# Study on Machine Learning for the Prediction of Tensile and Impact Properties of Aluminum Alloys by Incorporating Multi-Modal and Multi-Scale Information

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**Abstract:** Machine learning (ML) methods have played an increasingly important role in materials design. In this work, an explainable deep learning (DL) model was developed based on a multi-modal and multi-scale dataset for predicting the tensile properties of aluminum (Al) alloys. In addition, the internal mechanism of the model was analyzed by using a visualization technique. Further, a relationship of tensile property-impact property was established using a deep neural network (DNN) model. The correlation between tensile properties and impact properties was analyzed, providing scientific insight for the design of Al alloys with good comprehensive mechanical properties.

**Keywords:** machine learning; aluminum alloys; microstructure; tensile property; impact property

## 1 Introduction

By virtue of their high strength-to-weight ratio and high corrosion resistance, Al alloys are widely used in automotive industries. Recently, ML models have been incorporated to assist Al alloy design [1]. For instance, DL models, based on convolutional neural networks (CNN), can automatically extract features from images and analyze intricate correlations in high-dimensional data, which has been successfully used to predict tensile properties by compositions and microstructures [2].

Certain components in automotive applications are often exposed to dynamic impact loading during service life. Impact property [3], a measure of a material's ability to absorb energy and resist fracture under rapid loading, is a positive correlation both with ultimate tensile strength (UTS) and elongation (El). However, there is often a trade-off between UTS and El. Establishing the relationship model between tensile and impact properties can provide guidance for the design of Al alloys with good comprehensive mechanical properties.

In this work, we developed a DL model based on multi-scale microstructure information to predict the tensile properties. Then, by establishing a DNN model, the intrinsic connection between tensile and impact properties was further analyzed.

## 2 Experimental procedure

### Dataset construction

Al-7Si-0.35Mg alloys modified by adding 0.02wt.% Sr (ASr) and jointly modified by adding 0.02wt.% Sr and 0.1wt.% La (ASrLa) were prepared. The samples underwent solution treatment at 535 ℃ for 0-12 h, and then aging treatment at 170 ℃ for 0-24 h. To obtain the multi-scale microstructure information, optical microscope (OM) and scanning electron microscope (SEM) characterization were performed. Tensile testing and impact testing were conducted at ambient temperature. Finally, a “composition-microstructure-tensile property” dataset with 78 sets of data and a “tensile property-impact property” dataset with 41 sets of data was established.

### Construction of ML architectures

For the DL model, an OM image and an SEM image of each sample are combined as input to form the image features. The component information is input into the model to form text features. Then, the image and text features are spliced and trained together to predict the tensile properties. The architecture of the DNN model is “input layer-hidden layer 1-hidden layer 2-output layer”. The squared correlation coefficient ($R^2$) and mean absolute error (MAE) were used to evaluate the models' performance.

## 3 Results and discussion

### The relationship model of composition-microstructure-tensile property

For the UTS results of the DL model, the values of $R^2$ and MAE are 0.94 and 18.9 MPa, respectively. For the El result, the mean values of $R^2$ and MAE are 0.96 and 0.01%, respectively. The results indicate that the predicted values are in good agreement with the experimental values, demonstrating the model's high prediction accuracy.

To improve the interpretability of the DL model, the Gradient-weighted Class Activation Mapping (Grad-CAM) technique was applied. Grad-CAM can produce a heatmap in which regions with hotter spots indicate areas of the input image that contribute more to the prediction of the target value. The visual analysis of the DL model is performed using the SEM image of the ASrLa sample as an example (Figure 1). The results show a strong correlation between the UTS and the precipitates, as most of the hotspots coincide with the elliptical particles. This result proves that the visualization technology can reflect the mechanism knowledge learned by the DL model.

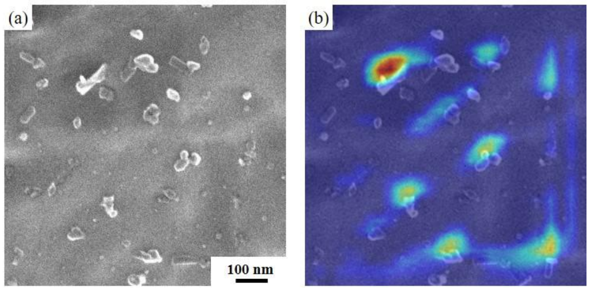


**Figure 1 The ASrLa sample: (a) original SEM image and (b) visualized results of UTS in stacked SEM image**

### The relationship model of tensile property-impact property

For the prediction results of the DNN model, the values of $R^2$ and MAE are 0.89 and 5.87 J, respectively. Figure 2 shows the 3D surface plot of the "UTS-El-impact property" predicted by the DNN model. Further, an analysis of the correlation between tensile properties and impact properties was carried out by calculating the sensitivity factors, which is the average partial derivative of the output with respect to the input. For solid solution state Al alloys, the sensitivity factors of UTS and El are -4.7 and 16.3, respectively. For aging state Al alloys, the sensitivity factors of UTS and El are 1.1 and 13.1, respectively. The results indicate that El has a stronger positive correlation with the impact properties of Al alloys compared to UTS. The relationship between UTS, El, and impact properties provides valuable insights for the design of impact-resistant Al alloys.

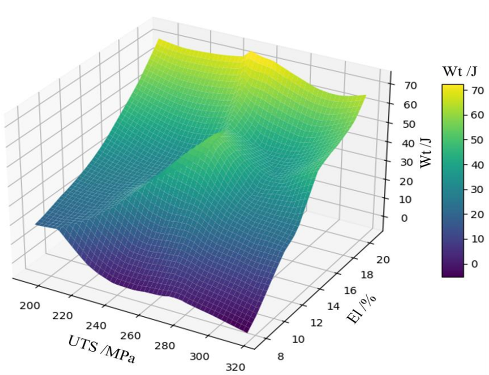


**Figure 2 The correlation results of "UTS-El-impact property"**

## 4 Conclusions

(1) The "composition-microstructure-tensile property" and "tensile property-impact property" relationship models were established using machine learning methods.

(2) The DL model can be used to comprehensively analyze the multi-scale microstructure information and the intrinsic mechanism was elucidated by visualization technology.

(3) The correlation between tensile properties and impact properties was analyzed, providing scientific insight for the design of Al alloys with good comprehensive mechanical properties.

## 5 Acknowledgment

The work was financially supported by Beijing Natural Science Foundation (L223001).

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