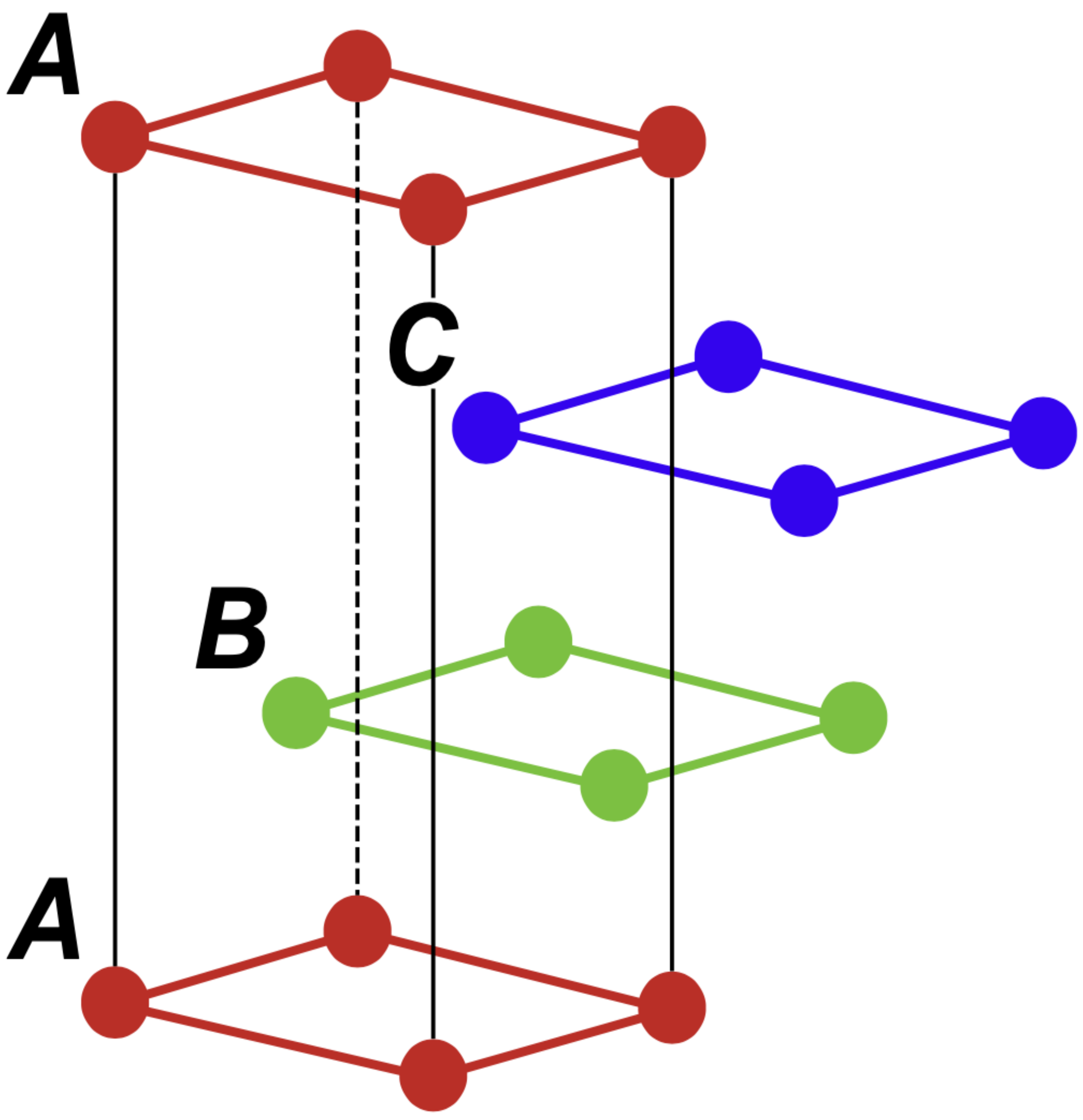
Predicting Stacking Fault Energy in High Entropy Alloys: A Machine Learning Approach

Exploring the potential of machine learning to predict stacking fault energy (SFE) in high-entropy alloys (HEAs). This presentation will examine the relationship between SFE, twinning-induced plasticity (TWIP), and the unique properties of HEAs.

A By Ali Tubayi & Morteza khodaei

Professor Abbas Zarei

TA : ENG Kamyar



HEAs: A New Breed of Materials

Compositional

More than 5 principal elements

Configurational

Entropy greater than 1.5R

High Entropy Effect

Stabilizes simple solid solution phases

Cocktail Effect

Unique combination of properties

George, E.P., Raabe, D. & Ritchie, R.O. High-entropy alloys. *Nat Rev Mater* **4**, 515–534 (2019). https://doi.org/10.1038/s41578-019-0121-4

Stacking Fault Energy: A Key Parameter

1 **Intrinsic Stacking Fault**

One layer displaced within the crystal structure

2 **Extrinsic Stacking Fault**

Two layers displaced within the crystal structure

3 **SFE and Mechanical Properties**

Low SFE favors twinning, high SFE favors slip

De Cooman, B.C., Y. Estrin, and S.K. Kim, Twinning-induced plasticity (TWIP) steels. Acta Materialia, 2018. 142: p. 283-362.

Twinning-Induced Plasticity (TWIP)

