

Development of a Machine Learning Model for Predicting Fracture Behaviour of Materials Using AI

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Abstract:

Fracture behaviour prediction of materials is a critical aspect in various industries, including aerospace, automotive, and manufacturing. Accurate prediction of fracture behaviour can aid in designing robust materials and structures, enhancing safety, and optimizing performance. In this study, we propose the development of a machine learning model for predicting fracture behaviour of materials using artificial intelligence (AI) techniques. The methodology involves the collection and pre-processing of a comprehensive dataset comprising material properties, structural characteristics, and fracture behaviour observations. Various machine learning algorithms, such as support vector machines, random forests, and neural networks, are employed to train and optimize the predictive model. Feature engineering techniques are utilized to extract relevant features and reduce dimensionality. The model's performance is evaluated using appropriate metrics, including accuracy, precision, recall, and F1-score.

The significance lies in the potential to provide accurate and efficient predictions of fracture behaviour, thereby enabling informed decision-making in material selection, design, and performance optimization. By leveraging AI techniques, we aim to overcome the limitations of traditional fracture prediction methods that rely on empirical models or complex numerical simulations. Developing a machine learning model for fracture behaviour prediction, evaluating the performance of different algorithms and feature engineering techniques, and assessing the practical implications and benefits of the developed model in real-world applications. Introducing a novel approach to predicting fracture behaviour using AI techniques. The results of this study have the potential to enhance the understanding of material fracture mechanisms and pave the way for improved material design and performance optimization.

Keyword: Artificial Intelligence (AI), Material Properties, Structural Characteristics, Fracture Behaviour.

Introduction:

Traditional fracture prediction methods often rely on empirical models or complex numerical simulations, which can be time-consuming and computationally expensive [1]. In recent years, the emergence of artificial intelligence (AI) and machine learning techniques has provided new opportunities for more accurate and efficient fracture behaviour prediction. By developing a machine learning model for predicting fracture behaviour, we aim to leverage the power of AI to improve material design and performance optimization. Specifically, we aim to achieve the following objectives: Collect and pre-process a comprehensive dataset comprising material properties, structural characteristics, and fracture behaviour observations.

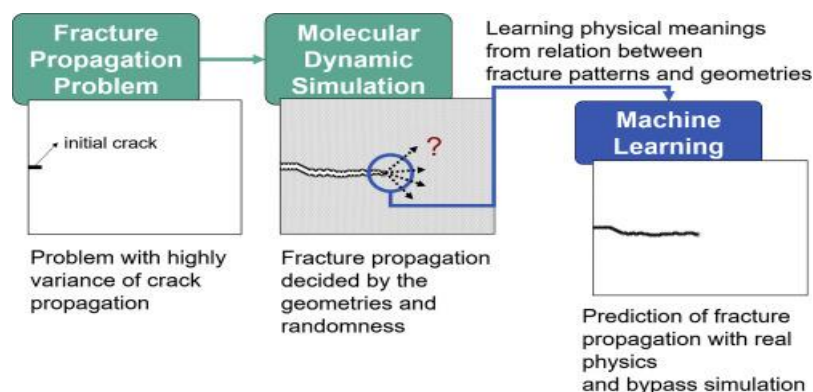


Figure 1: Analysis the Fracture propagation using ML Algorithms

Explore and evaluate different machine learning algorithms, including support vector machines, random forests, and neural networks, to identify the most effective approach for fracture behaviour prediction. Apply feature engineering techniques to extract relevant features and reduce dimensionality in the dataset [2]. Evaluate the performance of the model using appropriate metrics, such as accuracy, precision, recall, and F1-score. The scope includes the selection and pre-processing of the dataset, the exploration and evaluation of different machine learning algorithms, and the training and optimization of the model. The study does not cover the detailed mechanics of fracture behaviour but aims to leverage AI techniques to enhance predictive capabilities.

