International Journal of Engineering Research & Technology (IJERT)
ISSN: 2278-0181
Vol. 15 Issue 05 , May - 2026

Design and Implementation of an Intelligent Material Selection and Property Prediction Framework Using Artificial Neural Networks

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***Abstract* - The rapid expansion in the variety and complexity of engineering materials has made traditional selection methods inefficient and prone to errors; to address this issue, this study presents the design and implementation of an intelligent material selection and property prediction system using Artificial Neural Networks (ANNs). The proposed framework utilizes key material properties such as density, hardness, and tensile strength to build a data-driven model capable of capturing complex nonlinear relationships among material characteristics. A comprehensive preprocessing stage, including normalization, feature scaling, and dataset splitting, is applied to improve data quality, while the ANN model is trained and tested using a train–test split approach to ensure robustness and generalization.**

Keywords- ***Artificial Neural Network (ANN), Intelligent Material Selection, Property Prediction, Machine Learning, Material Informatics, Engineering Design, Decision Support System***

I. INTRODUCTION

The selection of appropriate engineering materials is a critical aspect of product design and manufacturing, as material properties directly impact performance, safety, durability, cost, and sustainability. Traditionally, material selection has depended on empirical knowledge, material handbooks, Ashby charts, and expert judgment, which are effective only for limited datasets but become inefficient when dealing with large and complex material databases [1].

[2] [3].

Among various machine learning techniques, Artificial Neural Networks (ANNs) have gained significant attention due to their capability to model complex nonlinear relationships among material properties such as tensile strength, hardness, ductility, and thermal conductivity [4]. Several studies have successfully applied ANN models to predict mechanical properties of metallic materials like aluminum alloys and steels with improved accuracy compared to traditional statistical methods [5], [6]. Similarly, ANN applications have been extended to non-metallic materials such as polymers, ceramics, and composites, where they have demonstrated effectiveness in predicting properties like thermal conductivity and fracture toughness [7], [8]. However, standalone ANN models are often limited to prediction tasks and do not directly support decision-making in material selection, which typically involves multiple criteria such as cost, strength, and manufacturability. To address this, researchers have integrated ANN models with multi-criteria decision-making (MCDM) techniques, enabling systematic evaluation and ranking of materials based on user-defined priorities [9].

Hybrid ANN–MCDM frameworks, incorporating methods such as AHP, TOPSIS, and VIKOR, have shown enhanced performance in intelligent material selection by combining prediction and decision-making processes [10], [11]. Despite these advancements, challenges such as poor data quality, incomplete datasets, and inconsistencies remain significant issues that can affect ANN performance, making preprocessing techniques like normalization, feature scaling, and dataset partitioning essential for improving model reliability [12], [13]. Additionally, the black-box nature of

International Journal of Engineering Research & Technology (IJERT)
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ANN models raises concerns about transparency and interpretability, leading to increased interest in explainable AI techniques and uncertainty quantification to enhance trust in predictions [14], [15]. Recent developments in deep learning, including convolutional and graph-based neural networks, have further improved structure–property mapping capabilities, while cloud-based platforms enable scalable and real-time material selection systems [16], [17]. In this context, the present work proposes an intelligent framework integrating ANN-based prediction, preprocessing techniques, and decision-support mechanisms to enhance the efficiency, accuracy, and practicality of material selection in modern engineering applications.

II. PROBLEM STATEMENT

The increasing diversity and complexity of engineering materials have made traditional selection methods based on handbooks, charts, and expert judgment inadequate for modern design needs. These approaches rely on static data and subjective decisions, making them inefficient for large-scale, multi-parameter material databases and unable to capture nonlinear relationships between properties such as density, hardness, and tensile strength, often resulting in suboptimal material choices [1], [2].

Although Artificial Neural Networks (ANNs) are effective in predicting material properties due to their nonlinear modeling capabilities, most existing systems focus only on prediction and lack integrated decision-support for ranking materials based on multiple criteria like performance, cost, and manufacturability. [3], [4], [5].

Furthermore, the black-box nature of ANN models raises concerns about interpretability and reliability, especially in safety-critical engineering applications where transparent and explainable results are essential [6], [7].