1

Mechanical Twinning

Formation of new crystallographic orientations

2

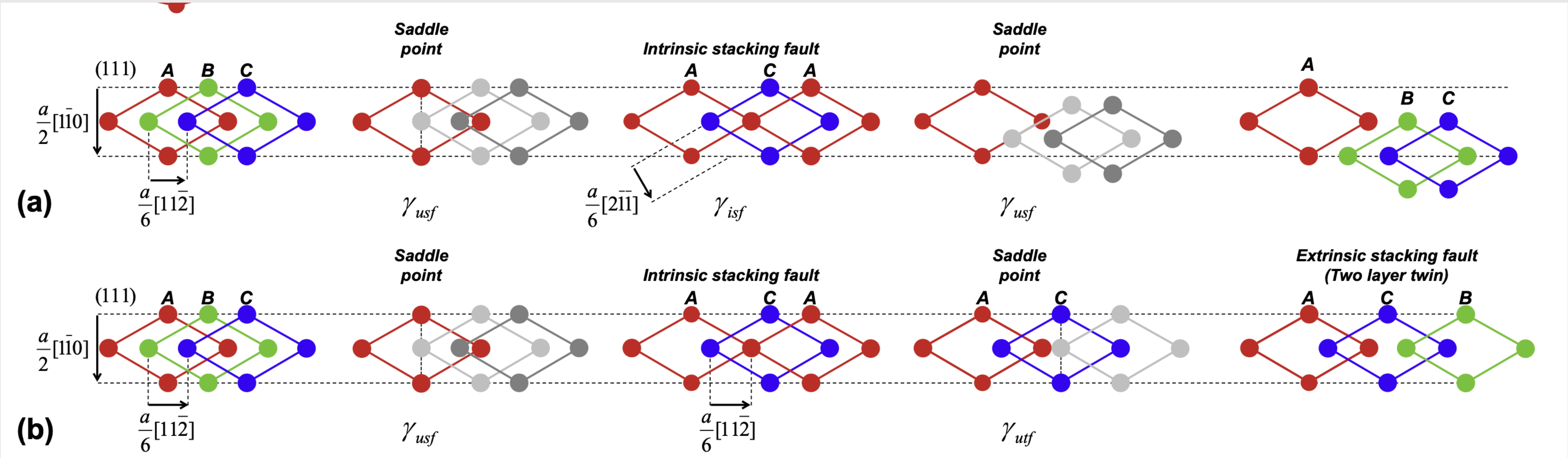
Coherency Loss

Interface between twin and parent crystal

3

Alloying Element Effect

Impact on twinning mechanism activation



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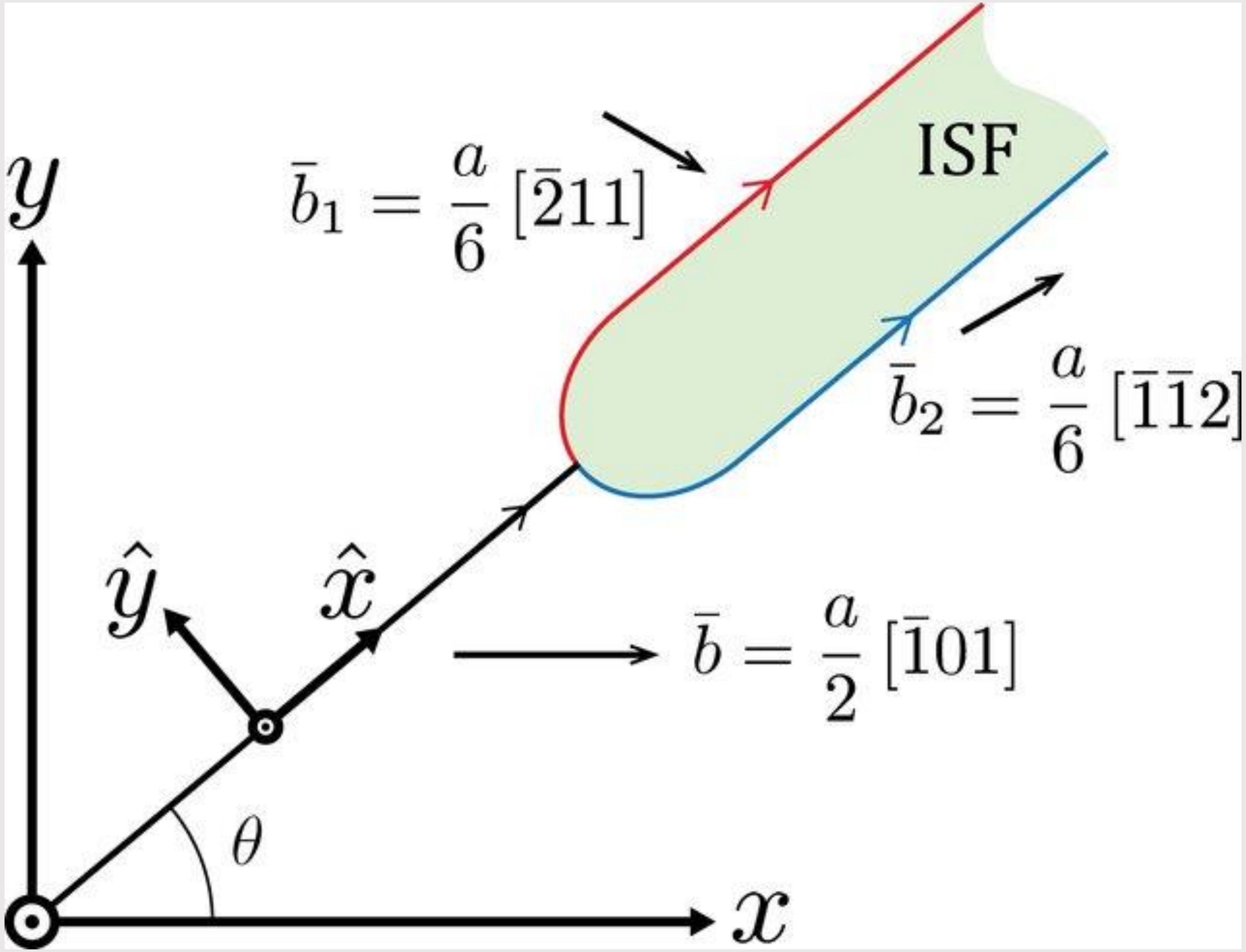

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Predicting SFE in HEAs: The Need for Machine Learning