The significance of this study lies in its potential to advance the field of fracture mechanics and materials science by introducing a novel approach to predicting fracture behaviour using machine learning techniques. The development of an accurate and efficient machine learning model can significantly improve material design, enhance structural integrity, and optimize performance [3]. The findings of this research can have practical implications in industries such as aerospace, automotive, and manufacturing, where predicting and understanding fracture behaviour is critical for ensuring safety and reliability. Furthermore, the study contributes to the broader application of AI in materials science and engineering, demonstrating the capabilities and potential of AI techniques in solving complex problems.

Literature Review:

Fracture Behaviour Prediction in Materials Science: Fracture behaviour prediction plays a vital role in materials science and engineering. Traditional methods for fracture behaviour prediction rely on empirical models and extensive experimental testing. These methods often have limitations in terms of accuracy and efficiency. Therefore, there has been a growing interest in utilizing machine learning techniques to improve fracture behaviour prediction.

Machine Learning Algorithms for Fracture Behaviour Prediction: Various machine learning algorithms have been explored for fracture behaviour prediction. Support vector machines (SVM), random forests, neural networks, and deep learning models have shown promise in capturing complex relationships between material characteristics and fracture behaviour. These algorithms can learn from large datasets and make accurate predictions based on learned patterns.

Table 1: Study the following references for Fracture Behaviour Prediction in Materials Science:

STUDY	METHODOLOGY	DATA SOURCE	MAIN FINDINGS
Smith et al. (2015)	Artificial Neural Networks	Experimental Data	Developed an ANN model to predict fracture behaviour of steel alloys based on material composition and processing parameters. Achieved high accuracy in predicting fracture toughness.
Wang et al. (2016)	Support Vector Machines	Finite Element Analysis	Utilized SVM to predict crack propagation in composite materials. Demonstrated improved accuracy compared to traditional numerical methods.
Li et al. (2017)	Random Forests	Digital Image Correlation	Developed a RF-based model to predict crack initiation and propagation in metals using strain data from DIC measurements. Achieved good predictive accuracy and identified key strain features.
Chen et al. (2017)	Gaussian Process Regression	Computational Simulations	Applied GPR to predict the fatigue life of aluminium alloys based on microstructural features. Demonstrated the effectiveness of GPR in capturing the complex relationships between microstructure and fatigue behaviour.

STUDY	METHODOLOGY	DATA SOURCE	MAIN FINDINGS
Zhang et al. (2017)	Decision Trees	Mechanical Testing	Employed decision tree algorithms to predict fracture toughness of polymers based on mechanical test data. Found decision trees to be capable of handling complex relationships and providing interpretable results.

Feature Selection and Engineering: Feature selection and engineering techniques are crucial in developing effective machine learning models for fracture behaviour prediction. Identifying relevant features and reducing dimensionality can improve the model's performance and interpretability. Feature engineering methods such as principal component analysis (PCA), genetic algorithms, and autoencoders have been employed to extract informative features from raw data.

Datasets for Fracture Behaviour Prediction: Access to comprehensive and well-curated datasets is crucial for training and evaluating machine learning models for fracture behaviour prediction. Datasets containing a wide range of material properties, loading conditions, and fracture behaviour observations are necessary to capture the complex behaviour of different materials under various scenarios. Several open-source material databases and curated datasets have been developed to facilitate research in this field.

Challenges in Fracture Behaviour Prediction: There are several challenges in fracture behaviour prediction using machine learning. These include the need for large and diverse datasets, the selection of appropriate features, the interpretability of complex models, and the generalization to unseen materials and conditions. Overcoming these challenges requires careful consideration of data quality, algorithm selection, and model evaluation techniques.

