absorb energy
- Thermal Conductivity shows a modest increase, highlighting TiAl's enhanced heat conduction capabilities with higher temperatures
- Specific Heat gradually rises, indicating TiAl's increased ability to store thermal energy as temperatures increase
- The close alignment between predicted and actual values underscores the ANN model's accuracy in estimating TiAl's complex thermal behavior
- These insights are pivotal for optimizing TiAl's performance in critical applications across the pharmaceuticals, automotive and manufacturing sectors

- The study reaffirms the ANN methodology's efficacy in materials science and engineering, emphasizing its potential for guiding future advancements in material design and optimization

Acknowledgment

The authors are all contributors to this study including North Carolina A&T State University and the National Science Foundation, NSF award NSF 2122067.

Use the same font size for the content of the acknowledgements section.

Funding Information

This research was carried out with financial support from the National Science Foundation (NSF) Partnership for Research and Education in Materials (PREM) program via grant number DMR-2122067.

Author's Contributions

Armaghan Shalbaftabar: Led research development, performed data cleaning and manipulation, conducted machine learning analysis and contributed to statistical analysis. Also participated in manuscript writing.

Kristen Rhinehardt: Provided the research topic, guided the research development and contributed to manuscript writing.

Dhananjay Kumar: Provided the research topic and contributed to manuscript writing.

Ethics

This article is an original research paper. No ethical issues are anticipated following its publication

References

Agatonovic-Kustrin, S., & Beresford, R. (2000). Basic Concepts of Artificial Neural Network (ANN) Modeling and Its Application IN Pharmaceutical Research. *Journal of Pharmaceutical and Biomedical Analysis*, *22*(5), 717–727. https://doi.org/10.1016/s0731-7085(99)00272-1

Agrawal, A., & Choudhary, A. (2016). Perspective: Materials informatics and big data: Realization of the "fourth paradigm" of science in materials science. *APL Materials*, *4*(5), 053208. https://doi.org/10.1063/1.4946894

Ahmad, M. R., Chen, B., Dai, J.-G., Kazmi, S. M. S., & Munir, M. J. (2021). Evolutionary artificial intelligence approach for performance prediction of bio-composites. *Construction and Building Materials*, *290*, 123254. https://doi.org/10.1016/j.conbuildmat.2021.123254

Aliyu, A. M., Choudhury, R., Sohani, B., Atanbori, J., Ribeiro, J. X. F., Ahmed, S. K. B., & Mishra, R. (2023). An Artificial Neural Network Model for the Prediction of Entrained Droplet Fraction in Annular Gas-liquid Two-phase Flow in Vertical Pipes. *International Journal of Multiphase Flow*, *164*, 104452. https://doi.org/10.1016/j.ijmultiphaseflow.2023.104452

Bak, T., Nowotny, J., Rekas, M., & Sorrell, C. C. (2003). Defect chemistry and semiconducting properties of titanium dioxide: I. Intrinsic electronic equilibrium☆. *Journal of Physics and Chemistry of Solids*, *64*(7), 1043–1056. https://doi.org/10.1016/s0022-3697(02)00479-1

Bao, M., Liu, Y., Wang, X., Yang, L., Li, S., Ren, J., Qin, G., & Zhang, E. (2018). Optimization of mechanical properties, biocorrosion properties, and antibacterial properties of wrought Ti-3Cu alloy by heat treatment. *Bioactive Materials*, *3*(1), 28–38. https://doi.org/10.1016/j.bioactmat.2018.01.004

Bewlay, BP, M Weimer, T Kelly, A Suzuki, and PR Bewlay, B. P., Weimer, M., Kelly, T., Suzuki, A., & Subramanian, P. R. (2013). The Science, Technology, and Implementation of TiAl Alloys in Commercial Aircraft Engines. *MRS Online Proceedings Library*, *1516*(1), 49–58. https://doi.org/10.1557/opl.2013.44

Clemens, H., & Smarsly, W. (2011). Light-Weight Intermetallic Titanium Aluminides–Status of Research and Development. *Advanced Materials Research*, *278*, 551–556. https://doi.org/10.4028/www.scientific.net/amr.278.551

Da Silva, L. F. M., & Adams, R. D. (2007). Measurement of the mechanical properties of a carbon reinforced bismaleimide over a wide range of temperatures. *Revista Da Associação Portuguesa de Análise Experimental de Tensões*, 7078.