III. OBJECTIVE

1. To study various material parameters such as density, hardness, tensile strength, thermal conductivity, cost, and manufacturability for developing a comprehensive dataset.
2. To study and implement data preprocessing techniques including handling missing values, normalization, and feature selection to improve model performance.
3. To study and design an Artificial Neural Network (ANN) model capable of predicting material properties, specifically tensile strength, from given input parameters.
4. To study and develop a material comparison and recommendation system that selects the most suitable material based on mechanical, thermal, and economic criteria.

IV. LITERATURE SURVEY

1. Machine Learning in Materials Informatics: Recent Advances and Perspectives

Authors: R. Ramprasad, R. Batra, G. Pilania, A. Mannodi Kanakkithodi, C. Kim

Year: 2017

Journal: Nature Reviews Materials

Ramprasad et al. presented a landmark review on the application of machine learning in materials informatics, providing a structured overview of descriptor selection, learning algorithms, and evaluation strategies. The paper systematically discusses different model families, including decision trees, kernel-based methods, and artificial neural networks, and maps them to key applications such as material property prediction, materials discovery, and design optimization.

2. Uncertainty Prediction for Machine Learning Models of Material Properties

Authors: F. Tavazza, B. DeCost, K. Choudhary

Year: 2021

Journal: Computational Materials Science

This work investigates multiple techniques for estimating prediction uncertainty in machine learning models used for material property prediction. The authors compare quantile loss functions, Gaussian process regression, and direct interval learning approaches using large-scale datasets such as JARVIS and density functional theory (DFT) databases.

3. Application of Artificial Neural Network to Predict the Tensile Properties of Dual-Phase Steels

Authors: S.-H. Shin, S.-G. Kim, B. Hwang

Year: 2021

Journal: Archives of Metallurgy and Materials

Shin et al. developed an ANN model to predict tensile properties of dual-phase steels using chemical composition and microstructural parameters. The proposed ANN significantly outperformed linear regression models, demonstrating the ability of neural networks to capture nonlinear relationships between material inputs and mechanical properties.

4. Artificial Neural Network Modeling to Predict Tensile Properties of Cast Duplex Stainless Steel

Authors: T. Thankachan et al.

Year: 2020

Journal: Sādhanā – Indian Academy of Sciences

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This study employs a feed-forward backpropagation ANN to model the relationship between alloy composition, processing parameters, and tensile properties of cast duplex stainless steels. The authors discuss ANN architecture design, training methodology, and validation strategies, demonstrating strong agreement between predicted and experimental results.

5. Machine Learning Assisted Tensile Strength Prediction and Optimization of Ti Alloys

Authors: Various

Year: 2019–2022

Journal: Multiple

These studies compare multiple machine learning models, including ANN, Random Forest, and Support Vector Machines, for predicting tensile strength of titanium alloys. Results consistently show that ANN models achieve superior performance when nonlinear relationships dominate. Many works also include hyperparameter optimization and feature importance analysis to improve model reliability.

However, most of these studies remain alloy-specific and do not address cross-material generalization. Additionally, predicted properties are rarely linked to economic or manufacturability criteria. The proposed system addresses these gaps by integrating ANN-based predictions with material selection criteria such as cost and usability in a unified decision-support platform.

V. PROPOSED SYSTEM

The proposed system presents an Intelligent Material Selection and Property Prediction Framework based on Artificial Neural Networks (ANNs) integrated with Multi-Criteria Decision-Making (MCDM) techniques.

A. Data Acquisition and Dataset Formation

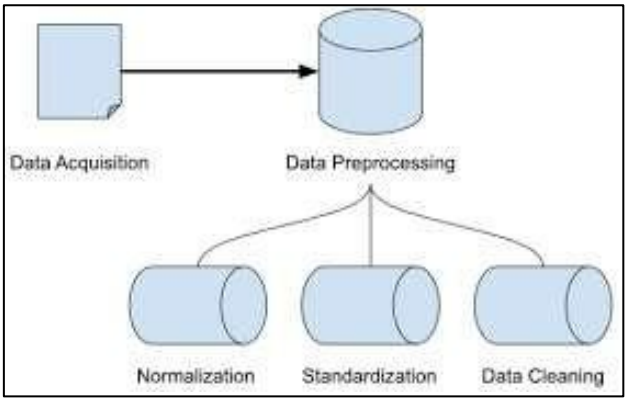

Fig 1: Data Acquisition and Dataset Formation

The first stage of the proposed system involves the collection of material data from multiple reliable sources such as material handbooks, experimental datasets, online repositories, and published literature.