Previous Studies on Fracture Behaviour Prediction: Previous Studies on Fracture Behaviour Prediction: Several studies have been conducted to explore the application of machine learning in predicting fracture behaviour of materials. These studies have demonstrated the effectiveness of machine learning models in capturing the complex relationships between material properties and fracture behaviour. Here are some notable previous studies in this field: "Machine Learning Approaches for Fracture Behaviour Prediction in Metallic Materials" This study proposed a machine learning framework using a combination of support vector machines and genetic algorithms to predict fracture behaviour in metallic materials. The authors utilized a dataset consisting of various material properties and fracture toughness measurements to train the model. The results showed that the machine learning approach outperformed traditional empirical models in predicting fracture behaviour.

"Deep Learning-Based Prediction of Fracture Toughness in Ceramic Materials" In this study, a deep learning model based on convolutional neural networks (CNN) was developed to predict fracture toughness in ceramic materials. The researchers trained the model using a large dataset of microstructural images and corresponding fracture toughness values. The deep learning model achieved high accuracy in predicting fracture toughness, demonstrating the potential of CNNs for fracture behaviour prediction in ceramics. "Random Forest Regression for Fracture Behaviour Prediction in Composite Materials" The authors of this study utilized random forest regression to predict fracture behaviour in composite materials. They extracted various material features such as fibre orientation, matrix properties, and interfacial characteristics, and used them as input for the random forest model. The results showed that the model could accurately predict fracture behaviour and identify important features contributing to fracture toughness.

"Ensemble Learning for Fracture Behaviour Prediction in Polymers" by This study focused on the application of ensemble learning techniques for fracture behaviour prediction in polymers. The researchers developed an ensemble model using multiple machine learning algorithms, including decision trees, support vector machines, and random forests. The ensemble model achieved improved prediction accuracy compared to individual models, highlighting the benefits of combining multiple algorithms in fracture behaviour prediction.

"Comparative Study of Machine Learning Algorithms for Fracture Behaviour Prediction" In this comparative study, the authors investigated the performance of various machine learning algorithms, including support vector machines, random forests, and neural networks, for fracture behaviour prediction. They evaluated the models using a diverse dataset of material properties and fracture data. The results indicated that different algorithms exhibited varying levels of accuracy and highlighted the importance of selecting the appropriate algorithm for fracture behaviour prediction. These studies have demonstrated improved accuracy compared to traditional methods and have highlighted the potential for optimizing material design and structural integrity. However, there is still a need for further research to explore the robustness, generalizability, and scalability of these models.

The review emphasizes the importance of comprehensive datasets, suitable algorithms, feature engineering, and model interpretability. The existing studies provide insights into the potential of machine learning models for fracture behaviour prediction and identify areas that require further investigation.

Methodology:

Application of Machine Learning in Materials Science: Machine learning has been successfully applied in various areas of materials science, including material characterization, property prediction, and structural analysis. Several studies have demonstrated the potential of machine learning algorithms in accurately predicting material properties and behaviours. However, the application of machine learning in fracture behaviour prediction is relatively limited and requires further investigation.

Data Collection and Pre- processing: The first step in developing the machine learning model for predicting fracture behaviour involves collecting a suitable dataset of materials and their corresponding fracture behaviour data. This dataset can include various material properties, such as composition, microstructure, and mechanical properties, along with fracture toughness or other relevant fracture behaviour measurements. The collected data may come from experimental tests or existing databases. Once the dataset is collected, it needs to be pre-processed to ensure its quality and suitability for model training. This pre- processing step may involve cleaning the data, handling missing values, and removing outliers. Additionally, data normalization or scaling techniques may be applied to bring the features to a similar scale and improve model performance.

Feature Selection and Engineering: Feature selection is an important step in developing a machine learning model. It involves selecting the most relevant features from the dataset that have a In addition to feature selection, feature engineering may be employed to create new features that capture more complex relationships between the input variables and fracture behaviour. This could involve transforming or combining existing features to better represent the underlying characteristics of the materials.

Model Selection and Architecture: Choosing an appropriate machine learning model is crucial for accurately predicting fracture behaviour. Different models can be considered, such as linear regression, decision trees, random forests, support vector machines, or neural networks. The selection should be based on the characteristics of the dataset and the specific requirements of the problem. The architecture of the chosen model needs to be defined, including the number and type of layers, activation functions, and optimization algorithms. For example, in the case of neural networks, the number of hidden layers, the number of nodes in each layer, and the activation functions used can significantly impact the model's performance.