Foteinopoulos, P., Papacharalampopoulos, A., & Stavropoulos, P. (2018). On thermal modeling of Additive Manufacturing processes. *CIRP Journal of Manufacturing Science and Technology*, *20*, 66–83. https://doi.org/10.1016/j.cirpj.2017.09.007

Hopkins, D. C., Baltis, T., Pitaress, J. M., & Hazelmyer, D. R. (2012). Extreme Thermal Transient Stress Analysis with Pre-Stress in a Metal Matrix Composite Power Package. *IMAPSource Proceedings*, *2012*(HITEC), 000361–000372. https://doi.org/10.4071/hitec-2012-tha25

Huan, T. D., Mannodi-Kanakkithodi, A., & Ramprasad, R. (2015). Accelerated materials property predictions and design using motif-based fingerprints. *Physical Review B*, *92*(1), 014106. https://doi.org/10.1103/physrevb.92.014106

Jha, D., Ward, L., Paul, A., Liao, W., Choudhary, A., Wolverton, C., & Agrawal, A. (2018). ElemNet: Deep Learning the Chemistry of Materials from Only Elemental Composition. *Scientific Reports*, *8*(1), 17593. https://doi.org/10.1038/s41598-018-35934-y

Junaid, M., Cheema, T. A., Haleem, H., Saad-ul-Fatah, Rahman, K., & Park, C. W. (2019). Effects of thermal material properties on precision of transient temperatures in pulsed laser welding of Ti6Al4V alloy. *Proceedings of the Institution of Mechanical Engineers, Part C: Journal of Mechanical Engineering Science*, *233*(9), 3170–3181. https://doi.org/10.1177/0954406218802604

Kertész, J., & Kovács, T. A. (2023). Effect of the Radial Constrain for the Impact Energy-Absorbing Behaviour of the Closed-Cell Metal Foam. *Vehicle and Automotive Engineering 4*, 139–150. https://doi.org/10.1007/978-3-031-15211-5_12

Khan, M. A., Aslam, F., Javed, M. F., Alabduljabbar, H., & Deifalla, A. F. (2022). New prediction models for the compressive strength and dry-thermal conductivity of bio-composites using novel machine learning algorithms. *Journal of Cleaner Production*, *350*, 131364. https://doi.org/10.1016/j.jclepro.2022.131364

Ling, J., Hutchinson, M., Antono, E., Paradiso, S., & Meredig, B. (2017). High-Dimensional Materials and Process Optimization Using Data-Driven Experimental Design with Well-Calibrated Uncertainty Estimates. *Integrating Materials and Manufacturing Innovation*, *6*(3), 207–217. https://doi.org/10.1007/s40192-017-0098-z

Pilania, G., Wang, C., Jiang, X., Rajasekaran, S., & Ramprasad, R. (2013). Accelerating materials property predictions using machine learning. *Scientific Reports*, *3*(1), 2810. https://doi.org/10.1038/srep02810

Raccuglia, P., Elbert, K. C., Adler, P. D. F., Falk, C., Wenny, M. B., Mollo, A., Zeller, M., Friedler, S. A., Schrier, J., & Norquist, A. J. (2016). Machine-learning-assisted materials discovery using failed experiments. *Nature*, *533*(7601), 73–76. https://doi.org/10.1038/nature17439

Ratner, B. D., Hoffman, A. S., Schoen, F. J., Lemons, J. E., Wagner, W. R., Sakiyama-Elbert, S. E., Zhang, G., & Yaszemski, M. J. (2020). 1.1.1 - Introduction to Biomaterials Science: An Evolving, Multidisciplinary Endeavor. In *Biomaterials Science* (4th Ed., pp. 3–19). Academic Press. https://doi.org/10.1016/b978-0-12-816137-1.00001-5

Spotose, L. (2022). *Identifying Ti-Cu-based alloys for biomedical applications*. Doctoral dissertation, Faculty of Engineering and the Built environment.

Wang, G., Dong, L., Wang, J., & Atluri, S. (2018). Three-dimensional Trefftz computational grains for the micromechanical modeling of heterogeneous media with coated spherical inclusions. *Journal of Mechanics of Materials and Structures*, *13*(4), 505–529. https://doi.org/10.2140/jomms.2018.13.505

Williams, D. F. (2008). On the mechanisms of biocompatibility. *Biomaterials*, *29*(20), 2941–2953. https://doi.org/10.1016/j.biomaterials.2008.04.023

Xie, B., Fan, Y. Z., Mu, T. Z., & Deng, B. (2017). Fabrication and energy absorption properties of titanium foam with $CaCl_2$ as a space holder. *Materials Science and Engineering: A*, *708*, 419–423. https://doi.org/10.1016/j.msea.2017.09.123

Yeadon, W. (2022). Multiphysics modelling of Gas Tungsten Arc Welding. *ArXiv:2205.07687*. https://doi.org/10.48550/arXiv.2205.07687

Zhao, P., Wang, Y., Jiang, B., Zhang, H., Cheng, X., & Fan, Q. (2023). Neural network modeling of titanium alloy composition-microstructure-property relationships based on multimodal data. *Materials Science and Engineering: A*, *879*, 145202. https://doi.org/10.1016/j.msea.2023.145202