論 文 の 要 旨

題 目 Microstructural Classification of Al-Si Casting Alloys with Machine Learning Techniques

（機械学習技術による Al-Si 鋳造合金の微細構造分類）

氏 名 邱 子翔

The development of materials science experienced 4 paradigms, from experiments to model-based theoretical science, then computational science, or called simulations. And now, big data-driven materials informatics is becoming the 4th paradigm. Materials informatics can provide "inverse models" for design and optimization, which is the process of optimizing a property while adhering to certain restrictions. Using processing, composition, and structure to forecast the ultimate characteristic, materials informatics may also provide "forward models" for predictive analytics.

The analysis of microstructure is one of the most important parts in the characterization of metallic materials. Traditionally, the majority of microstructure characterization has been done manually by experts, which involves subjectivity-related uncertainties. With the development of computer technology in recent years, multiple intelligent image analysis techniques have emerged, providing new perspectives on microstructure analysis. In order to increase the precision and effectiveness of microstructure analysis in comparison to traditional approaches, numerous attempts have been made to classify and evaluate the microstructures using machine learning techniques and related technology.

Al-Si casting alloys are widely used for commercial applications mainly due to their low density and good mechanical properties. The Si-phase in the eutectic is plate-like of this alloy, which will lead to low mechanical properties. Usually, there are two ways to improve it. One is increasing the cooling rate, which could refine the size of all microstructural features, including eutectic Si-phase, secondary dendrite arm spacing (SDAS), and all the other intermetallic compounds. But the morphology is not changed. Sr modification as one of the most commonly used modification treatments could change the eutectic from plate-like into coralline-like structures, leading to an impressive increment of mechanical properties.

The final purpose of the present research is to develop a system that uses machine learning to analyze the interrelationships among processes, microstructures, and material properties. This study focuses on microstructural analysis with the help of machine learning techniques, in order to help improve the accuracy and efficiency of this process. In this study, we attempted to classify the microstructures of Al-Si casting alloy at different stages of the T6 heat treatment process, Al-Si alloy casting at different cooling rates, and after Sr modification treatment by machine learning techniques, and quantitatively analyze the morphology and distribution of eutectic Si-phase particles using our originally developed methods. The conclusions of this thesis are summarized as follows:

1. The study on microstructural classification of Al-Si casting alloy after aging treatment (Chapter 2).

A machine learning-based image classification technique was attempted to be applied to the classification of microstructures of Al-4 %Si-0.5 %Mg alloy at each stage of the T6 heat treatment process. A classification rate of 100% accuracy was obtained when comparing the microstructures from the casting and other T6 process stages. The feature values that contributed significantly to the classification were the average value and standard deviation of IMFP. This is because the solution treatment causes the eutectic Si-phase to become spherical that leading to the increase of the IMFP value, which is the free path length. In the case of classification using SVM, the classification rate was generally higher when statistical data were used. This is thought to be due to overlearning when the histogram data (frequency distribution of the features) is applied. Comparing the algorithms used for classification, the classification rate was higher when Random Forest was used as a classifier than SVM.

2. The study on microstructural classification of Al-Si alloy casting at different cooling rates (Chapter 3).

The Al-7%Si-0.3%Mg alloys were solidified in a copper mold at three different cooling rates. The microstructures of the samples were similar because of the approximate cooling rates, so originally developed machine learning-based image classification techniques were used to detect the difference between the microstructures of the samples. The mechanical properties of the three samples were slightly increased with the increase of cooling rates, proving the differences between the samples.

The classification of the microstructures was accomplished by using machine learning techniques, and high classification rates of about 80% to 90% were obtained. The classification rate was highest when using the statistical data and using SVM as classifier. Besides, the classification rate was higher when the difference of cooling rates of samples was bigger. In order to get the highest classification rate in shortest time, a suitable number of images for training was 60 to 80 during the machine learning process in this study.

3. The study on microstructural classification of unmodified and strontium modified Al-Si casting alloys (Chapter 4).

The Al-7%Si-0.3%Mg casting alloys (wt%) were solidified and modified with the additive of Sr. The microstructural classification of the samples and quantitative analysis of the eutectic Si-phase changes before and after modification were accomplished by machine learning-based image classification techniques. The large areas of eutectic-Si structure and finer eutectic-Si particles could be found in the microstructures of the samples after modification.

The classification rate of unmodified and 0.02% Sr modified samples reached the highest point of 97.5% accuracy when using the statistical data and SVM as classifier. The results of PCA shown that LN2DRvar was the first principal component during the classification, which indicated the importance of second phase distribution on differentiating the microstructures of the samples before and after the modification. The modification changed the arrangement of the eutectic-Si particles from random to clustering distribution, which lead to a significantly increment of LN2DRvar value.

The tensile properties of the samples were significantly increased after modification because of the refinement effect of Sr to the eutectic-Si phase. Therefore, the feature Diameter was negatively correlated to tensile properties. The feature LN2DRvar was the first principal component and increased with more addition of Sr, which reflected the distribution change of eutectic Si phase before and after Sr modification. However, it is still worth discussing and further investigating about why the increase of LN2DRvar lead to the enhancement of tensile properties.