Phase-field modeling of corrosion in alloys

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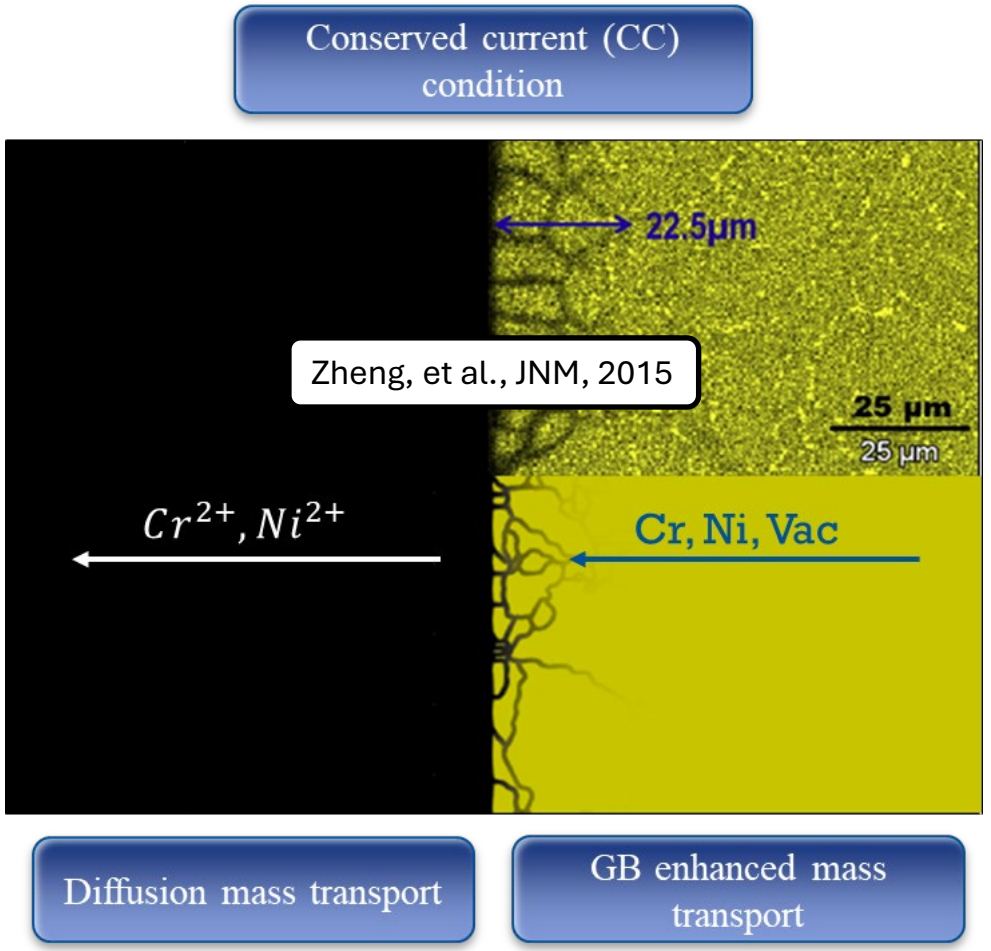
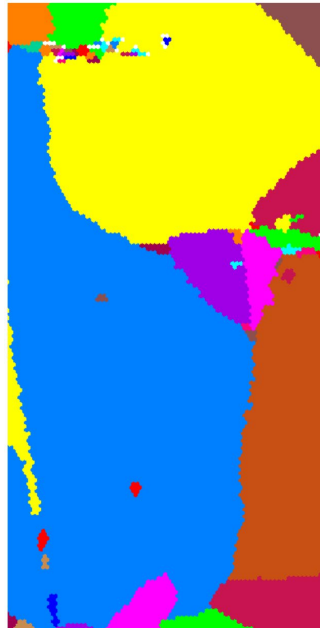
MSR Annual Campaign