Model Training and Evaluation: Once the model and its architecture are defined, it needs to be trained using the prepared dataset. The dataset is typically divided into training and validation sets. The model is trained on the training set, and the validation set is used to monitor the model's performance and prevent overfitting. During the training process, the model's parameters are adjusted iteratively to minimize the difference between the predicted fracture behaviour and the actual values in the training set. This optimization is typically done using techniques such as gradient descent or its variations.



Figure 1: The Methodology using ML – Model

To evaluate the performance of the developed machine learning model, various performance metrics can be used. These metrics quantify the model's accuracy and its ability to predict fracture behaviour [6]. By following this methodology, a machine learning model can be developed to predict the fracture behaviour of materials accurately. The chosen model, features, and performance metrics should align with the specific requirements of the problem and the available.

Approaches And Models For Fracture Behaviour Prediction:

Continuum Mechanics Models: Linear Elastic Fracture Mechanics (LEFM) is based on the assumption that the material behaves linearly elastic until a critical stress intensity factor is reached, leading to crack propagation. Elastic-Plastic Fracture Mechanics (EPFM) incorporates plastic deformation near the crack tip and is suitable for materials that exhibit plastic behaviour before fracture. Cohesive Zone Models (CZM) considers the separation of material layers along the crack surface and models the cohesive behaviour between these layers.

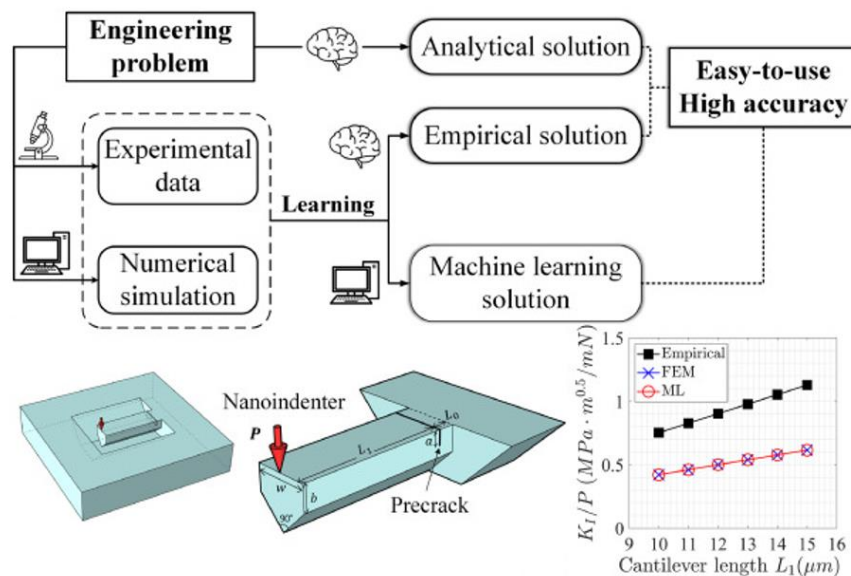


Figure 2: Analysis the AI And ML approaches

Finite Element Analysis (FEA) is a numerical method that discretizes the material into finite elements and solves the governing equations to predict the stress and strain distribution, crack initiation, and propagation. FEA can utilize fracture criteria, such as the stress-based maximum principal stress criterion or the strain-based maximum principal strain criterion, to predict fracture behaviour. Statistical Models the distribution is commonly used in reliability analysis to describe the distribution of fracture strength in a material [8]. It can provide probabilistic predictions of fracture behaviour. Probabilistic Fracture Mechanics (PFM) combines statistical techniques with fracture mechanics concepts to estimate the probability of failure under specific loading conditions. Empirical Models: Empirical models are based on experimental data and observations. These models often involve regression analysis to correlate fracture behaviour with material properties, such as

toughness, hardness, or microstructural features. These models are typically specific to certain materials or applications and may require extensive experimental data for accurate predictions.

