Material Parameter Estimation from Microstructure Morphologies with Machine Learning

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I. Introduction

The application of machine learning in predicting the initial parameters of phase-field models is beneficial in understanding the spinodal decomposition of metal alloys. It enables the characterization of the microstructural variables that affect the transition of an alloy from a single phase to two unique phases. An evaluation of the prediction model will then give the accuracy of the results.

II. Background

As an alloy experiences heat stress over an extended period, the alloy's composition begins to change. This process is known as Spinodal Decomposition, the spontaneous separation of a single thermodynamic phase into two unique phases. A solution, or in this case a metal alloy containing Iron and Chromium, starts out with evenly distributed concentrations of its components. As the alloy goes through Spinodal Decomposition, we no longer see one distinct concentration, but the emergence of areas of two unique concentrations. The Cahn-Hilliard equation is an important component in understanding this phenomenon. This equation describes the phase separation mathematically.

$$\frac{\partial c}{\partial t} = \nabla \cdot M(c) \nabla \left(\frac{\partial f_{loc}(c)}{\partial c} - \kappa \nabla^2 c \right)$$

Figure I: Cahn-Hilliard Equation

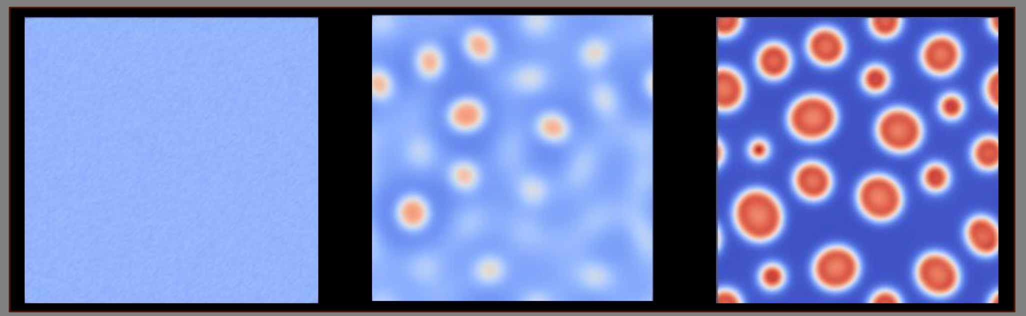

Figure II: Images depicting Spinodal Decomposition

III. Methods

With the application of the physics-based software, MOOSE, accurate images replicating the process of spinodal decomposition were created using the Cahn-Hilliard Equation with controlled initial parameters. The initial concentration was set to be forty percent Chromium and the phase separation was tracked over a one-hundred-hour time period at five-hundred degrees Celsius. This ran one-hundred different times with varying kappa and mobility values which are expressed in the Cahn-Hilliard equation. The data collected from these runs, the images along with the recorded kappa and mobility values, are then ready for analysis through a neural network built using TensorFlow.

Due to the relatively small number of images generated, the use of transfer learning to build our convolutional neural network (CNN) was necessary to produce reliable results. EfficientNetB7 was used to generate the initial layers of our network, then trained more convolutional and fully connected layers to better improve results. The network teaches itself to predict the kappa and mobility values based on the images, using the dataset to check itself. From there we can determine the accuracy of the network.