Complexity of HEAs

Many elements, wide range of compositions

Experimental Limitations

Time-consuming and expensive

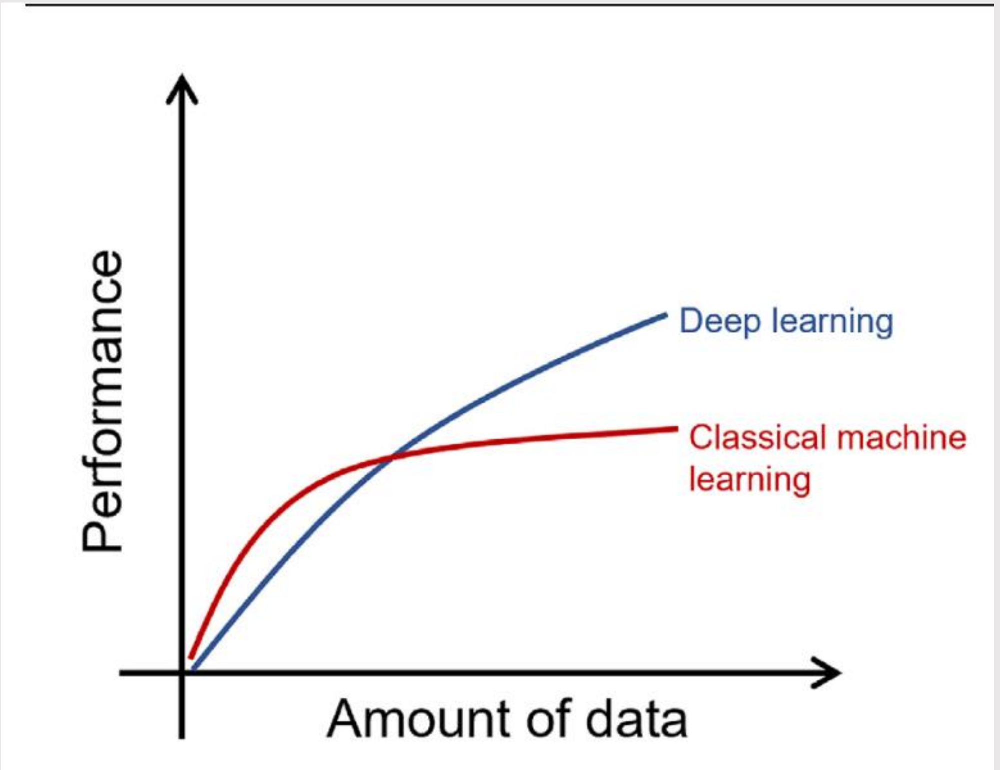
ML for Prediction

Fast and efficient, can handle large datasets

Machine Learning Approach: Data and Model

Dataset Construction

Experimental data, DFT calculations, databases



Classification Model

Prediction of SFE ranges through location

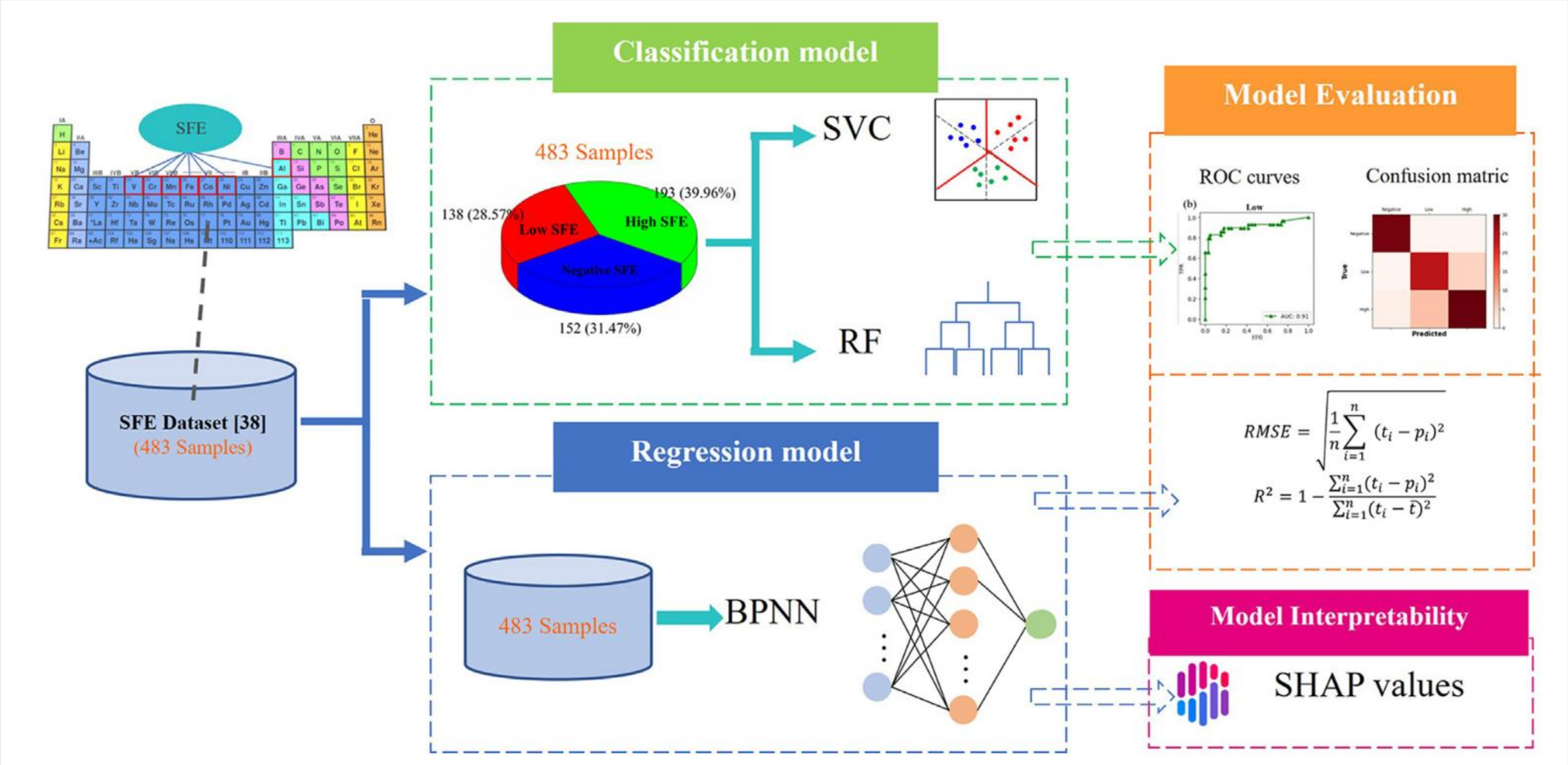
Regression Model

Predict the numerical value range of SFE

$$RMSE = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(t_i - p_i)^2}$$

$$R^2 = 1 - \frac{\sum_{i=1}^{n}(t_i - p_i)^2}{\sum_{i=1}^{n}(t_i - \bar{t})^2}$$

Machine Learning Approach: Data and Model



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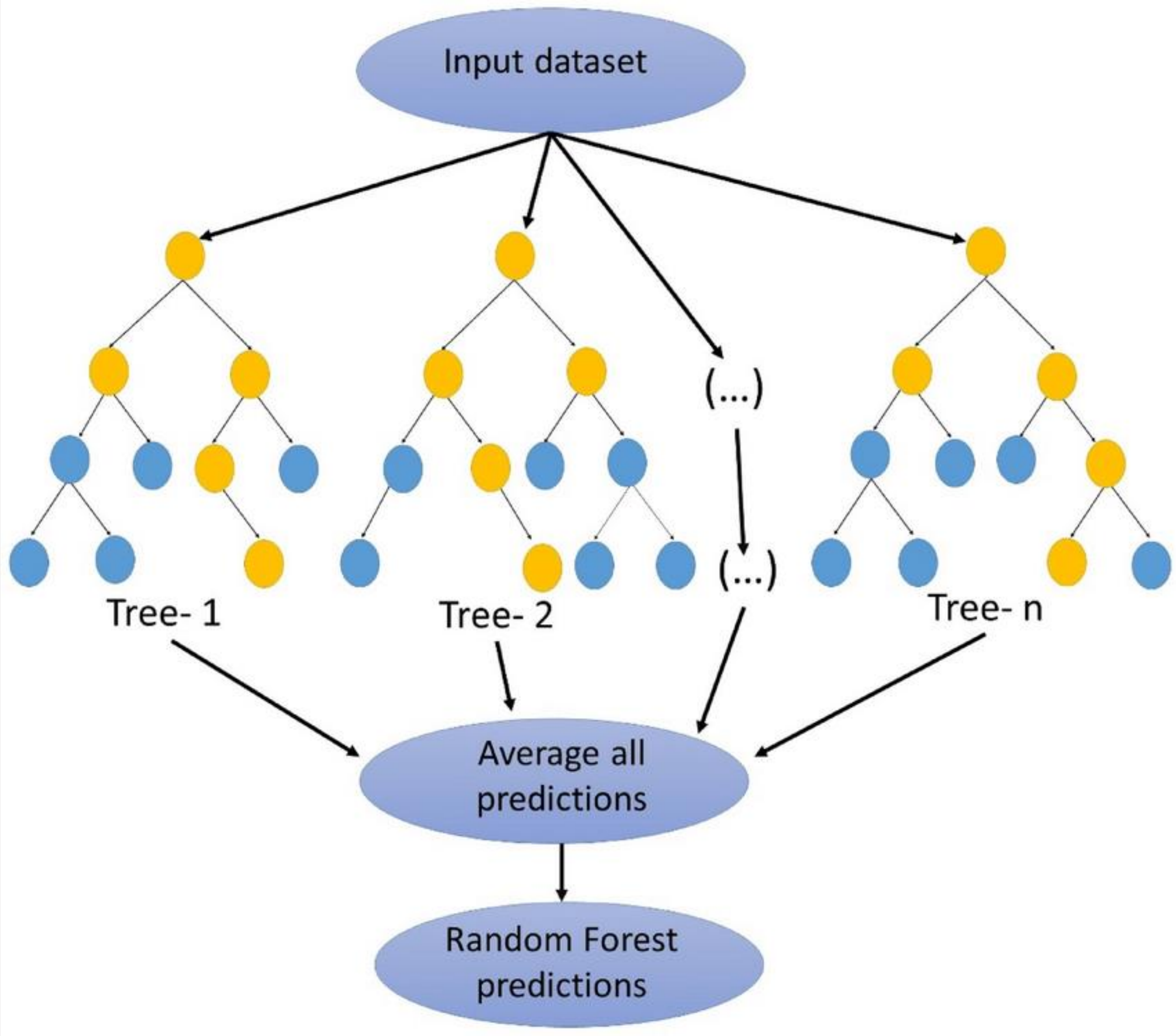