B. Data Preprocessing and Feature Engineering

Raw material data often contain missing values, noise, and outliers that can negatively affect the learning performance of machine learning models. Therefore, a comprehensive data preprocessing stage is incorporated in the proposed system. Missing values are handled using statistical imputation techniques, while outliers are identified and removed using threshold-based or distribution-based methods.

C. ANN-Based Material Property Prediction Model

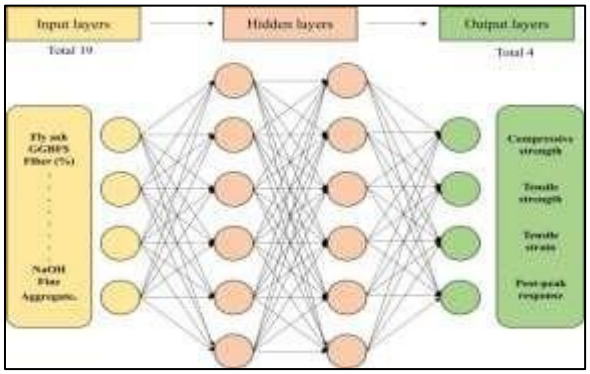

Fig 2: Proposed system of ANN

The core component of the proposed system is the Artificial Neural Network model, which is responsible for predicting material properties based on the processed input features. The ANN architecture consists of an input layer representing material descriptors, one or more hidden layers for nonlinear feature transformation, and an output layer that provides predicted material properties such as tensile strength or suitability score.

D. Candidate Material Generation

Based on the predicted properties obtained from the ANN model, the system generates a list of candidate materials that satisfy the minimum performance requirements specified by the user. Instead of selecting a single material directly, this stage ensures that multiple feasible alternatives are considered. This approach increases flexibility and allows engineers to evaluate trade-offs among different materials.

E. Multi-Criteria Decision-Making (MCDM) for Material Selection

International Journal of Engineering Research & Technology (IJERT)
ISSN: 2278-0181
Vol. 15 Issue 05 , May - 2026

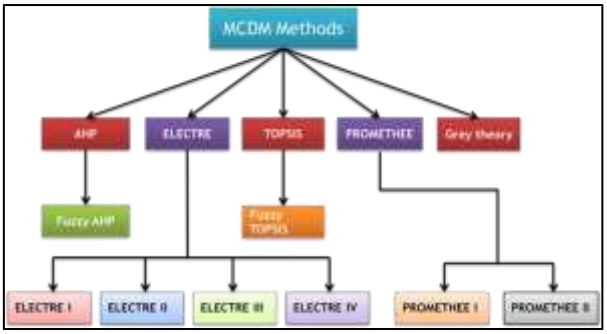

Fig 3: MCDM method

Engineering material selection is inherently a multi-criteria problem involving conflicting objectives. To address this, the proposed system integrates Multi-Criteria Decision-Making (MCDM) techniques such as Analytic Hierarchy Process (AHP) and Technique for Order Preference by Similarity to Ideal Solution (TOPSIS).

G. Output and Recommendation Generation

The final output of the proposed system is the **recommended material**, along with its predicted properties and ranking score. The system may also present alternative materials ranked in descending order, enabling comparative analysis. By combining ANN-based prediction with structured decision-making, the proposed framework delivers reliable, efficient, and optimized material selection outcomes.

