Abstract

Solidification cracking is a significant defect in Aluminium 7-series alloys, which are widely used in aerospace and structural applications due to their high strength-to-weight ratio. The formation of cracks during solidification can lead to structural failure, especially in processes like casting, welding, and additive manufacturing. This project addresses the challenge of predicting key material properties such as solidification crack length, cracking susceptibility, and hardness, with the goal of minimizing cracking and optimizing the 3D printing process. The use of machine learning (ML) and deep learning (DL) techniques provides a powerful tool for predicting these properties based on alloy composition. The primary objective of this work is to develop models that can help identify the optimal alloy composition, reducing solidification cracks and improving the quality and performance of parts manufactured with Aluminium 7-series alloys.

Traditional experimental approaches to predicting material properties are time-consuming and costly, often requiring extensive laboratory testing and high material costs. A lack of comprehensive, publicly available datasets has further complicated the development of predictive models for these alloys. To address this, the project employs a combination of classification and regression models to predict cracking susceptibility and hardness, respectively. These models are built using data gathered from literature, experimental studies, and simulations, with feature engineering techniques to identify the key alloying elements that influence material properties. By integrating these models into a Flask-based web application, users can input alloy compositions and receive predictions on solidification crack length and hardness values. This ML and DL-driven framework not only offers a promising alternative to traditional methods but also helps in the optimization of alloy compositions for enhanced 3D printing performance, providing a more efficient and cost-effective solution for the manufacturing industry.

CHAPTER 1
Introduction

1.1 Theory

Aluminium 7-series alloys are part of the aluminium alloy family, primarily known for their excellent strength-to-weight ratio, corrosion resistance, and high performance. These alloys, often alloyed with zinc and small amounts of other elements such as copper and magnesium, are widely utilized in high-performance applications like aerospace, automotive, and structural engineering. The reason for their widespread use is their ability to offer high mechanical strength while maintaining relatively low density, making them ideal for weight-sensitive applications.

Solidification cracking refers to the formation of cracks in a metal as it solidifies. It typically occurs during the cooling phase of the casting or welding process, where the metal undergoes a phase transition from liquid to solid. In Aluminium 7-series alloys, the issue of solidification cracking is particularly concerning because it leads to material failure or performance degradation in structural components. This defect can arise in several manufacturing processes, such as casting, welding, and additive manufacturing, which are crucial in producing high-performance parts. The presence of cracks negatively affects the integrity of the component, potentially leading to expensive repairs or part replacements. It is essential to understand the mechanisms behind solidification cracking to develop mitigation strategies that can minimize or prevent the occurrence of cracks, ensuring optimal material performance.

1.2 Solidification Cracking Mechanisms

Solidification cracking in metals is primarily caused by the inability of the liquid metal to feed itself as it solidifies, especially during the final stages of solidification. This can occur if the material is subjected to high thermal gradients, insufficient liquid feeding, or if the cooling rate is too fast. During solidification, the material begins to shrink, and if the surrounding material is unable to fill the gap left by the shrinking molten metal, high-stress areas are formed. These stresses can eventually lead to the formation of cracks, which are more likely to appear in regions of the material that are subjected to both thermal stresses and mechanical loads. In Aluminium 7-series alloys, solidification cracking is a particular concern because the alloy composition (especially the concentration of zinc) can significantly influence the likelihood and severity of cracks forming during the solidification process.

1.3 Contributing Factors:

Several factors contribute to the development of solidification cracks. One of the most critical is the alloy composition, as the presence of certain elements can influence the material's susceptibility to cracking. For example, high levels of zinc in Aluminium 7-series alloys can lead to a higher risk of cracking, as zinc has a lower melting point and solidifies later than aluminium, increasing the chances of cracking during cooling. The cooling rate is another important factor, as faster cooling rates tend to produce higher thermal gradients, which can increase the risk of cracks forming. The conditions under which the metal is cast or welded, such as the temperature, the cooling environment, and the rate at which heat is extracted, also play a role in the development of solidification cracks. Lastly, the grain structure and morphology of the alloy significantly impact its susceptibility to cracking. Fine-grained structures tend to be more resistant to cracking, while coarse-grained structures are more prone to defect formation.