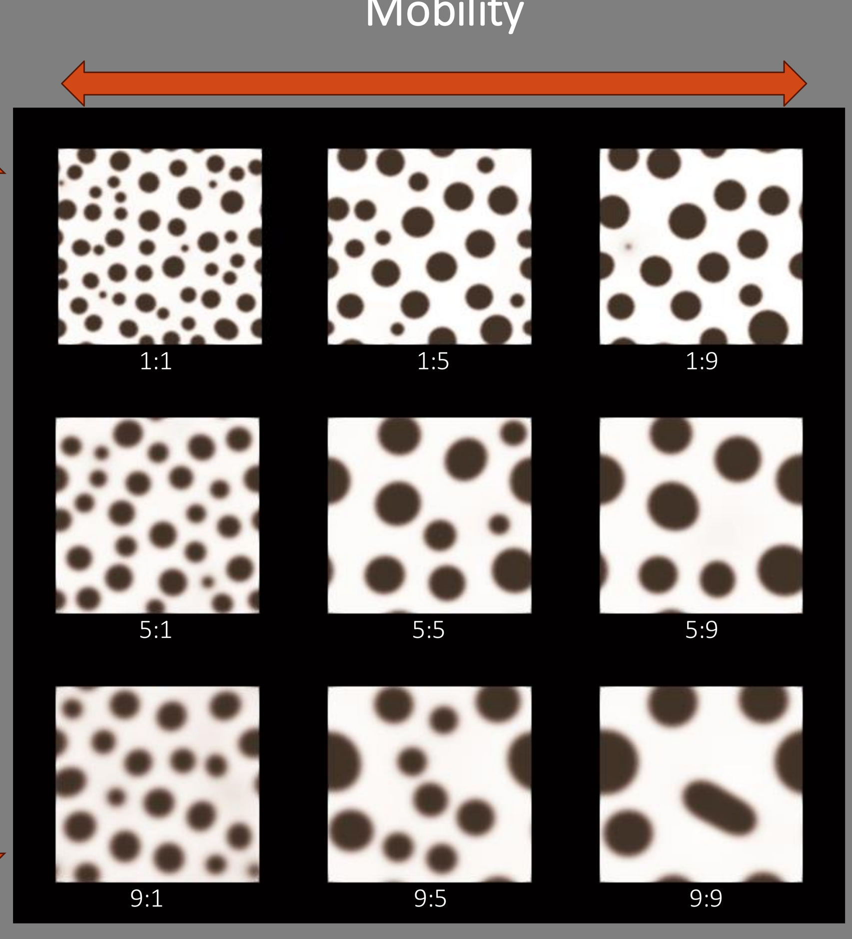

Figure III: Selection of images that show the trends of Mobility and Kappa

IV. Results

kappa accuracy:
R-squared: 0.9894004648111793
MSE: 0.08560891254170902

mob accuracy:
R-squared: 0.9760375872254436
MSE: 0.2155521535867542

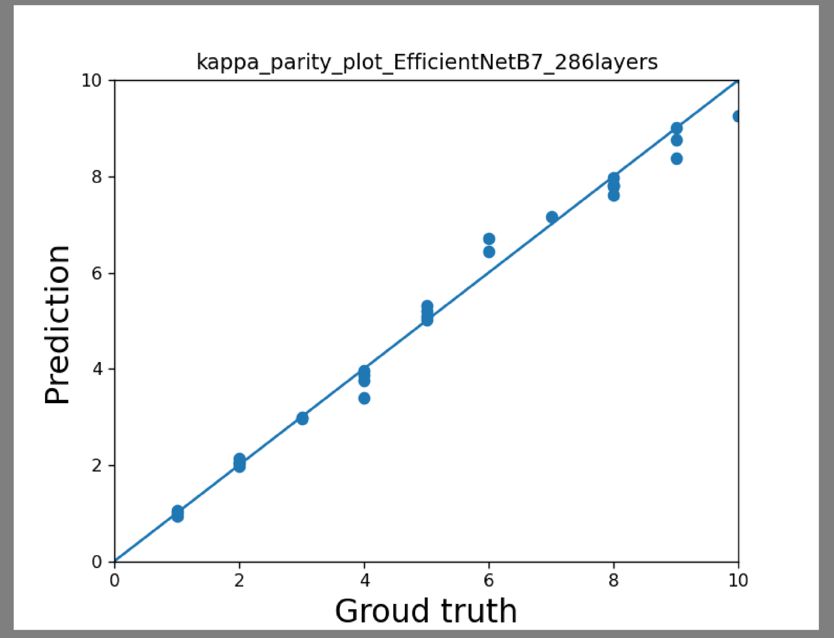

Figure IV: Parody plot of the kappa prediction accuracy

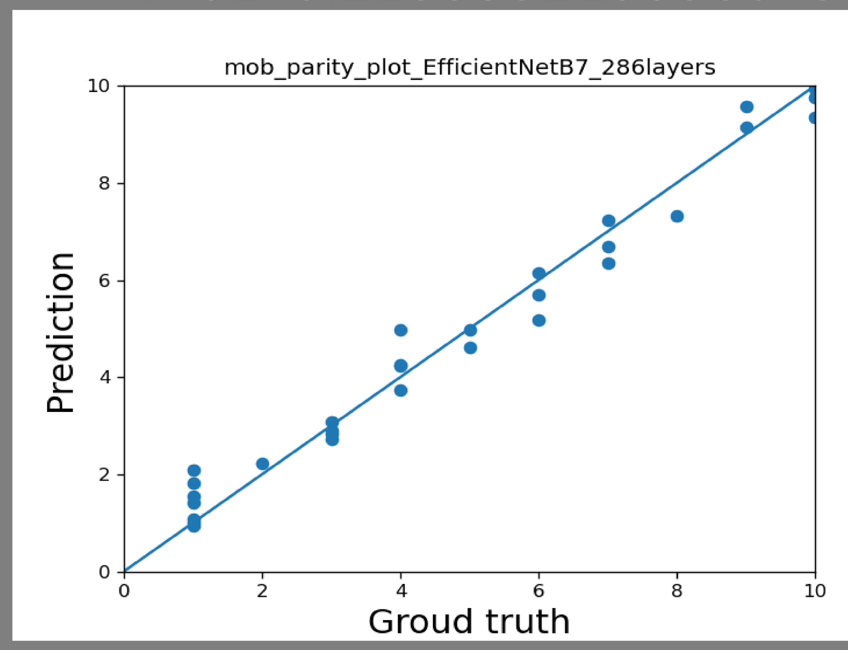

Figure V: Parody plot of the mobility prediction accuracy

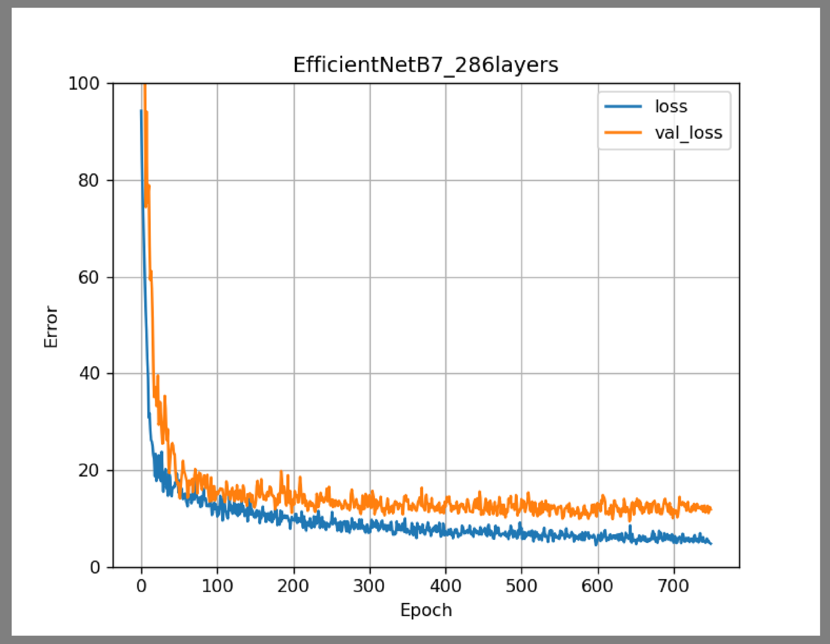

Figure VI: Error graph of the training and test data

V. Discussion

The results show that the neural network was able to successfully predict the kappa and mobility values associated with the phase-field models. The data was also not overfit, which means the model was not only effective at predicting the training data, but the test data as well. Machine learning is a viable option in analyzing and understanding spinodal decomposition

VI. Acknowledgements

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