Sahour, Hossein & Gholami, Vahid & Torkman, Javad & Vazifedan, Mehdi & Saeedi, Sirwe. (2021). Random forest and extreme gradient boosting algorithms for streamflow modeling using vessel features and tree-rings. Environmental Earth Sciences. 80. 10.1007/s12665-021-10054-5.

Machine Learning Approach: Data and Model

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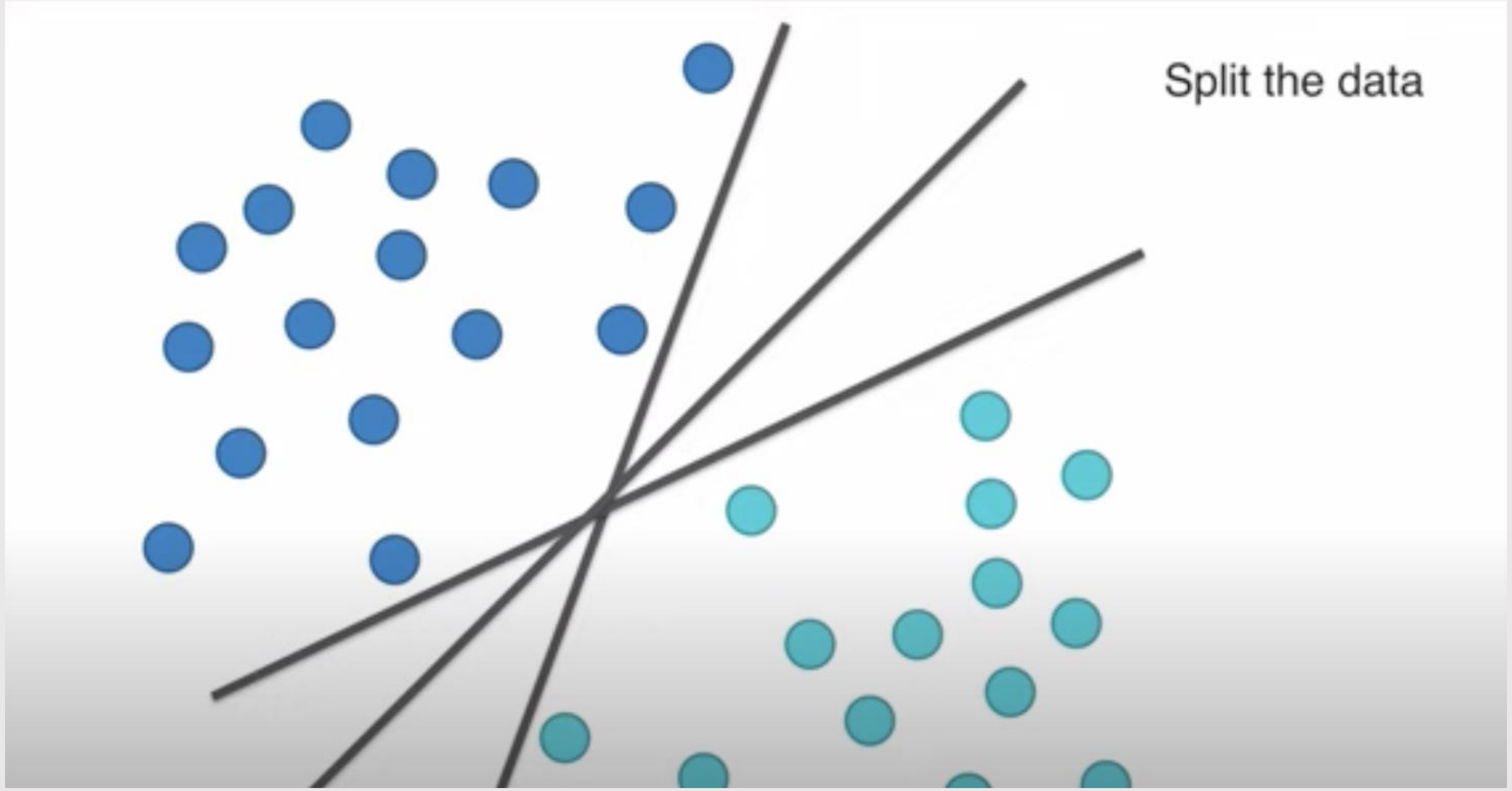
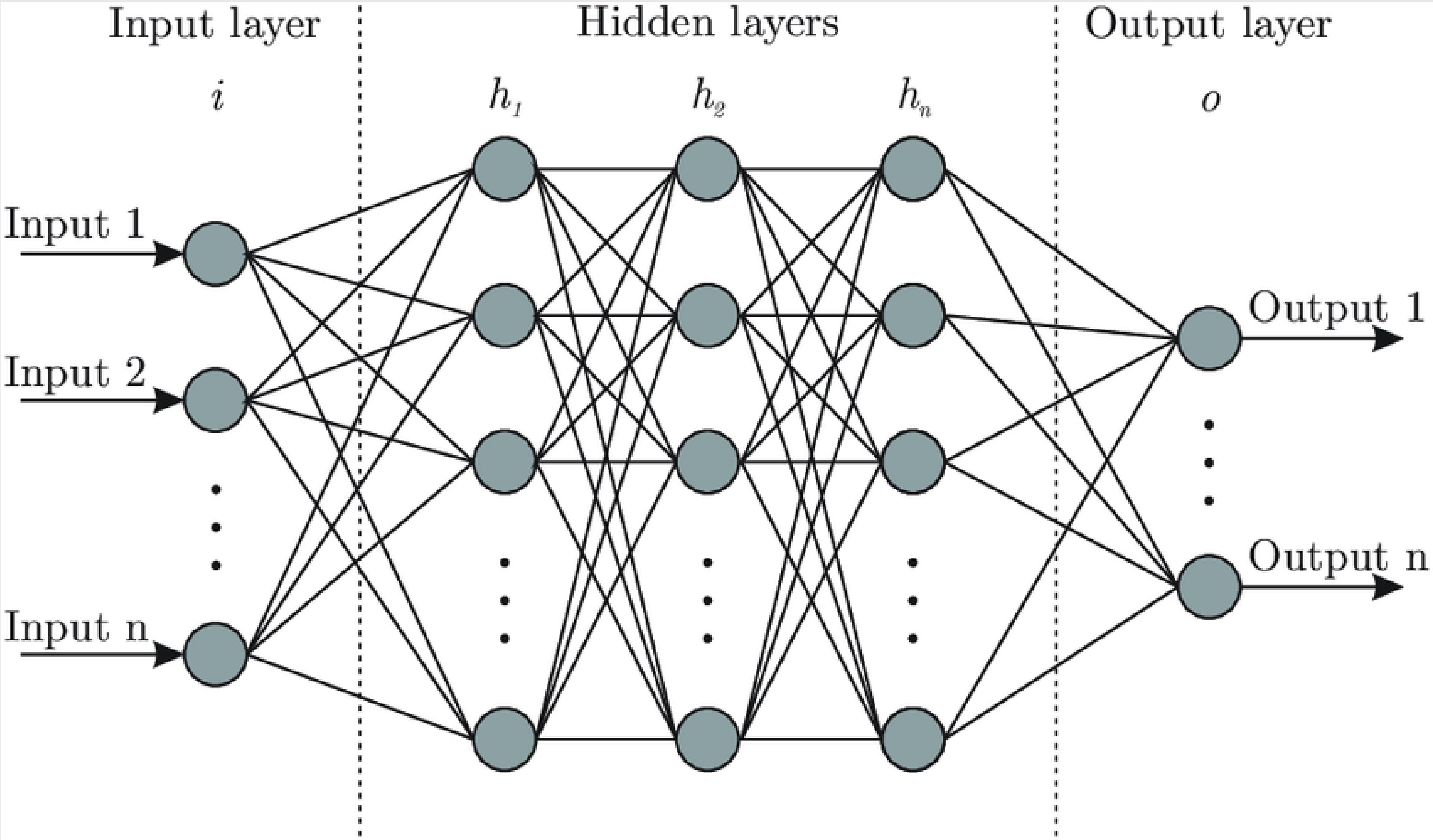


