Supplementary Materials

An integrated design of novel RAFM steels with targeted microstructures and tensile properties using machine learning and CALPHAD

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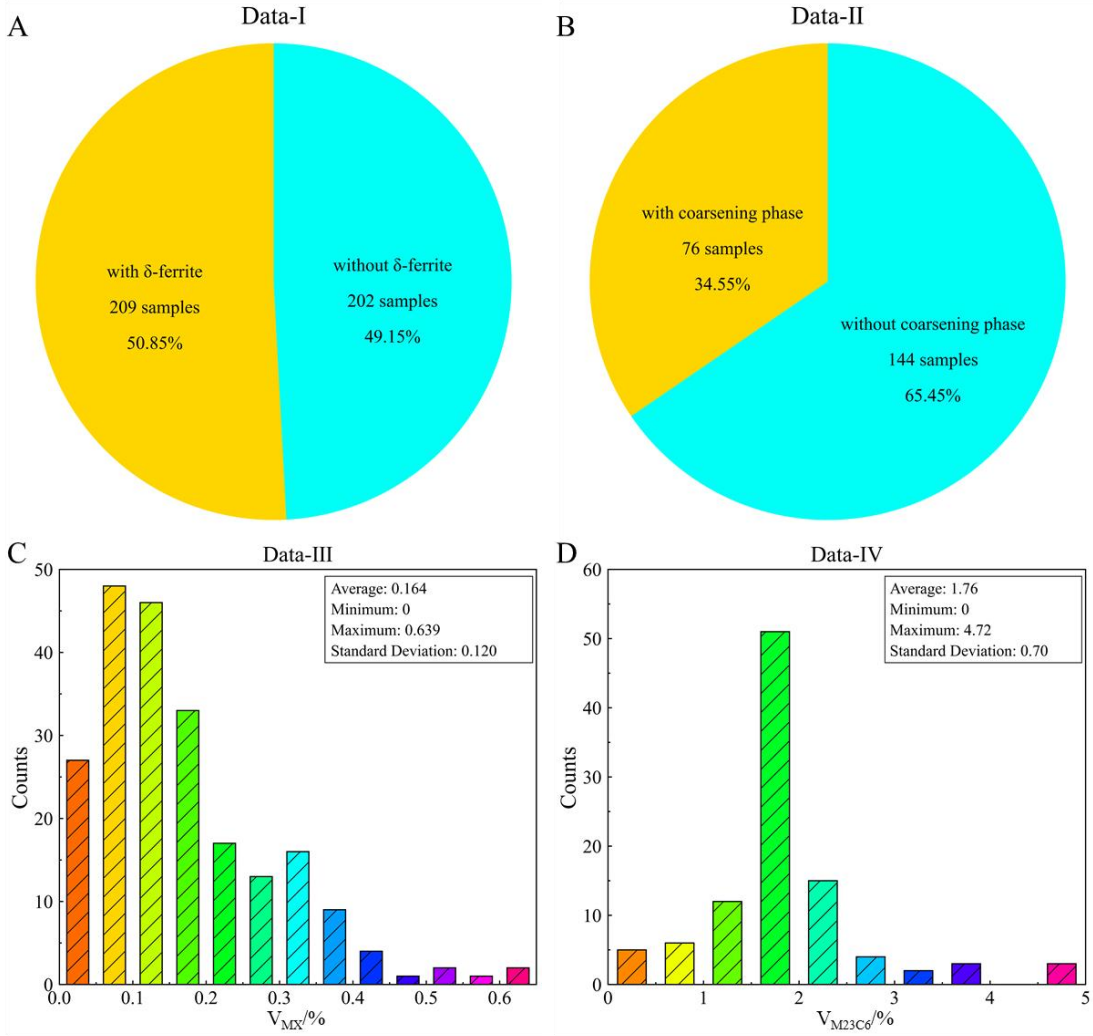
1. Supplementary information on the data distribution of the microstructural dataset



Supplementary Figure 1. The data distribution of the microstructural dataset.

2. Supplementary information on the overview of commonly used machine learning algorithms

In this study, various machine learning algorithms which were commonly used in materials research, such as decision tree (DT), random forest (RF), support vector machine (SVM), gradient boosting (GB), k-nearest neighbor (KNN), and artificial neural network (ANN) were used to develop classification and regression models. The following section provides an overview of these algorithms, highlighting their unique strengths and limitations.

DT is a robust and prevalent algorithm that utilize a tree-like flowchart to effectively partition data into groups for solving classification and regression problems. It does not require complex domain knowledge [1], making them accessible for various applications. However, DT can readily result in significant prediction deviations from actual results [2]. Additionally, it is more suitable for predicting categorical features than for estimating numerical variables [3].

RF is highly regarded for its strength, flexibility, and capability in processing high-dimensional data [4]. It helps reduce overfitting compared to individual decision trees, leading to improved predictive performance. RF works well with large datasets, can accommodate a wide range of input features, and excels at determining feature importance [5]. Furthermore, it effectively handles missing values and addresses class imbalances [5]. However, using RF requires careful attention to hyperparameter tuning, such as the number of trees and the features chosen for splits. Due to its ensemble nature, the model is less interpretable than a single decision tree, making it

challenging to understand the contribution of each individual tree.

SVM is a supervised binary classification method introduced by VaPnik [6]. It is primarily designed to identify a separating hyperplane that maximizes the margin in the feature space, leading to higher classification accuracy. This segmentation maximizes the margin, transforming the problem into a convex optimization challenge. Initially designed for linear classification, SVM has evolved to tackle non-linear and high-dimensional data while effectively addressing overfitting [7]. It is known for its robustness and accuracy in managing complex, high-dimensional, and small-sample challenges [8]. However, SVM requires high computational resources and relies heavily on selecting an optimal hyperplane [9]. Despite this, its framework is effortlessly generalized for various issues, making it highly versatile [10].

GB is a machine learning algorithm for regression and classification that builds models in stages but extends this approach by optimizing a chosen differentiable loss function [11]. This algorithm assembles multiple weak models, usually decision trees, to form a more powerful predictive model [12]. The effectiveness of GB stems from the proven superiority of ensemble methods over other machine learning algorithms in various situations, making it particularly powerful for complex predictive tasks [13–15]. However, GB builds models in a stage-by-stage way [12], which may result in higher computational costs and difficulty in achieving parallelization.

KNN is a non-parametric supervised machine learning algorithm utilized for both classification and regression tasks [16]. It classifies a new data point by finding its ‘k’ nearest neighbors in the training set based on similarity. The prediction for the new

data point is then calculated as the average or weighted average of the outcomes from its ‘k’ nearest neighbors [17]. KNN is a straightforward algorithm suitable for applications across various fields and supports multiple distance measures (e.g., Euclidean, Manhattan, Minkowski), making it adaptable to different data types and problem requirements. Despite its usefulness, the KNN algorithm can be sensitive to outliers in the data, which may disproportionately affect its prediction performance.

ANN is non-linear computational model inspired by biological neural networks in the brain, utilizing interconnected neurons and weighted connections to recognize the pattern and tackle complex problems [18]. ANN is particularly effective for non-linear problems and perform well with large datasets. A basic ANN algorithm consists of input, hidden, and output layers: the input layer receives primary data, the hidden layer processes it, and the output layer generates results [19]. Common types of ANN include Feed Forward Neural Network (FFNN), Back Propagation Neural Network (BPNN), etc., among which FFNN is the most widely used [20]. ANN is well-suited for tasks like pattern recognition and matching, grouping, and classification, but they require extensive computational resources and large datasets to perform effectively and often lack interpretability.

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