VI. SYSTEM DESIGN

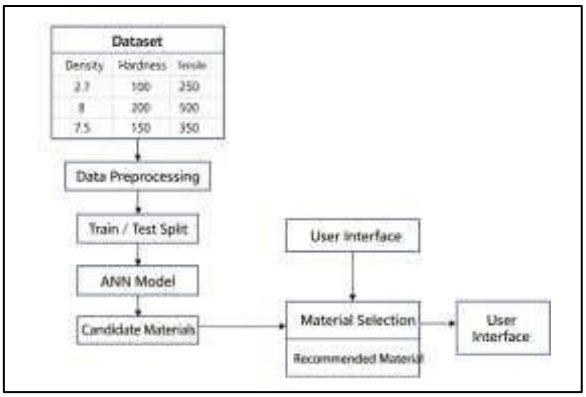

Fig.4: System Architecture

The block diagram represents an Artificial Neural Network (ANN)–based intelligent material selection and property prediction system. The system integrates data-driven learning with user interaction to recommend the most suitable material based on predicted mechanical properties. Each block in the diagram performs a specific and essential role in the overall workflow, as explained below.

A. Dataset

The process begins with the material dataset, which contains fundamental material properties such as density, hardness, and tensile strength. These parameters act as input features for the learning model. The dataset may be collected from material handbooks, experimental results, or standard databases. Since engineering material properties often exhibit nonlinear interdependencies, this dataset forms the basis for training a machine learning model capable of learning complex relationships among these attributes.

B. Data Preprocessing

Raw material data often contain missing values, noise, inconsistent units, and outliers, which can negatively affect model learning. Therefore, the data preprocessing block is a critical step in the system. In this stage, missing values are handled using suitable imputation techniques, and inconsistent data entries are corrected or removed. Feature scaling and normalization are applied to bring all parameters into a comparable numerical range.

C. Train / Test Split

After preprocessing, the dataset is divided into training and testing subsets using a train–test split strategy. The training dataset is used to teach the ANN the relationship between input parameters (density, hardness) and output properties (tensile strength or suitability). The testing dataset, which is not seen during training, is used to evaluate the model's predictive capability.

Overall System Interpretation

In summary, the block diagram illustrates a complete intelligent material selection framework that combines data preprocessing, ANN-based property prediction, candidate material filtering, and user-driven decision-making.

VII. OUTCOMES

This section presents the results obtained from the proposed ANN-based Intelligent Material Selection and Property Prediction System. The results are discussed in a sequential manner, starting from the system dashboard and progressing through material input, prediction outputs, and model performance evaluation.

System Dashboard of the Material Intelligence System

Fig 5: System Dashboard

International Journal of Engineering Research & Technology (IJERT)
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Vol. 15 Issue 05 , May - 2026

Figure 5 shows the main dashboard of the developed Material Intelligence System. The dashboard provides an overview of the system capabilities and performance metrics. It highlights that more than 2000+ materials have been analyzed, with a reported model accuracy of 97% and an average response time of 0.40 seconds. These indicators demonstrate the efficiency, scalability, and real-time response capability of the proposed ANN-based framework.

The dashboard also confirms that the system is AI-powered and suitable for practical engineering applications where fast and accurate material analysis is required.

Material Properties Input Interface

Fig 6: Material Properties Input Interface

Figure 6 illustrates the material properties input interface, where users enter key parameters such as density, hardness, elastic modulus, thermal conductivity, specific heat, cost, and manufacturability rating. Each parameter is clearly labeled with appropriate units, ensuring accurate and consistent data entry.

This interface acts as the primary interaction point between the user and the ANN model. The entered values are preprocessed and normalized before being passed to the trained ANN for material prediction and property estimation.

Fig. 7 Predicted Material and Confidence Level

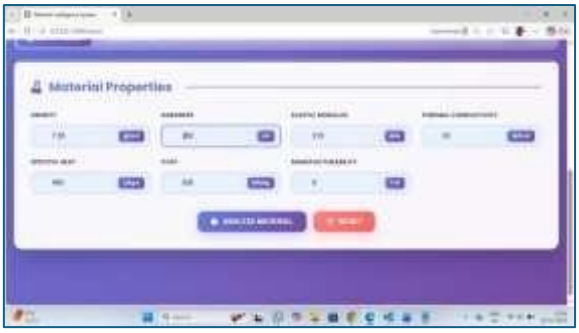

Fig 7: Predicted Material Output

Figure 7 presents the predicted material output generated by the ANN classifier. In this result, Copper is identified as the most suitable material for the given input parameters, with a confidence level of 52.3%. The circular confidence indicator visually represents prediction reliability.