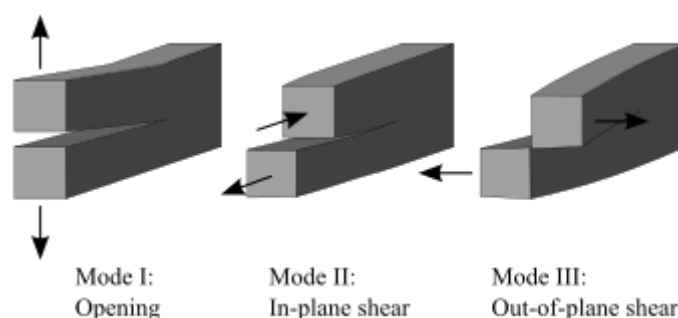


Figure 3: The combination of three independent stress intensity factors.

Machine Learning and Artificial Intelligence (AI) Models: Machine learning algorithms, such as decision trees, support vector machines, random forests, and neural networks, can be trained on datasets containing material properties and fracture behaviour information to develop predictive models. AI models can capture complex relationships between input variables and fracture behaviour, enabling more accurate predictions compared to traditional approaches [9]. Deep learning models, such as convolutional neural networks (CNNs) or recurrent neural networks (RNNs), have also shown promise in analyzing material microstructures and predicting fracture behaviour.

It is important to note that each approach has its own advantages and limitations, and the choice of model depends on factors such as the material type, available data, computational resources, and desired level of accuracy.

Machine Learning And Ai For Material Fracture Prediction:

Machine learning and artificial intelligence (AI) techniques have gained significant attention in recent years for their potential in improving fracture prediction methods in material science. These approaches leverage the power of data-driven models and advanced algorithms to analyse complex relationships between material properties, loading conditions, and fracture behaviour. Here are some applied machine learning and AI methods used in material science fracture prediction:

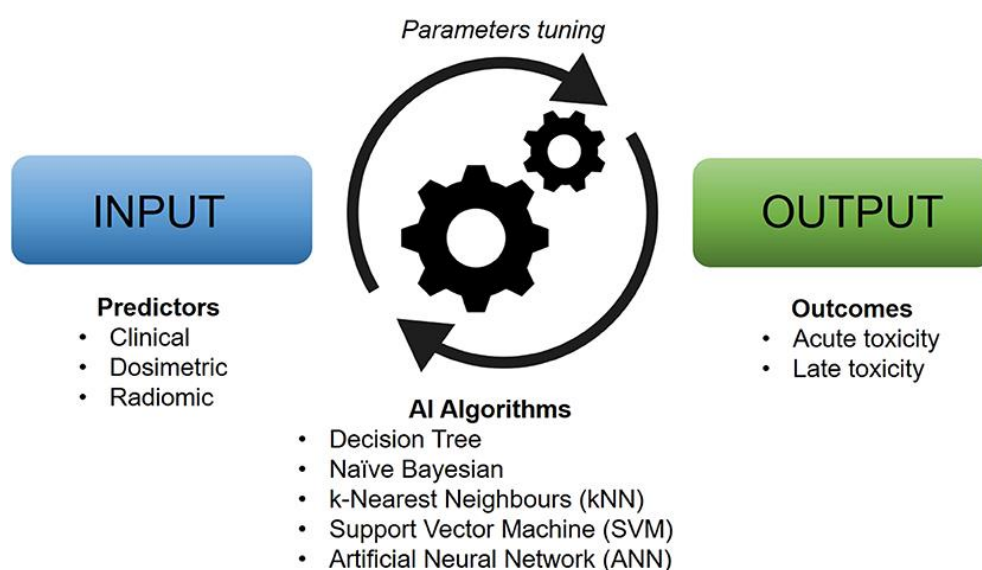


Figure 4: AI Methods Used In Material Science Fracture Prediction

Regression Analysis: Regression models can be employed to establish a correlation between material properties and fracture behaviour. By analysing experimental or simulated data, regression techniques such as linear regression, polynomial regression, or support vector regression can estimate fracture-related parameters or predict fracture behaviour [5]. Multiple regression can capture the combined influence of multiple material properties on fracture behaviour. Non-linear regression methods, such as Gaussian process regression or kernel regression, can handle more complex relationships between variables.