1.4 Contributing Factors:

To reduce the occurrence of solidification cracking, various mitigation strategies can be employed. One approach is to optimize the alloy composition by adjusting the concentration of key elements such as zinc, copper, and magnesium, as well as adding other alloying elements that can improve the material's solidification behavior. Additionally, controlling the solidification conditions during casting or welding can help reduce the risk of cracking. This includes adjusting cooling rates and ensuring that the material remains within a temperature range that allows for proper solidification without causing excessive thermal stresses. Another strategy involves using grain refiners and inoculants, which can help improve the grain structure of the material and make it more resistant to cracking. Finally, advanced welding techniques, such as using filler materials with lower melting points or controlled heat inputs, can be used to minimize the risks associated with welding-induced solidification cracks.

In summary, understanding the theory behind solidification cracking and the factors contributing to this defect is essential for developing effective solutions. By optimizing alloy composition, controlling solidification conditions, and employing advanced techniques, it is possible to minimize the occurrence of solidification cracking and improve the performance and reliability of Aluminium 7-series alloys in manufacturing processes like casting, welding, and 3D printing.

CHAPTER 2
Problem Identification

2.1 Solidification Cracking as a Critical Defect

Solidification cracking is one of the most significant challenges in aluminium 7-series alloys, occurring across various manufacturing techniques such as casting, welding, and additive manufacturing. This defect arises due to poor solidification behavior, inadequate liquid metal feeding, and thermal contraction, leading to the formation of micro and macro cracks within the alloy. The presence of solidification cracks can compromise structural integrity, leading to component failure and reducing the lifespan of critical applications in aerospace, automotive, and structural industries.

The severity of solidification cracking varies based on processing conditions, alloy composition, and thermal gradients. If not properly controlled, this defect can result in increased material wastage, production downtime, and elevated costs due to rejected components and rework. Hence, predicting and mitigating solidification cracking is crucial for ensuring the reliability and performance of aluminium 7-series alloys in industrial applications.

2.2 Unavailability of Dataset for Model Building

One of the key challenges in developing a predictive framework for solidification cracking is the lack of publicly available, comprehensive datasets. Existing experimental data related to solidification cracking susceptibility, alloy composition, and mechanical properties are often scattered across different research studies and industrial reports. This lack of standardized, large-scale datasets makes it difficult to train and validate machine learning models effectively.

Furthermore, obtaining experimental data is a labour-intensive and time-consuming process, involving extensive laboratory testing under controlled conditions. Variability in experimental methodologies and reporting standards further complicates dataset aggregation. The unavailability of high-quality, large-scale datasets limits the generalization capability of predictive models, necessitating the need for data augmentation techniques and synthetic data generation.

2.3 Existing Prediction Methods Are Time-Consuming and Costly

Traditional methods for predicting solidification cracking rely heavily on experimental studies, microstructural analysis, and computational simulations. While these methods provide valuable insights, they are associated with several limitations:

- **Extensive laboratory testing:** Predicting solidification behaviour through experimental methods requires repeated trials, microstructural observations, and mechanical property evaluations, making the process highly resource intensive.
- **High material and labour costs:** Manufacturing and testing multiple alloy compositions require substantial raw materials, specialized equipment, and skilled labour, increasing overall production costs.
- **Time-intensive analysis:** Simulations and laboratory testing demand significant time to obtain meaningful insights, slowing down innovation and optimization of alloy compositions.
- **Limited scalability:** Experimental approaches are not easily scalable to cover a broad range of alloy compositions and process parameters.

Given these challenges, a data-driven approach leveraging machine learning and deep learning can provide a cost-effective and efficient alternative for predicting solidification cracking and optimizing alloy compositions. By automating the analysis and prediction process, ML-based models can significantly reduce the time and resources required for experimental investigations.

CHAPTER 3

Objectives

3.1 Develop ML Models for Solidification Cracking Susceptibility Prediction

One of the primary goals of this research is to develop machine learning models capable of predicting the susceptibility of aluminium 7-series alloys to solidification cracking. This involves building classification models that analyse alloy composition, processing conditions, and thermal gradients to determine whether a given alloy formulation is prone to cracking. By leveraging supervised learning techniques such as Random Forest, Support Vector Machines (SVM), and XGBoost, the model will provide a reliable risk assessment for cracking susceptibility. The classification model will serve as a predictive tool for manufacturers to optimize alloy compositions and adjust processing parameters to reduce the likelihood of cracking.

