Prediction of Onsager and Gradient Energy Coefficients from Microstructure Images with Machine Learning

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Introduction

Spinodal decomposition is a simple process of phase separation that is modeled by the **Cahn-Hilliard equation**.[1] Parameters such as the **Onsager coefficients** and **gradient energy coefficient** affect the rate of separation, and they can be very difficult to estimate with experimentation.[2] As an alternative, **machine learning** can be used to estimate these parameters without the need for costly experiments. Therefore, the goal of this work is to estimate material parameters for the spinodal decomposition of an **FeCrCo alloy** using a database of microstructure images.

Background

Spinodal Decomposition

- Spinodal decomposition is the **separation** of a uniform mixture of elements into regions of unique phase compositions[2]
- For FeCrCo, this process occurs between 850 and 970 K (Fig. 1)[1]

Figure 1: *Spinodal decomposition of FeCrCo at 950 K, showing high Fe composition as red and low Fe composition as blue.*

Cahn-Hilliard (CH) Equation

$$\frac{\partial c_i}{\partial t} = \nabla \cdot \left(M_{ii} \nabla \frac{\partial G_{sys}}{\partial c_i} + M_{ij} \nabla \frac{\partial G_{sys}}{\partial c_j} \right)$$

- The CH equation (above) uses the **phase field method** to describe the change in composition of an element over time[2]
- Phase decomposition occurs in order to attain a **minimum** in total Gibbs free energy (G_{sys})[1,2]

$$G_{sys} = \int_r \left[G_c + \frac{1}{2} \kappa \sum_{i=1}^{3} (\nabla c_i)^2 \right] dr$$

- Compositions: c_1 is Fe, c_2 is Cr, and c_3 is Co
- Free energy density: G_c
- Onsager coefficients (mobilities): $M_{22}, M_{23}, M_{32}, M_{33}$
- Gradient energy coefficient: κ

Parameter Ranges

- M_{ij} and κ are assumed to be **independent** of composition
- Ranges for M_{ij} and κ were determined based on the values that promote spinodal decomposition

Table 1. *Ranges for each parameter in which separation occurs.*

Parameter	Minimum	Maximum
M_{22}	2.5e-28	2.5e-24
M_{23}	No effect	
M_{33}	No effect	
κ	1.0e-15	1.0e-13

Database Generation

- A database of 573 microstructure images was generated by simulating the spinodal decomposition of FeCrCo at 873 K with an atomic composition of 46% Fe, 31% Cr, and 23% Co (the experimental conditions used in Okada et al.)[3]
- The simulations were conducted using the **Multiphysics Object-Oriented Simulation Environment (MOOSE)**, which utilizes the finite element method to solve the CH equation
- The inputs to the simulation were 1035 combinations of M_{22} and κ within the determined ranges
- Microstructure images were extracted after 100 hours of decomposition using **Paraview** (Fig. 2), and the images that showed less than 0.05 units of separation for c_1 were removed

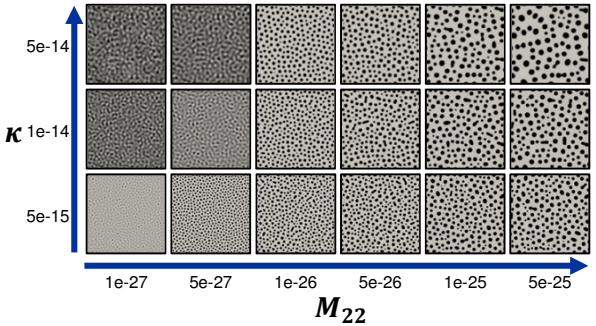
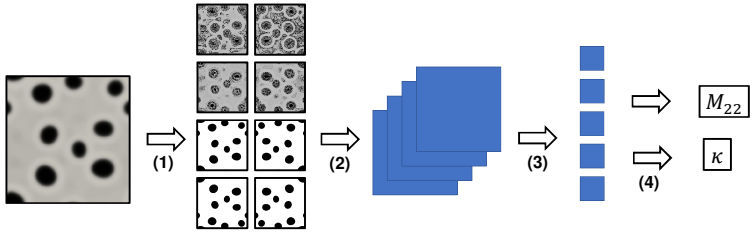


Figure 2: *Representative microstructure images of FeCrCo after 100 hours of decomposition at 873 K, showing high Fe composition as light and low Fe composition as dark.*

Model Development

- **TensorFlow** was used to compile a machine learning model that extracts the features from each microstructure image to predict M_{22} and κ
- A 70-30 train-test split was utilized with an input image resolution of 128 × 128 pixels
- The model was trained for 4,000 epochs with the Adam optimizer, a batch size of 8, a learning rate of 1e-3, and a learning rate decay of 5e-6 per batch[1]



1. Augmentation & Preprocessing	2. Convolution & Pooling Layers (x3)	3. Flatten	4. Dense Layers
• Horizontal reflection • Vertical reflection • Inversion through origin • Binarization • Min/max scaling	• Convolution (3x3) • Batch normalization • Max pooling (2x2) • Repeated with 16, 32, and 64 filters		• Dense (256) • Batch normalization • Dropout (0.5) • Dense (64, 16, 8, 2)

Results

- On average, the M_{22} prediction was **6.4%** different and the κ prediction was **2.5%** different from actual
- Predictions for both parameters were very accurate and precise throughout their respective ranges (Fig. 3)

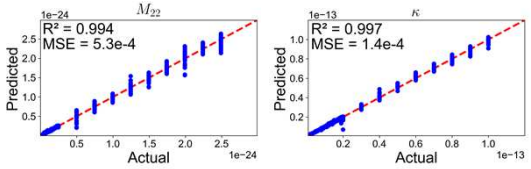
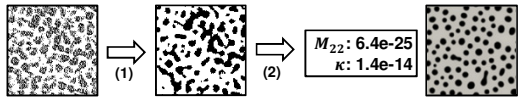


Figure 3. *Parity plots for M_{22} (left) and κ (right).*

TEM Image Analysis

A total of 17 experimental **transmission electron microscopy (TEM)** images from Okada et al. were preprocessed by binarization and noise reduction **(1)**, and then put into the machine learning model **(2)** to estimate the parameters.[3] A corresponding image from MOOSE with the estimated parameters (right) is displayed for comparison.



Conclusions

- Machine learning was used to estimate M_{22} and κ for images in the test dataset with high accuracy and precision
- The TEM image predictions were inconsistent, illustrating how multiple parameter combinations can yield similar microstructures
- Future work should confirm the model's accuracy using newer, higher-resolution TEM images with known parameter values

References

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