Phase-field modeling molten salt corrosion

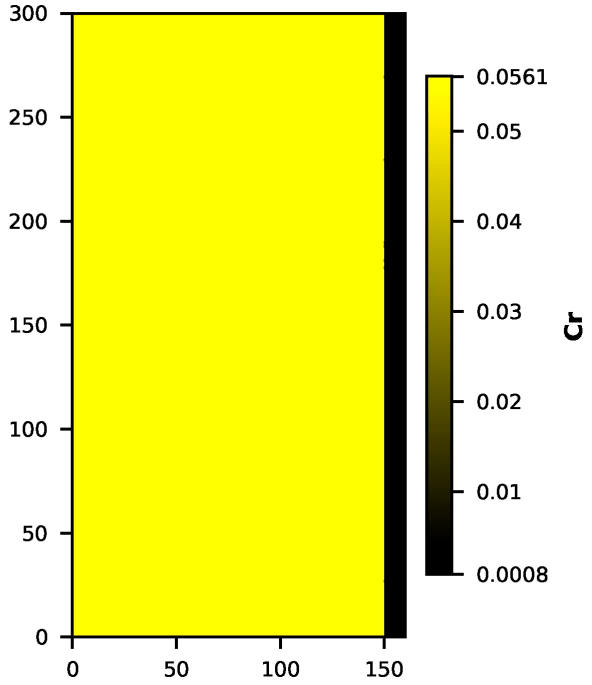
- Molten salt corrosion is driven by chemical potential gradients for structural alloy elements between metal and salt
- Diffusion of components in alloy is enhanced on grain boundaries
- At the interface, we enforce the conserved current condition to ensure charge conservation