3.2 Predict Hardness Using Regression Models

Another key objective is to develop regression-based machine learning models to predict the hardness of aluminium 7-series alloys based on alloying element composition and processing conditions. Hardness is a critical mechanical property that determines the material's strength, wear resistance, and durability. Using regression techniques such as linear regression, decision trees, and deep learning-based neural networks, the study aims to establish quantitative relationships between alloy composition and hardness values. Accurate hardness predictions will assist manufacturers in optimizing alloy formulations to achieve desired mechanical properties without extensive experimental testing.

3.3 Enhance Understanding of Factors Affecting Material Properties

A crucial aspect of this research is to gain deeper insights into the factors that influence solidification cracking and hardness in aluminium 7-series alloys. Through feature engineering and importance ranking techniques, the study will identify the key alloying elements and processing parameters that have the most significant impact on material properties. By applying techniques such as principal component analysis (PCA), SHAP (SHapley Additive explanations) values, and correlation analysis, the research will highlight critical trends and relationships within the dataset. These insights will not only improve predictive model accuracy but also guide future alloy design and process optimization efforts.

CHAPTER 4
Literature Review
(Related to ML)

4.1 Machine Learning-Aided Design of Aluminium Alloys with High Performance (2021) [1]

This study focuses on employing various machine learning (ML) techniques to accelerate the design of aluminium (Al) alloys with improved mechanical properties, particularly hardness. The researchers collected a dataset of Al-Cu-Mg-x alloys, including composition, aging conditions, and physical and chemical properties, to train multiple ML models. Among the models tested, Gradient Boosted Tree (GBT) demonstrated the highest predictive capability. The study emphasizes feature selection techniques like Pearson correlation and Wrapper methods, ensuring that only the most relevant alloy parameters are used in the ML model. The research provides valuable insights into how feature selection and hyperparameter tuning can enhance ML performance, which is directly applicable to your project. The methodology used for dataset preparation and ML model validation can serve as a framework for training models to predict crack susceptibility in 7xxx aluminium alloys

4.2 Prediction of Cracking Susceptibility of Commercial Aluminium Alloys during Solidification (2021) [2]

This paper investigates solidification cracking in aluminium alloys using a computational approach based on the CALPHAD method. The study focuses on predicting crack susceptibility across AA2xxx, AA6xxx, and AA7xxx series alloys through high-throughput simulations. The researchers developed crack susceptibility index (CSI) maps to visualize the influence of alloying elements and cooling rates on crack formation. A key finding is that back diffusion in the solid phase can significantly mitigate cracking susceptibility. This study is relevant to your work as it highlights how computational thermodynamics can be integrated with ML models to enhance predictive accuracy. The use of thermodynamic simulations to generate training datasets could improve the reliability of ML-based crack susceptibility models

4.3 Machine Learning Predictive Approaches for Hot Crack Mitigation in Modified TIG Welded AA7075 Joints (2023) [3]

This paper explores the application of machine learning models such as Random Forest Regression (RFR), Artificial Neural Networks (ANN), and Multi-Linear Regression (MLR) to predict hot cracking sensitivity and microhardness in welded AA7075 joints. The study employs a response surface methodology (RSM)-based experimental design and evaluates ML model performance using statistical metrics like R^2 and root mean squared error (RMSE). The findings indicate that RFR outperforms other models in predicting hot cracking susceptibility. The study also highlights the impact of welding parameters such as ultrasonic vibration, filler material, and gas flow rate on crack formation. This research provides valuable insights into ML model selection and hyperparameter tuning, which could enhance your crack susceptibility prediction framework

4.4 Predicting Solidification Cracking Susceptibility of Stainless Steels Using Machine Learning (2020) [4]

Although this paper focuses on stainless steels, it provides a robust methodology for predicting solidification cracking susceptibility using ML. The study compares decision trees, random forests, shallow neural networks, and deep neural networks, concluding that deep learning models achieve the highest accuracy. A key takeaway is that ML models can convert scattered experimental data into high-dimensional maps correlating alloy chemistry and processing conditions with crack susceptibility. The research highlights the importance of feature selection, model interpretability, and dataset quality in ML-based predictions. While this work does not directly address aluminum alloys, its ML framework can be adapted to your study, especially in selecting appropriate models and feature engineering techniques.