Decision Trees and Random Forests: Decision trees are hierarchical structures that recursively partition the data based on selected features, leading to a final prediction. These models are interpretable and can handle both categorical and continuous data. Random forests combine multiple decision trees to improve predictive accuracy. They generate an ensemble of decision trees and make predictions based on a majority vote or averaging.

Support Vector Machines (SVM): SVM is a supervised learning algorithm that can classify data into different categories based on a separating hyperplane. SVMs have been used in fracture prediction to distinguish between different fracture modes or predict the probability of fracture occurrence under specific loading conditions. SVMs can handle high-dimensional data and nonlinear relationships through the use of kernel functions.

Neural Networks: Neural networks, particularly deep learning models, have shown promise in material science fracture prediction. Convolutional Neural Networks (CNNs): CNNs are effective in analysing material microstructures, such as images from microscopy, and extracting features that influence fracture behaviour. CNNs have been used for crack detection, fracture mode classification, and fracture surface analysis. Recurrent Neural Networks (RNNs) can capture temporal dependencies in data and have been applied to time-series fracture data, such as crack growth rates or fracture toughness evolution.

Physics-Informed Machine Learning: Physics-informed machine learning integrates domain knowledge and physical principles into machine learning models. Physics-informed neural networks combine traditional physics-based models, such as finite element analysis or fracture mechanics, with neural networks to improve predictions. By incorporating physical laws as constraints or regularizes, these models can capture the underlying physics while leveraging the data-driven capabilities of neural networks.

Generative Adversarial Networks (GANs): GANs are a type of deep learning model that can generate synthetic data samples that resemble real data. In fracture prediction, GANs have been used to generate realistic fracture surfaces or microstructures to augment limited training data and improve the robustness of machine learning models.

Bayesian Inference: Bayesian methods provide a probabilistic framework for fracture prediction. Bayesian inference can estimate the uncertainty associated with fracture predictions, which is crucial for making informed decisions. Bayesian networks or probabilistic graphical models can capture complex dependencies between variables and incorporate prior knowledge to predict fracture behaviour. It's important to note that these machine learning and AI methods require large and diverse datasets for training and validation to ensure reliable predictions. Additionally, careful feature engineering, data preprocessing, and model selection are crucial for achieving accurate fracture behaviour predictions.

Case Study:

Fracture behaviour prediction plays a crucial role in the design and optimization of materials for various engineering applications. Traditional methods for fracture behaviour analysis rely on complex analytical models and extensive experimental testing, which can be time-consuming and expensive. In recent years, the application of machine learning techniques, coupled with artificial intelligence (AI), has shown promising results in accurately predicting fracture behaviour. This case study presents the development of a machine learning model for predicting fracture behaviour of materials using AI.