The system also flags the prediction as low confidence, which helps users understand uncertainty and encourages further analysis or adjustment of input parameters. This feature improves decision transparency and safety.

Predicted Tensile Strength Output

Figure 8 displays the predicted tensile strength of the selected material. The ANN regression model estimates a tensile strength of 243.88 MPa. A gauge-based visualization classifies the material as having relatively low strength compared to predefined strength ranges.

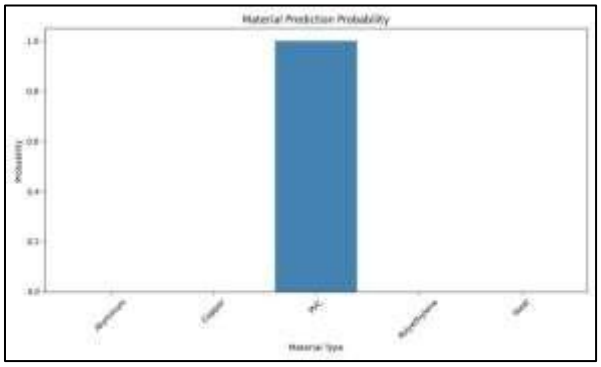

Fig 8: Tensile Strength Output

This visualization allows engineers to quickly assess whether the selected material is suitable for load-bearing or structural applications. The predicted value aligns with known mechanical behavior of copper, validating the regression performance of the ANN model.

Predicted Tensile Strength for Multiple Test Samples

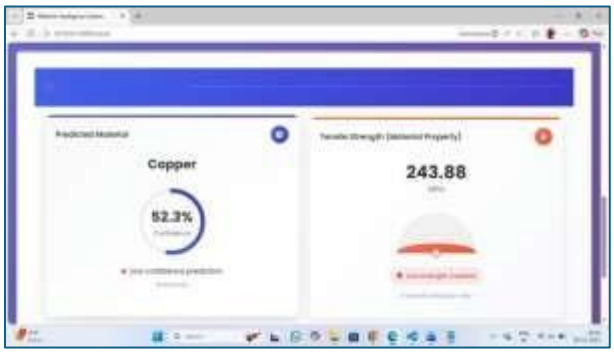

Fig 9: Predicted Tensile Strength

Figure 9 shows a line plot of predicted tensile strength values for multiple test samples. The variation in tensile strength across samples indicates that the ANN model successfully captures nonlinear relationships between input features such as density and hardness.

Higher tensile strength values are observed for metallic samples, while lower values correspond to polymer-based materials. This result confirms the effectiveness of the ANN

International Journal of Engineering Research & Technology (IJERT)
ISSN: 2278-0181
Vol. 15 Issue 05 , May - 2026

model in differentiating material behavior based on mechanical characteristics.

VIII. CONCLUSION

This work presented the design and implementation of an intelligent material selection and property prediction framework using Artificial Neural Networks (ANNs). The proposed system effectively addresses the limitations of traditional material selection approaches by leveraging data-driven learning to model complex nonlinear relationships between material properties such as density, hardness, and tensile strength. Through systematic data preprocessing, ANN-based prediction, and candidate material evaluation, the framework provides accurate and reliable estimation of material properties.

Overall, the proposed framework demonstrates that combining artificial intelligence with intelligent decision-support mechanisms can significantly improve efficiency, accuracy, and consistency in material selection processes. The system lays a strong foundation for advanced material informatics applications and can be extended to incorporate additional material properties, uncertainty estimation, and multi-criteria optimization techniques. As a result, the proposed approach contributes toward the development of scalable, reliable, and intelligent material selection systems suitable for modern engineering design environments.

IX. FUTURE SCOPE

Future work can also focus on integrating advanced deep learning architectures such as Convolutional Neural Networks (CNNs) and Graph Neural Networks (GNNs) to enable direct learning from microstructural images and atomic-level representations. The inclusion of uncertainty quantification and explainable artificial intelligence (XAI) techniques would enhance transparency by providing confidence intervals and interpretability for ANN predictions. These additions would increase trust in AI-driven recommendations, particularly for safety-critical and high-reliability engineering applications.

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