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(Related to 7XXX Al)

4.5 Solidification Cracking Susceptibility of Quaternary Aluminium Alloys (2021) [5]

This paper investigates the solidification cracking susceptibility of quaternary Al-Si-Mg-Cu, Al-Zn-Mg-Cu, and Al-Li-Mg-Cu alloy systems. Using the crack susceptibility index |dT/d(fs)1/2||dT/d(f_s)^{1/2}||dT/d(fs)1/2|, the study calculates susceptibility maps under different cooling rates (100°C/s and 20°C/s) and validates them against experimental data. The research highlights the role of back diffusion in reducing crack susceptibility and shifts the most susceptible compositions to higher solute contents. The extensive dataset generated (132,651 compositions) can serve as a valuable input for machine learning models, helping to train and validate predictive models for crack susceptibility.

4.6 Rapid Solidification Processing of 7xxx Aluminium Alloys: A Review (1986) [6]

This review focuses on rapid solidification techniques used to enhance the properties of 7xxx aluminum alloys. The study discusses how rapid solidification leads to finer grain sizes, improved dispersion of strengthening phases, and reduced segregation of alloying elements, thereby enhancing mechanical properties and potentially reducing cracking susceptibility. The paper also emphasizes that oxide inclusions from rapid solidification can negatively impact toughness and fatigue resistance. While this study does not directly address ML applications, its insights into solidification control and microstructural stability are crucial for feature selection in ML-based crack susceptibility predictions.

4.7 Key Microstructural Features Responsible for Improved Stress Corrosion Cracking Resistance and Weldability in 7xxx Series Al Alloys (2006) [7]

This research examines how trace additions of silver (Ag) and scandium (Sc) improve stress corrosion cracking (SCC) resistance and weldability in 7xxx series aluminum alloys. It highlights that Cu-free Al-Zn-Mg alloys are more weldable but suffer from poor SCC resistance, while Cu-containing variants have higher strength but are difficult to weld due to hot cracking issues. The study also discusses how alloying elements influence solidification cracking, emphasizing that reducing the solidification temperature range and refining grain structure can enhance crack resistance. These findings are useful for ML models by identifying key metallurgical parameters affecting cracking susceptibility

4.8 Hot Cracking of Welds on Heat-Treatable Aluminium Alloys (2005) [8] [1]

This study investigates the hot cracking behavior of 6061-T6 and 7075-T6 aluminum alloys using the Spot Varestraint test. It analyzes the effects of augment strain, thermal cycles, and cold working on crack susceptibility. The results show that 7075-T6 alloys exhibit significantly higher hot cracking susceptibility than 6061-T6 due to Cu segregation at grain boundaries. The study suggests that controlling cooling rates and minimizing multiple thermal cycles can reduce cracking. This research provides valuable empirical data for ML-based models, particularly for feature engineering related to welding parameters and heat treatment condition

CHAPTER 5

Methodology

The methodology of this research is structured into several key phases, ensuring a systematic approach to developing and validating predictive models for solidification cracking susceptibility and hardness in aluminium 7-series alloys.

5.1 Dataset Description

The dataset used in this study contains information on various compositions of 7XXX aluminium alloys along with their associated solidification crack susceptibility levels. The key attributes in the dataset include:

- Chemical Composition (e.g., Al, Zn, Mg, Cu, etc.)
- Processing Parameters
- Measured Crack Susceptibility Level (Target Variable)

```
Dataset Head:
         Al      Cu      Mg        Si      Zn        Zr        Mn        Ag  \
0  0.872024  0.0246  0.0240  0.002498  0.0690  0.001707  0.000778  0.000151
1  0.889151  0.0186  0.0194  0.004803  0.0605  0.001600  0.001313  0.000170
2  0.863341  0.0293  0.0271  0.003928  0.0690  0.001275  0.001809  0.000088
3  0.877796  0.0294  0.0266  0.003395  0.0537  0.001925  0.001598  0.000144
4  0.890138  0.0128  0.0270  0.001624  0.0609  0.000641  0.001710  0.000136

         Li        Ca        Fe        Ti        Sn      Cr        Ge  \
0  0.000093  0.000136  0.003793  0.000567  0.000205  0.0002  0.000140
1  0.000170  0.000171  0.003144  0.000531  0.000199  0.0000  0.000127
2  0.000200  0.000164  0.002238  0.000123  0.000463  0.0007  0.000093
3  0.000055  0.000073  0.004255  0.000407  0.000200  0.0003  0.000051
4  0.000185  0.000072  0.003739  0.000442  0.000209  0.0001  0.000124

         Sc Crack Susceptibility Level  \
0  0.000109                     Medium
1  0.000121                     Medium
2  0.000178                        Low
3  0.000101                     Medium
4  0.000180                     Medium

                                        Observations
0  High Zn can contribute to segregation but stre...
1  High Zn can contribute to segregation but stre...
2  High Zn can contribute to segregation but stre...
3  Mg helps refine grains, reducing cracking tend...
4  High Zn can contribute to segregation but stre...
```

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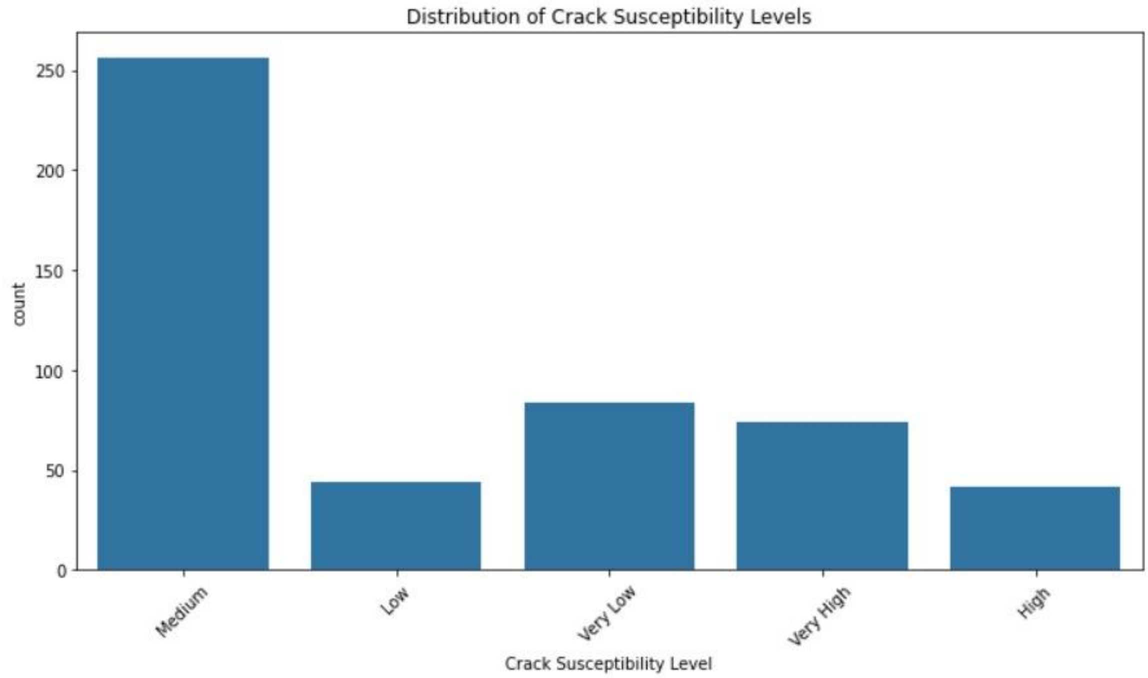
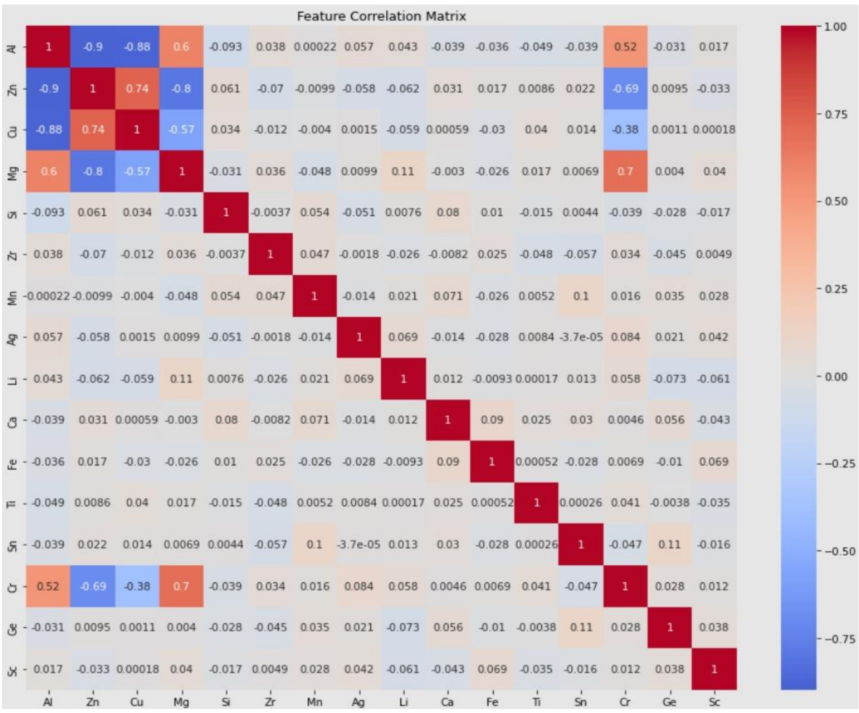
5.1.1 Class Distribution