Lagrange multiplier

Machine Learning Approach: Data and Model

Regression Model

Predict the numerical value range of SFE



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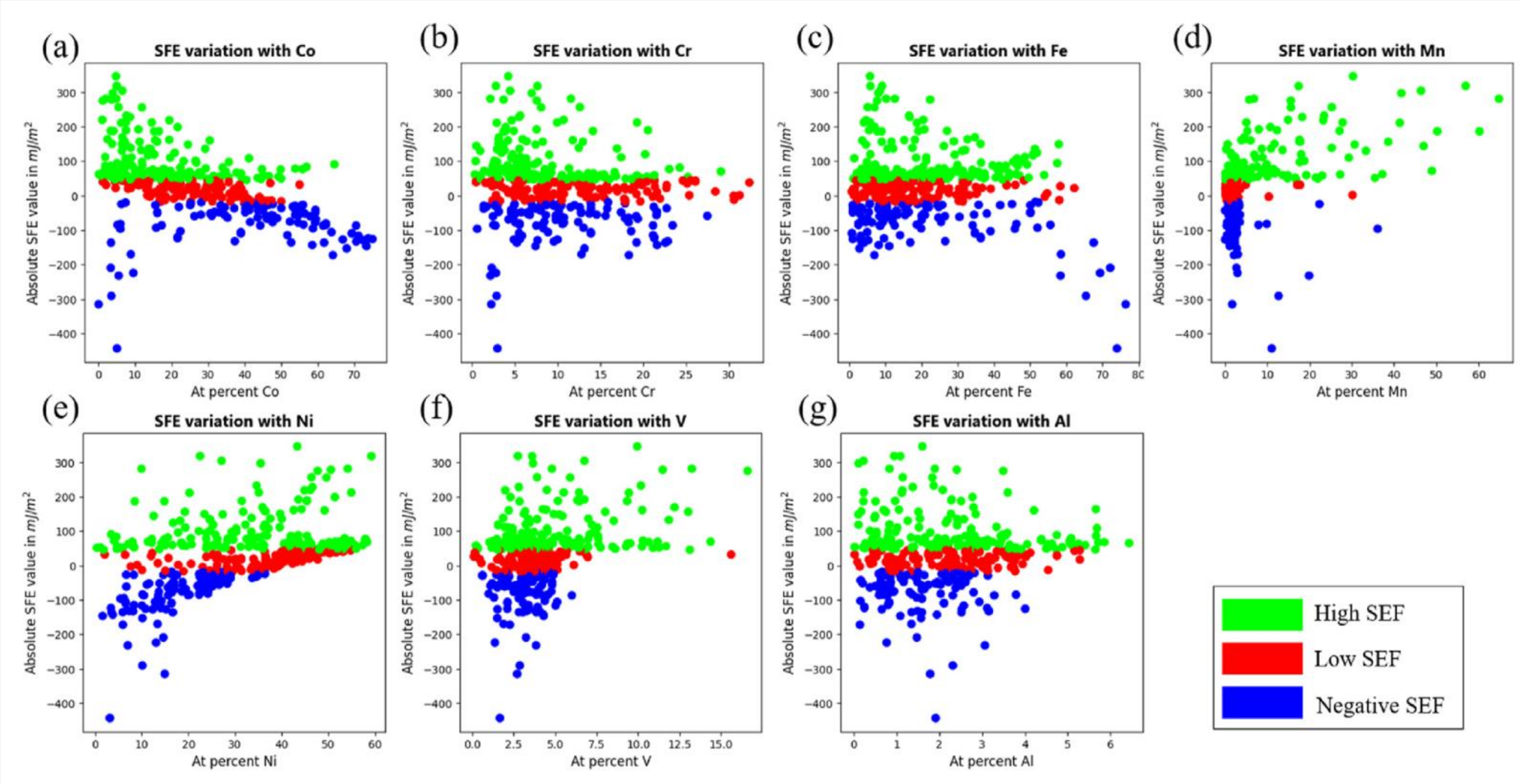
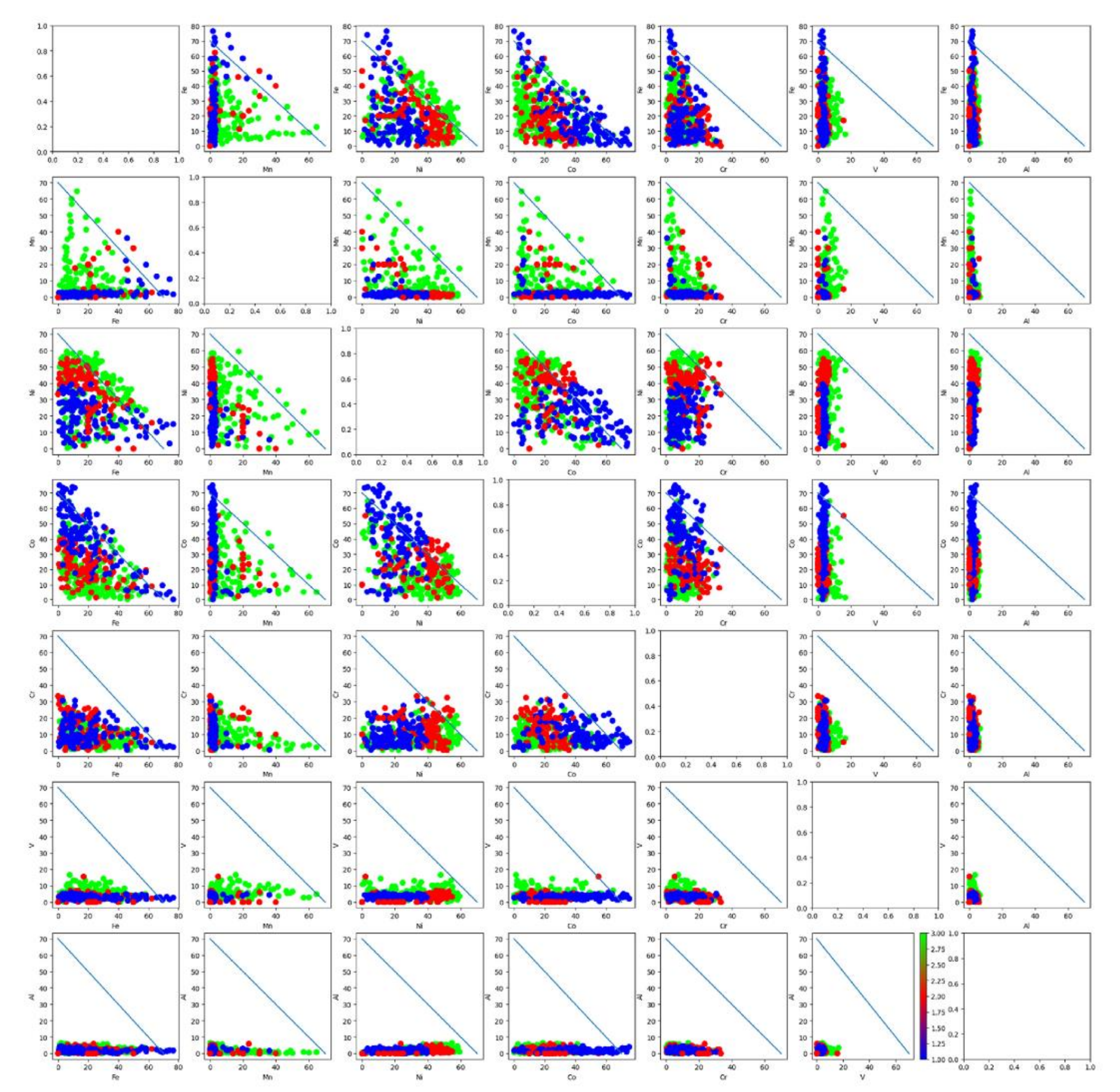
results

Data visualization



Zhang, X., et al., Predicting the stacking fault energy in FCC high-entropy alloys based on data-driven machine learning. Journal of Materials Research and Technology, 2023. 26: p. 4813-4824