We can simulate corrosion directly on characterized microstructures

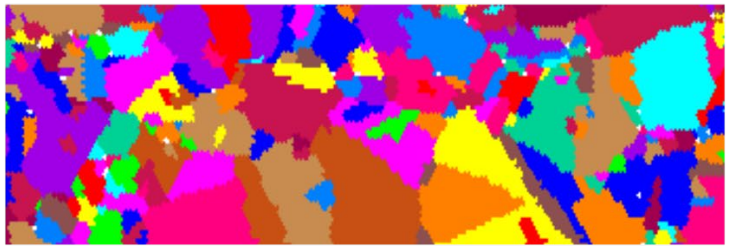


EBSD

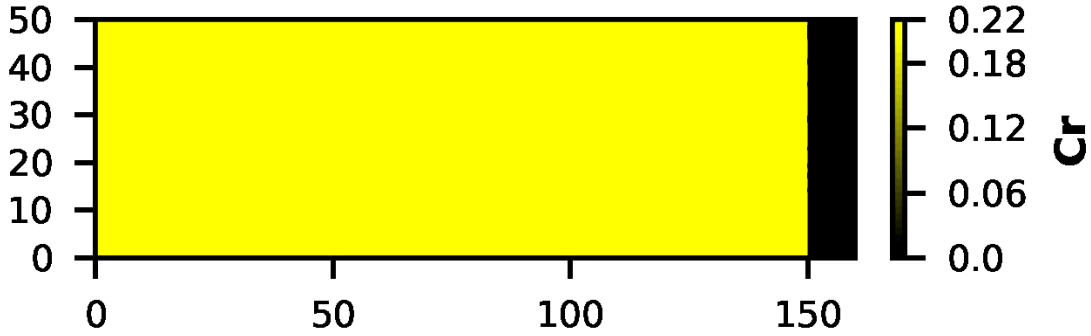


Simulation

Cr depletion in Ni-5Cr alloy



EBSD

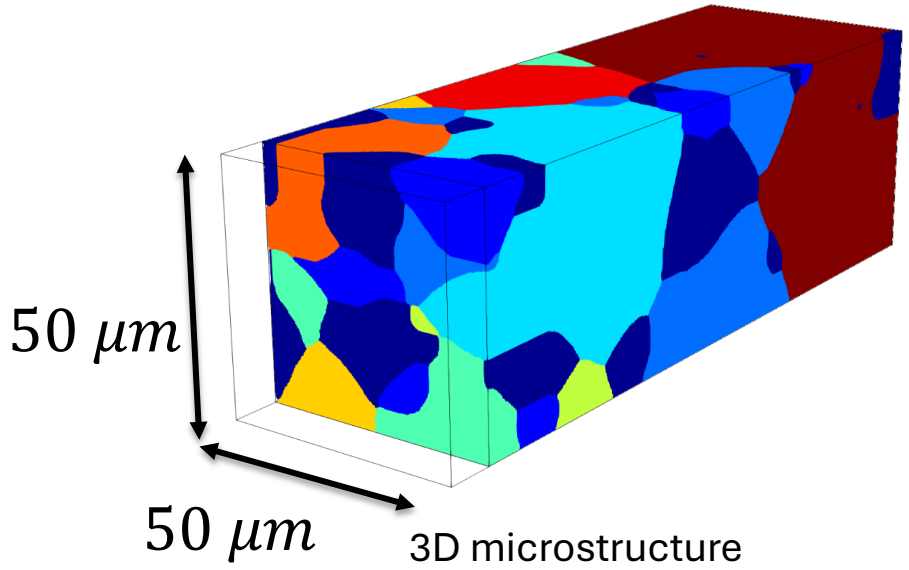


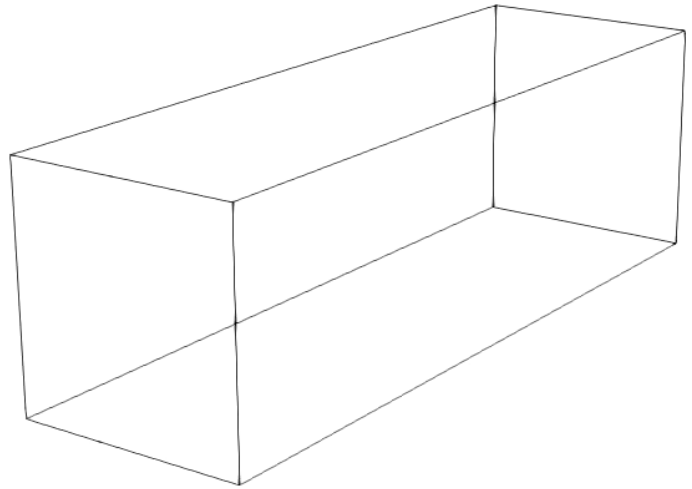
Simulation

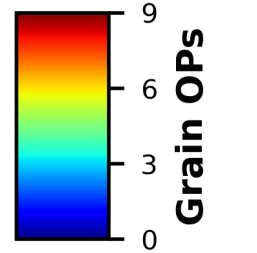
Cr depletion in Ni-20Cr alloy

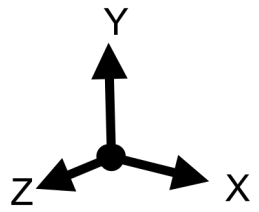
Chaitanya Vivek Bhave, Guiqiu Zheng, Kumar Sridharan, Daniel Schwen, Michael R Tonks, An electrochemical mesoscale tool for modeling the corrosion of structural alloys by molten salt, Journal of Nuclear Materials (2023)

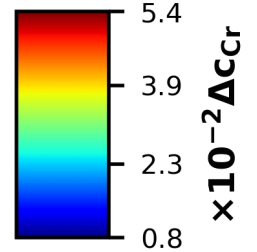
3D simulations most accurately account for the microstructure