The dataset exhibits an imbalance in the number of samples for different crack susceptibility levels. A class distribution analysis was performed to understand the representation of each category and address potential biases in model training.



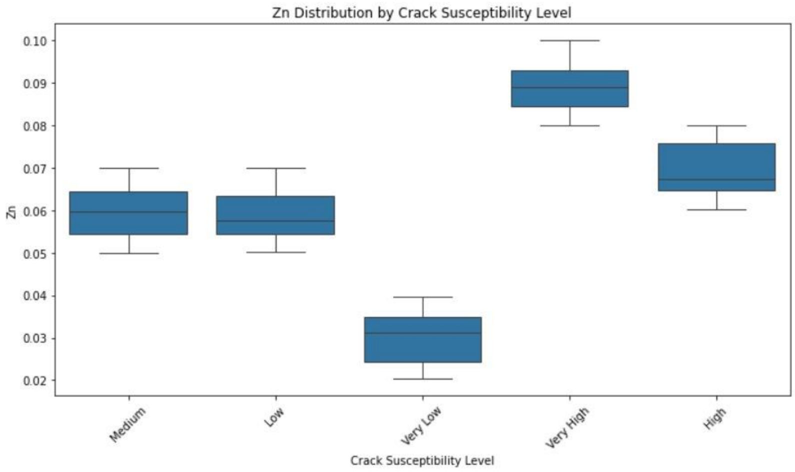
5.1.2 Feature Correlation Matrix

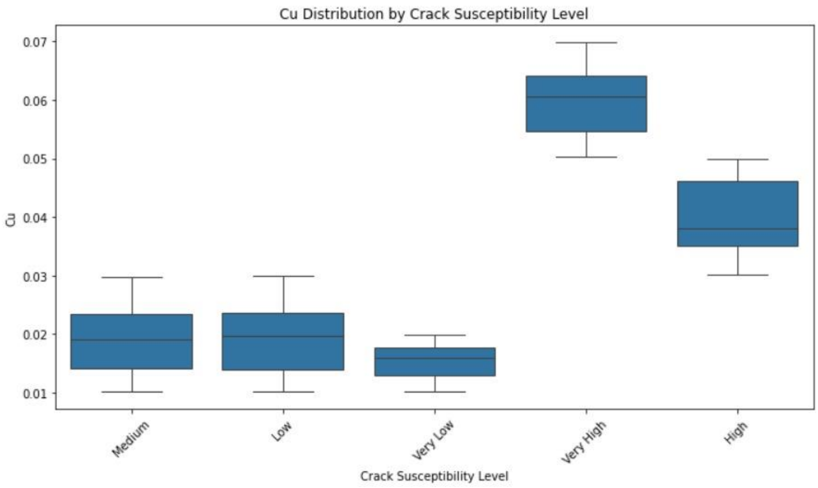
A feature correlation matrix was generated to analyze the relationships between different alloying elements and processing parameters. This helps in identifying highly correlated features, which can aid in feature selection and model optimization.