Scater diagram of bi-element system

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Model Evaluation and Validation

Accuracy

How well the model predicts the outcome

Precision

How reliable the model's predictions are

Recall

How well the model identifies all relevant cases

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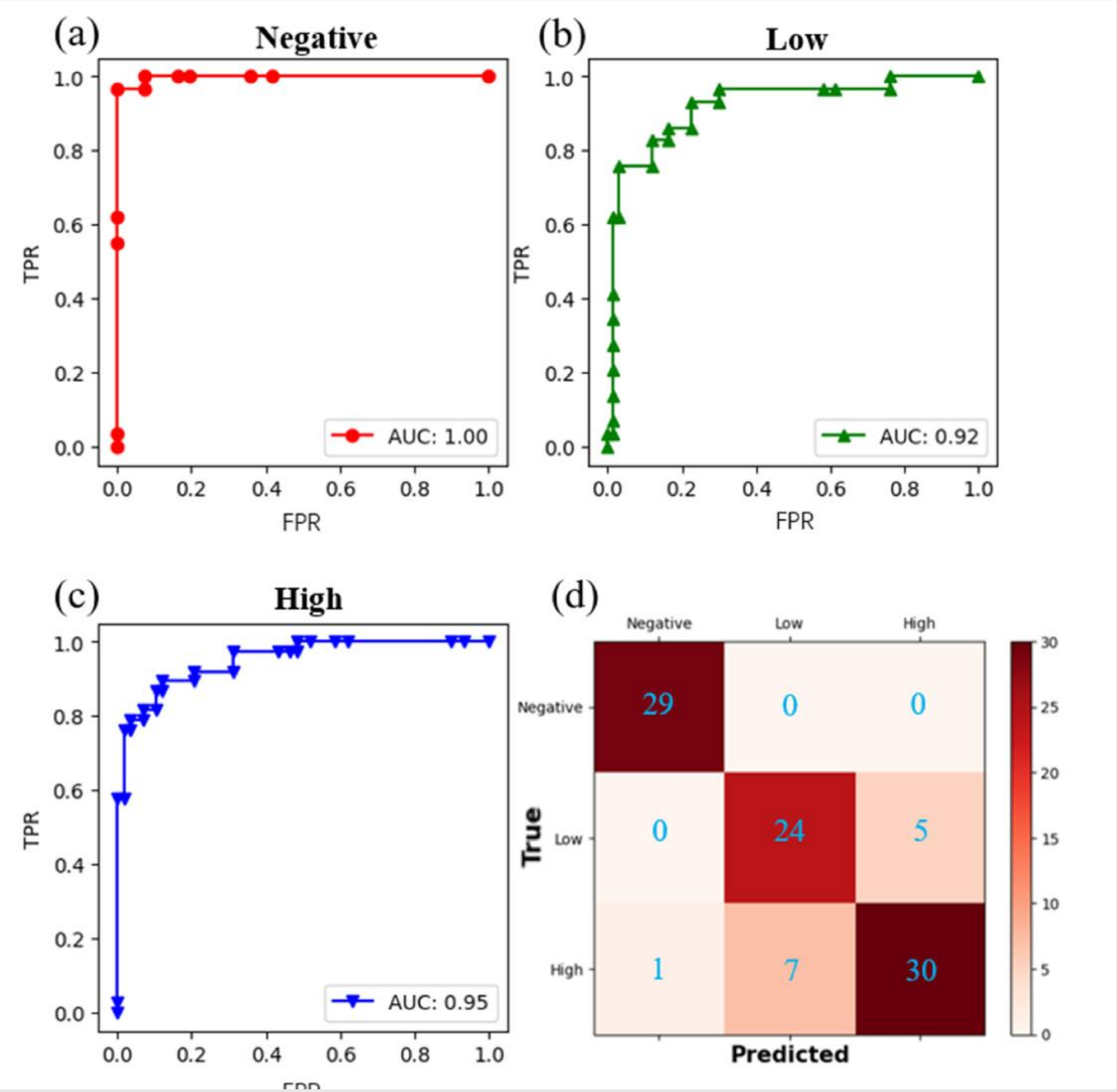