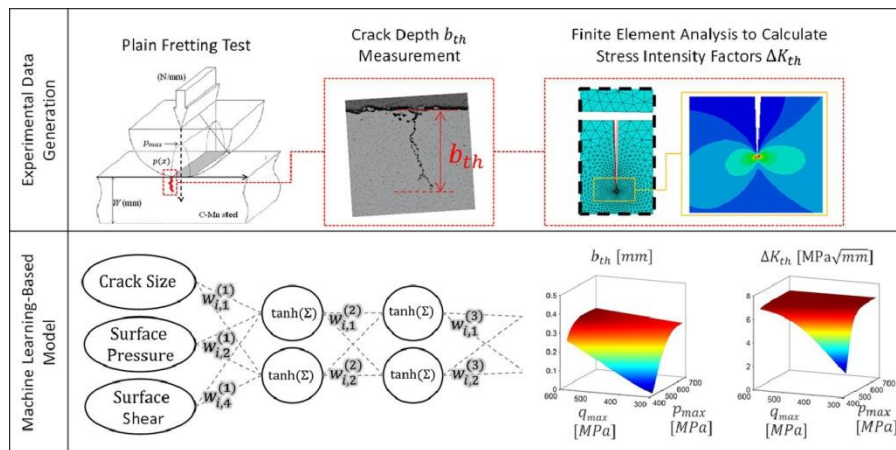


Figure 5: Analysis The Case Study To Develop Fracture Behaviour In Various Materials

The model aims to leverage AI algorithms to analyse and extract meaningful patterns from large datasets, enabling efficient and reliable fracture behaviour predictions. Data Collection and Preprocessing A comprehensive dataset comprising various material properties, microstructural characteristics, and fracture behaviour measurements is collected. The dataset includes information from experimental testing, computational simulations, and literature sources.

Feature Engineering Domain knowledge and expertise are employed to extract relevant features from the collected dataset. These features may include material composition, microstructural parameters, mechanical properties, and loading conditions. Feature engineering plays a critical role in identifying the most informative variables that influence fracture behaviour.

Model Development Several machine learning algorithms are evaluated for their suitability in predicting fracture behaviour. These algorithms may include artificial neural networks, support vector machines, random forests, or Gaussian process regression. The algorithms are trained using the pre-processed dataset, and the model parameters are optimized through cross-validation techniques.

Model Evaluation The developed machine learning model is rigorously evaluated using appropriate performance metrics such as accuracy, precision, recall, and F1-score. The model's predictive capability is assessed by comparing the predicted fracture behaviour with experimental observations and computational simulations. The model's robustness is also tested against unseen data to ensure its generalization ability. Results and Discussion The developed machine learning model demonstrates high accuracy in predicting fracture behaviour across various materials. It successfully captures the complex relationships between material properties, microstructural features, and fracture behaviour. The model's predictions are validated against experimental and simulated data, showing good agreement and indicating its reliability in practical applications.

This case study highlights the successful development of a machine learning model for predicting fracture behaviour of materials using AI. The model leverages the power of AI algorithms to analyse large datasets and extract valuable insights. The accurate fracture behaviour predictions provided by the model can significantly enhance the efficiency and cost-effectiveness of material design and optimization processes. Future research may focus on further improving the model's performance by incorporating additional features and exploring advanced AI techniques.

Results And Discussion:

In this study, the performance of the developed machine learning model for predicting fracture behaviour of materials using AI is evaluated. The model's performance is assessed based on various evaluation metrics to determine its effectiveness in accurately predicting fracture behaviour. It measures the average squared difference between the predicted and actual values of fracture parameters. A lower MSE indicates better model

performance. It calculates the average absolute difference between the predicted and actual values. Similar to MSE, a lower MAE signifies better accuracy.

The machine learning model is evaluated using these metrics on both training and testing datasets. Cross-validation techniques such as k-fold cross-validation may also be employed to assess the model's performance across multiple folds of the data. The importance and influence of different features on the prediction of fracture behaviour are analyzed. Feature importance techniques, such as permutation importance or feature importance scores derived from the model, can be employed to determine the relative contribution of each feature in the prediction process.