DREAM.3D
BlueQuartz Edition

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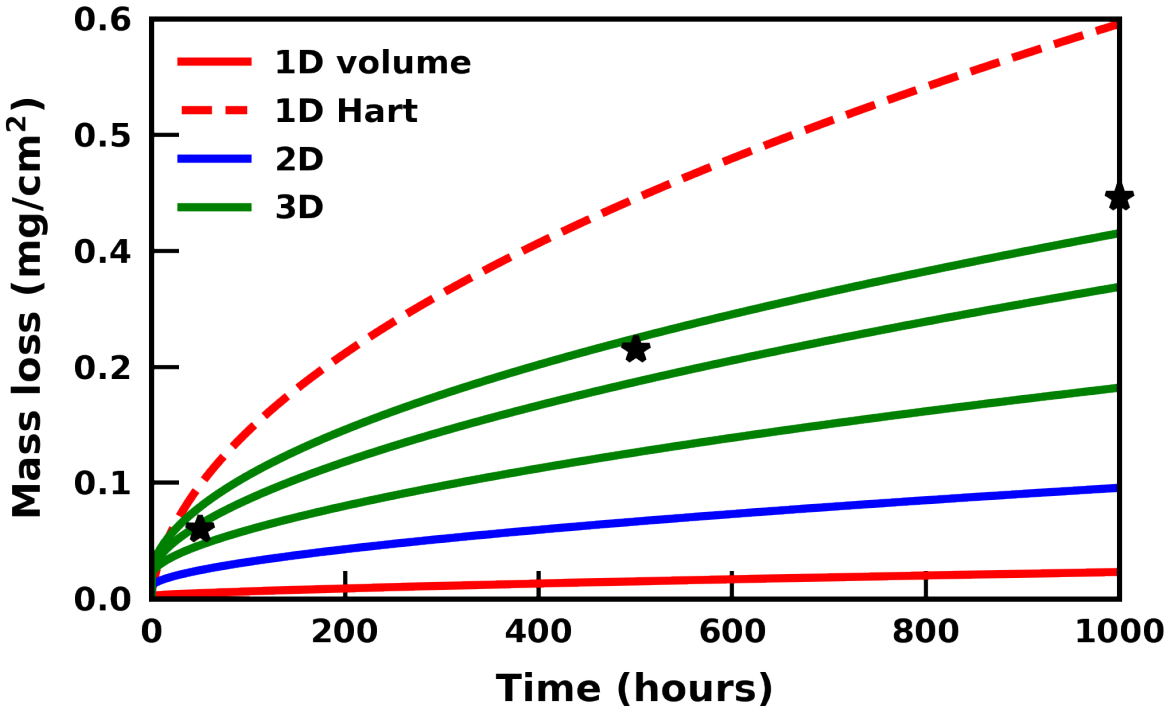
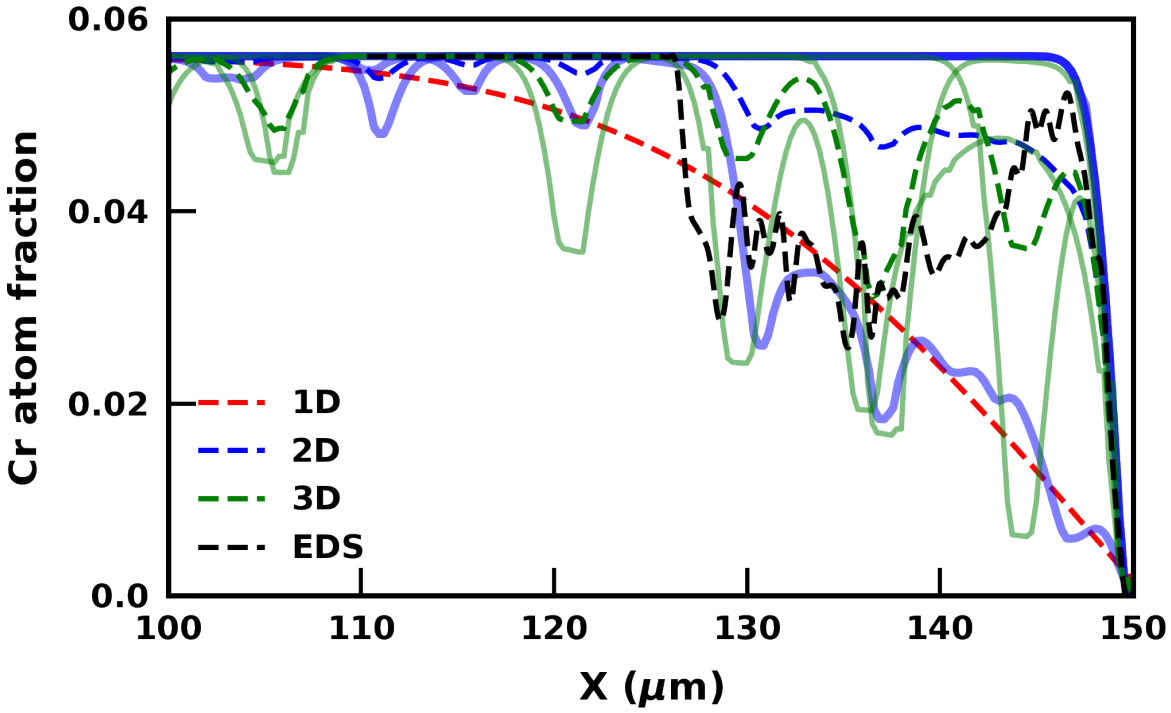
The phase-field model has been validated against experiments for Ni-Cr alloys



