Materials Parameter Estimation from Microstructures with Deep Learning: Thermodynamic Parameters Database Generation

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Background:

- FeCrCo undergoes spinodal decomposition between 850-970K at 46% Fe, 31% Cr, and 23% Co [1]
- FeCrCo alloys can be simulated with different chemical and physical parameters
- Machine learning can be a useful tool for predicting parameter from microstructure images
- **Cahn-Hilliard Equation**[2]

$$\frac{\partial c_i}{\partial t} = \nabla \cdot \left(\sum_{j=2}^{3} M_{ij} \nabla \frac{\delta G_{sys}}{\delta c_j} \right), \quad i = 2, 3.$$

Total Free Energy of FeCrCo[2]

$$G_{sys} = \int_{\mathbf{r}} \left[G_c + \frac{1}{2} \kappa_c \sum_{i=1}^{3} (\nabla c_i)^2 \right] d\mathbf{r}$$

- **The Gibbs free energy of α phase in a Fe-Cr-Co system**[2]

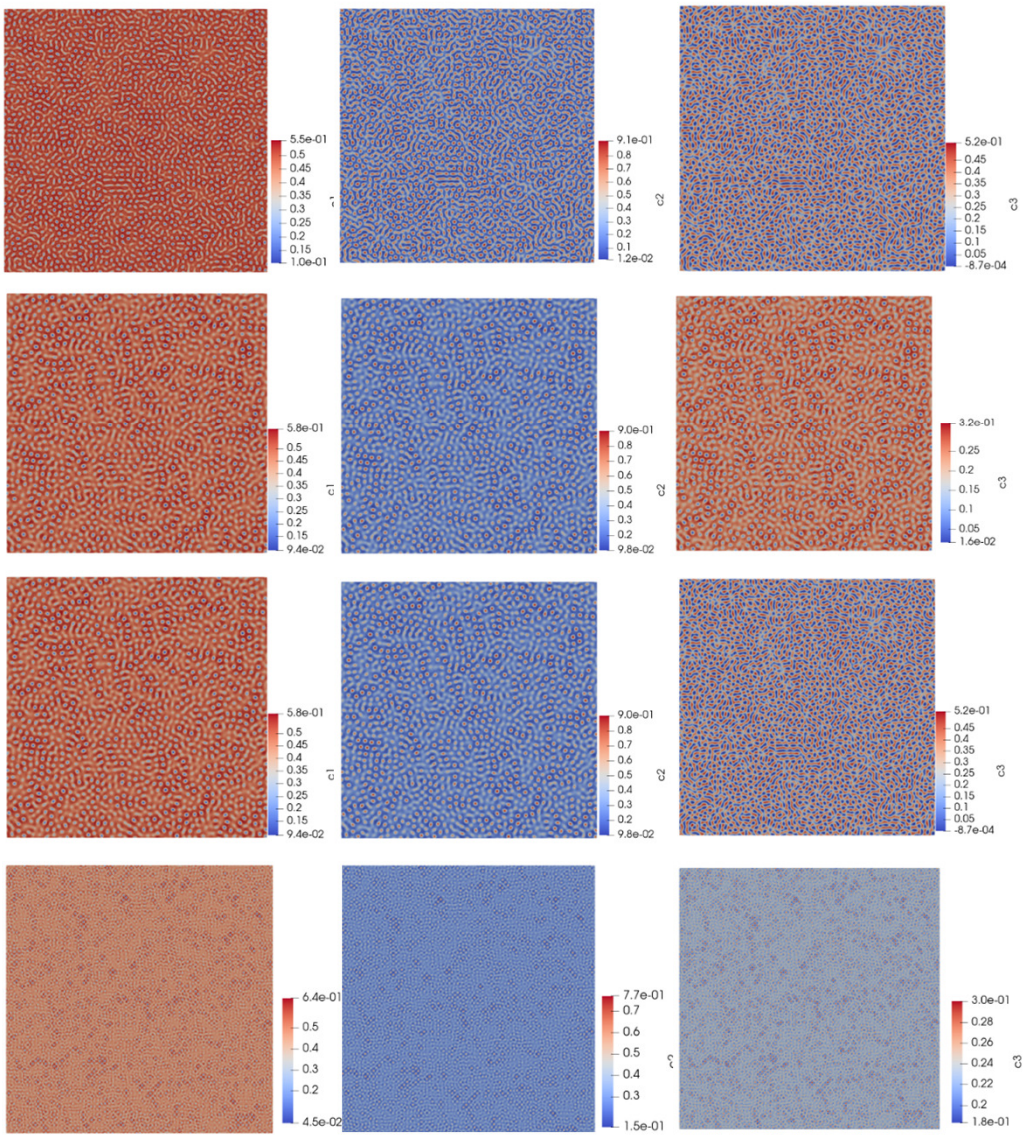
$$G_c^{\alpha}(c_i, T) = \sum_{i=1}^{3} {}^{\circ}G_i^{\alpha} c_i + RT \sum_{i=1}^{3} c_i \ln c_i + {}^{E}G^{\alpha} + {}^{mg}G^{\alpha}$$

Current Research Goal:

- Simulate the interaction parameters in excess free energy that result in spinodal decomposition and the change of the microstructure morphology

Proposed Solution:

- We plan to continue database generation for a wider combination of parameters



Method : Simulate the microstructure evolution ofFeCrCo alloy using interaction parameters in excess free energy using:

MOOSE

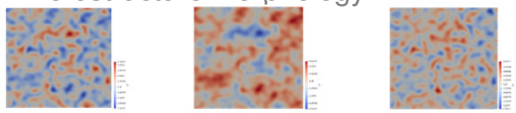
An open-source, parallel finite element framework developed by INL

ParaView

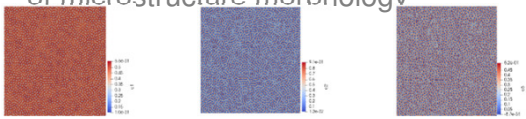
Open-source data analysis and visualization tool

Results:

- Homogenous changes in interaction parameters do not change the microstructure morphology.



- Heterogeneous changes in interaction parameters do result in changes the of microstructure morphology



The range was selected to be 0.1 - 10 x

Future Work:

- Use images in a Convolutional Neural Network to predict thermodynamic parameters based on microstructure morphologies
- Apply machine learning to other metal alloys
- Explore the different parameters between the range of 0.1 X-10 X

References

[1]Okada, M., Thomas, G., Homma, M., & Kaneko, H. (1978). Microstructure and magnetic properties of spinodal Fe--Cr--Co Alloys. IEEE Transactions on Magnetics, 14(4), 245–253. https://doi.org/10.2172/6627188
[2]Koyama, T., & Onodera, H. (2004). Phase-field simulation of phase decomposition in fe–cr–co alloy under an external magnetic field. Metals and Materials International, 10(4), 321–326. https://doi.org/10.1007/bf03185980

Acknowledgements

This work was supported by the National Science Foundation via the Research Experience for Undergraduates Site: Materials for Society (Award No. 1950305)
Thank you Dr. Rick Ubic for this Opportunity