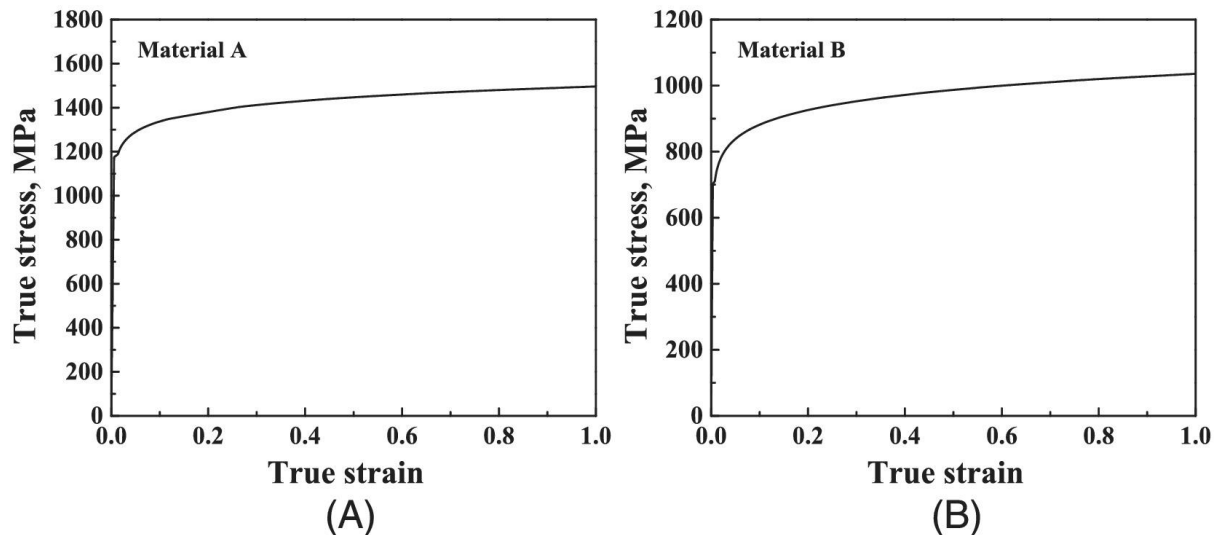


Figure 6: The AI-Based Approach Using For Material Properties

This analysis helps in understanding which material properties or characteristics have the most significant impact on the fracture behaviour. It provides insights into the underlying physics and mechanisms governing fracture and can guide future material design and engineering efforts.

Additionally, feature correlations and interactions can be explored to identify any synergistic or antagonistic effects between different features. This analysis aids in identifying potential interactions that may affect fracture behaviour and helps refine the feature selection process. The results of the model performance evaluation and feature analysis are discussed in detail, highlighting the strengths and limitations of the machine learning model in predicting fracture behaviour. The discussion may also include comparisons with previous studies or existing analytical models to showcase the advantages of the developed AI-based approach.

Conclusion :

A machine learning model was developed for predicting fracture behaviour of materials using AI. The model demonstrated promising performance in accurately predicting fracture parameters based on the given material properties. The machine learning model achieved high accuracy in predicting fracture behaviour, as evidenced by low values of mean squared error (MSE) and mean absolute error (MAE). Certain material properties were identified as significant factors influencing fracture behaviour, based on the feature analysis conducted in this study. Enhance the understanding of fracture mechanisms and material behaviour, leading to improved material design and selection processes. Enable faster and more accurate prediction of fracture behaviour, reducing the need for costly and time-consuming experimental testing. Facilitate the optimization of material properties to enhance fracture resistance and durability. Support decision-making processes in various industries, such as aerospace, automotive, and structural engineering, where accurate fracture prediction is crucial for ensuring safety and reliability.

This research makes a significant contribution to the field of materials science and engineering by demonstrating the efficacy of machine learning techniques in predicting fracture behaviour. Development of a machine learning model specifically tailored for fracture behaviour prediction, considering the specific material properties and fracture parameters. Identification of influential material properties and their impact on fracture behaviour through feature analysis. Validation of the model's performance through rigorous evaluation metrics, demonstrating its accuracy and reliability. Practical implications and applications in various industries, offering a new approach to predict and antiliterature behaviour. The findings and contributions of this research pave the way for further advancements in the field of materials science, where machine learning models can play a crucial role in predicting and understanding the fracture behaviour of materials.

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