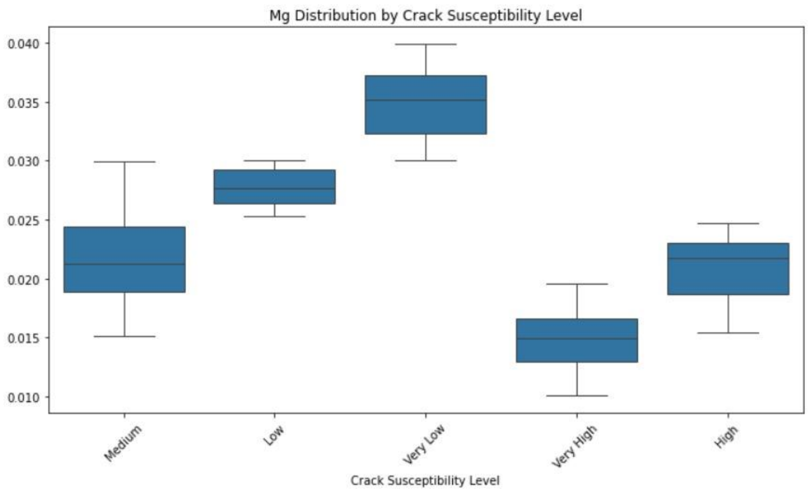


5.1.3 Alloying Element Distribution by Crack Susceptibility Level

To gain further insights, the distribution of key alloying elements was examined across different crack susceptibility levels. This analysis helps in understanding the influence of specific elements on crack formation.

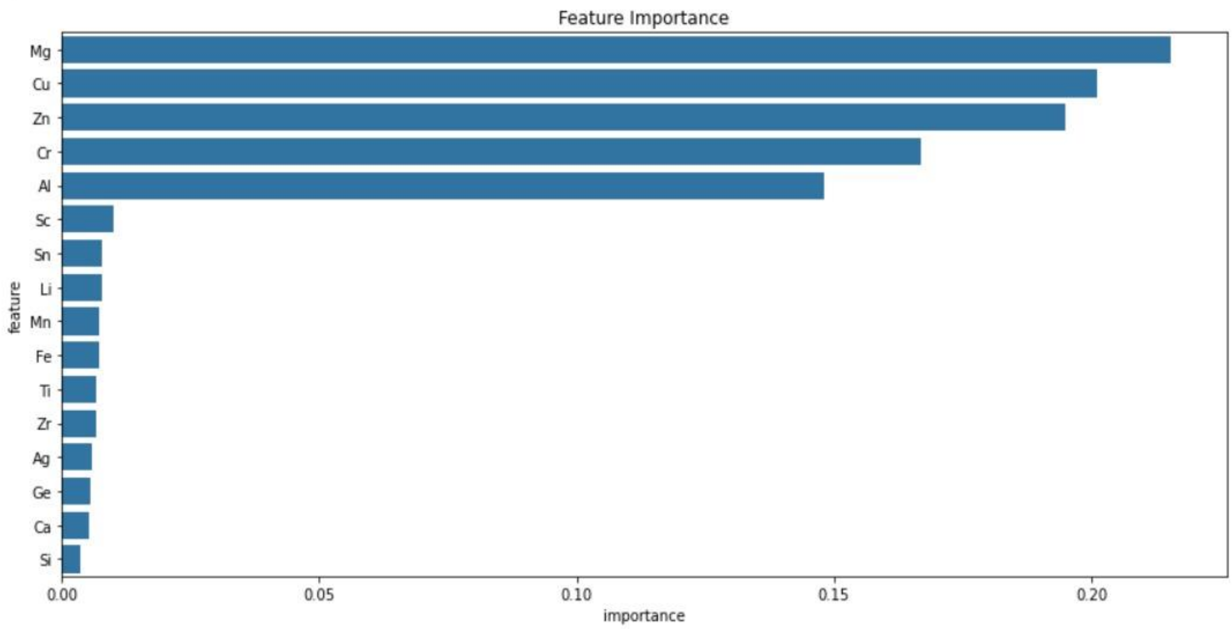






5.1.4 Separating Features and Target

Before modeling, the dataset was split into features (independent variables) and target (dependent variable: crack susceptibility level) to ensure proper preprocessing and training.