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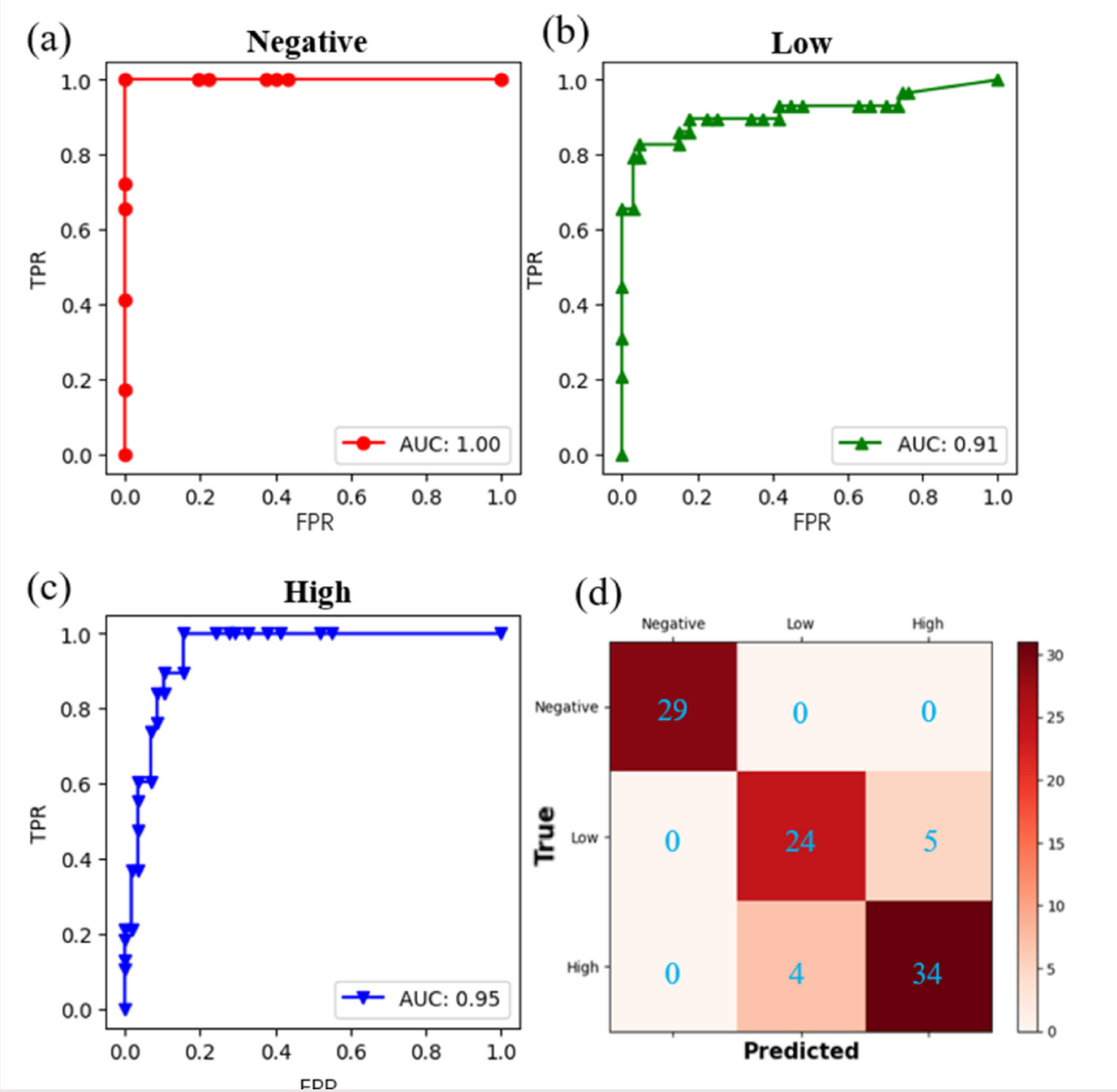

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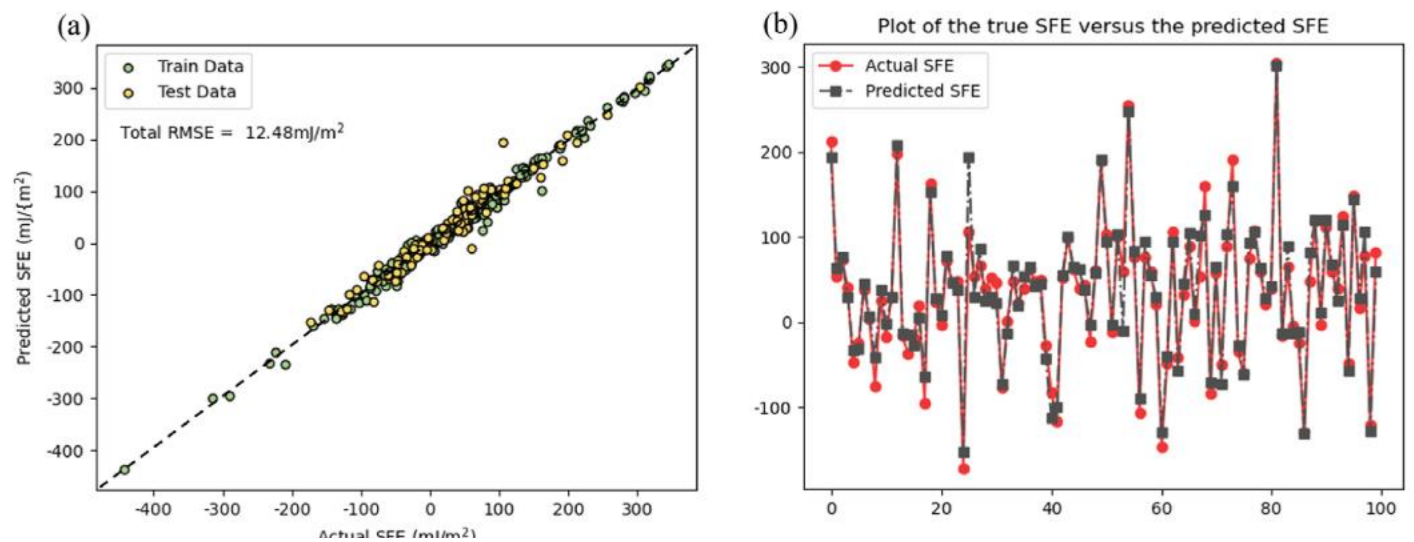