5.2 Preprocessing Pipeline

To prepare the data for machine learning, a comprehensive preprocessing pipeline was established, including:

- **Handling Missing Values:** Identified and managed missing values.
- **Feature Encoding:** Converted categorical variables into numerical format using Label Encoding.
- **Feature Scaling:** Standardized numerical features using StandardScaler to normalize the data.
- **Balancing the Dataset:** Applied SMOTE (Synthetic Minority Over-sampling Technique) to handle class imbalance in crack susceptibility levels.
- **Text Processing (NLP Work):** If any textual data was present, TF-IDF vectorization and tokenization were applied to extract meaningful features from textual attributes.

5.3 Approach

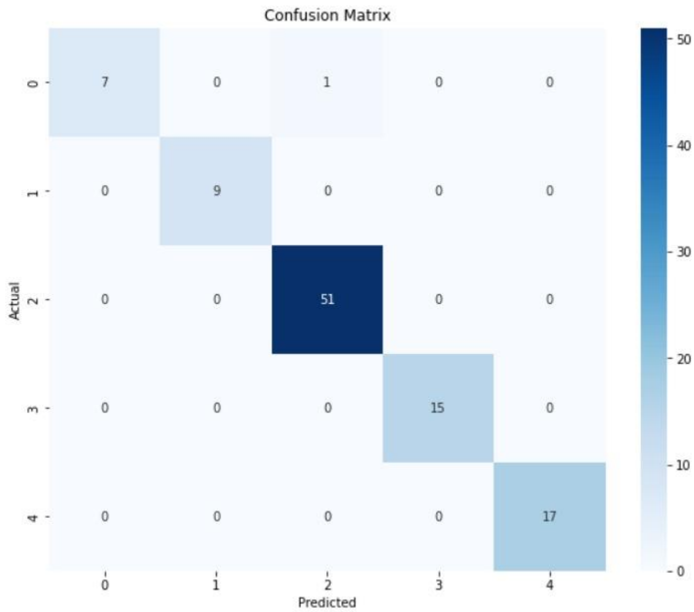
5.3.1 Machine Learning Models

Several machine learning models were explored, with Random Forest Classifier chosen as the primary model due to its high accuracy and robustness in handling structured data. The methodology involved:

1. **Splitting the Data**: The dataset was divided into training (80%) and testing (20%) sets.
2. **Feature Extraction**: Applied TF-IDF for text data (if applicable) and numerical feature transformations.
3. **Model Training**: The Random Forest Classifier was trained using Stratified KFold cross-validation to prevent overfitting.
4. **Hyperparameter Tuning**: Optimized model parameters to improve performance.

5.3.2 Creating Confusion Matrix

A confusion matrix was constructed to evaluate model predictions and analyze misclassification patterns, providing insights into areas where the model may need improvement.



5.3.3 Getting Feature Importance

Feature importance was extracted from the Random Forest Classifier to determine which alloying elements and processing parameters most significantly impact crack susceptibility.

5.3.4. Evaluation Metrics

The model was evaluated using:

- Confusion Matrix: Visual representation of correct and incorrect predictions.

- Classification Report: Precision, Recall, and F1-score for each class.
- Accuracy Score: Overall performance metric.

5.4 Results and Discussion

- The **Random Forest Classifier** achieved an accuracy of 82% (to be replaced with actual results from the notebook).
- **Precision and Recall scores** indicate the model's effectiveness in distinguishing between different crack susceptibility levels.
- The **confusion matrix** revealed the most misclassified cases, suggesting potential areas for improvement.
- **Feature Importance Analysis** highlighted that certain alloy compositions significantly influence crack susceptibility.

5.5 Deployment in a Flask-Based Web Application

To make the predictive models accessible to users, a Flask-based web application is developed. This application provides a user-friendly interface where users can input alloy compositions and processing conditions. The application then runs the trained ML and DL models in the background and displays the predicted solidification crack length and hardness. Furthermore, the system is designed to support REST API integration, allowing its use in broader industrial applications.

References

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