$$\varphi_i(v) = \sum_{S \subseteq N \setminus \{i\}} \frac{|S|!(|N|-|S|-1)!}{|N|!}\left(v(S \cup \{i\}) - v(S)\right)$$

$$g(x') = \varphi_0 + \sum_{i=1}^{n} \varphi_i$$

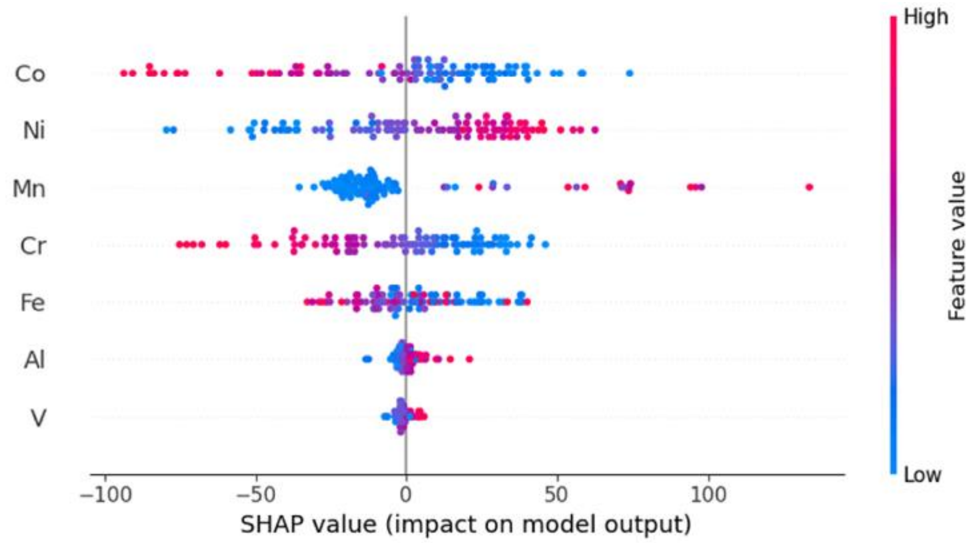

Fig. 8 – The summary plots of the SHAP values for each feature in each sample.

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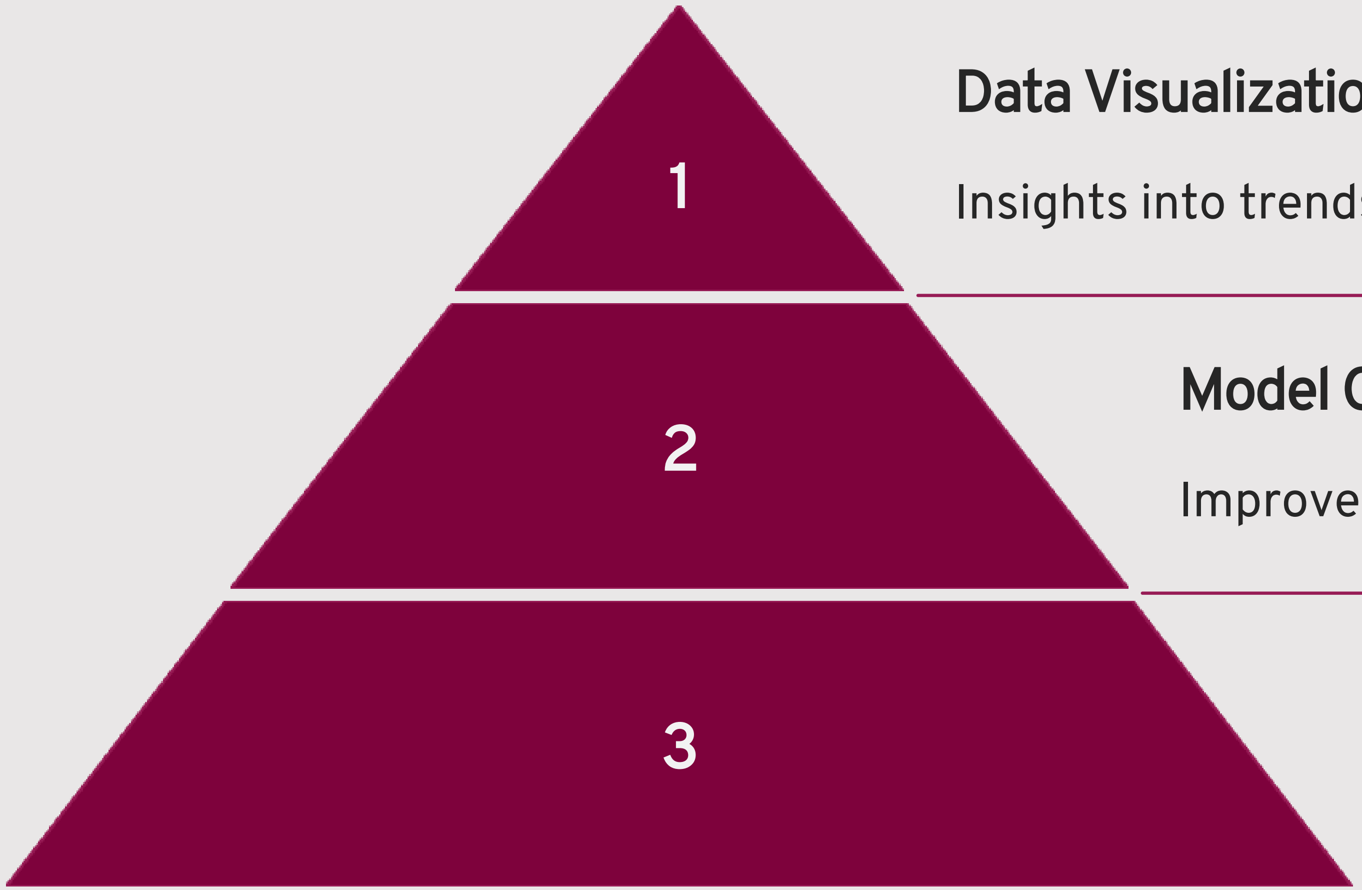
Future Directions and Implications



Data Visualization

Insights into trends and relationships

Model Optimization

Improved accuracy and efficiency

Real-World Application

Accelerated HEA design and development