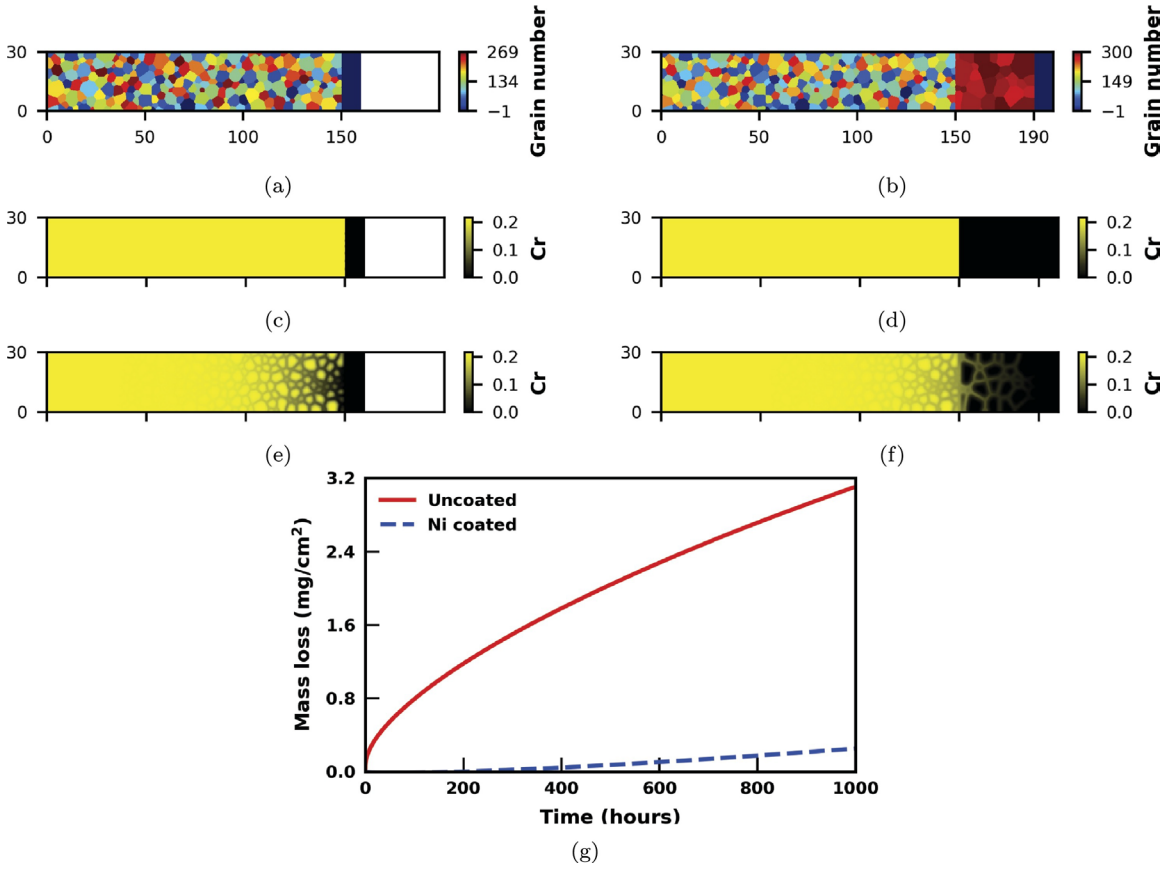
Mass loss comparison



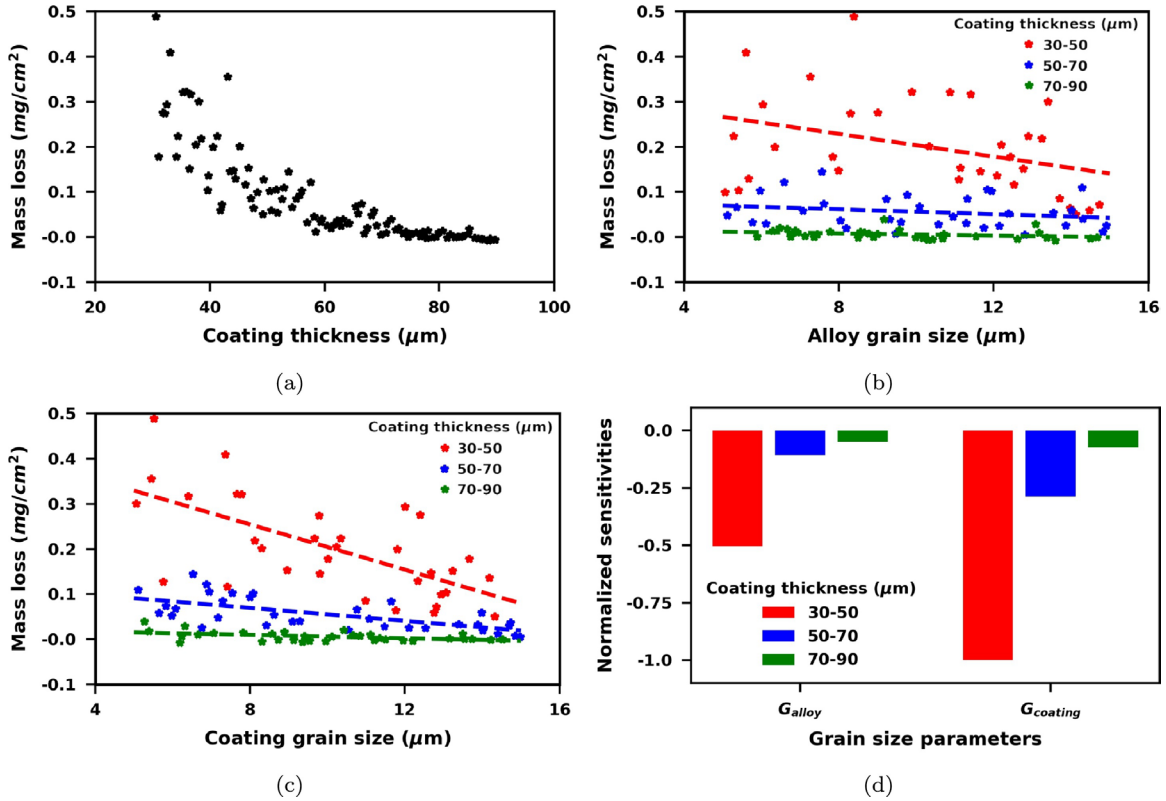
Cr depletion line plot

Chaitanya Vivek Bhave, Guiqiu Zheng, Kumar Sridharan, Daniel Schwen, Michael R Tonks, An electrochemical mesoscale tool for modeling the corrosion of structural alloys by molten salt, Journal of Nuclear Materials (2023)

We can model inert diffusion barrier coatings for corrosion



Ni-coated versus uncoated microstructure corrosion



Latin Hypercube Sampling (LHS) study on effect of Ni-coating parameters on corrosion

Chaitanya Bhave, Michael Tonks, *The effect of nickel coatings on corrosion of nickel-chrome alloys in molten FLiBe determined using a phase-field model*, Journal of Nuclear Materials (2025)

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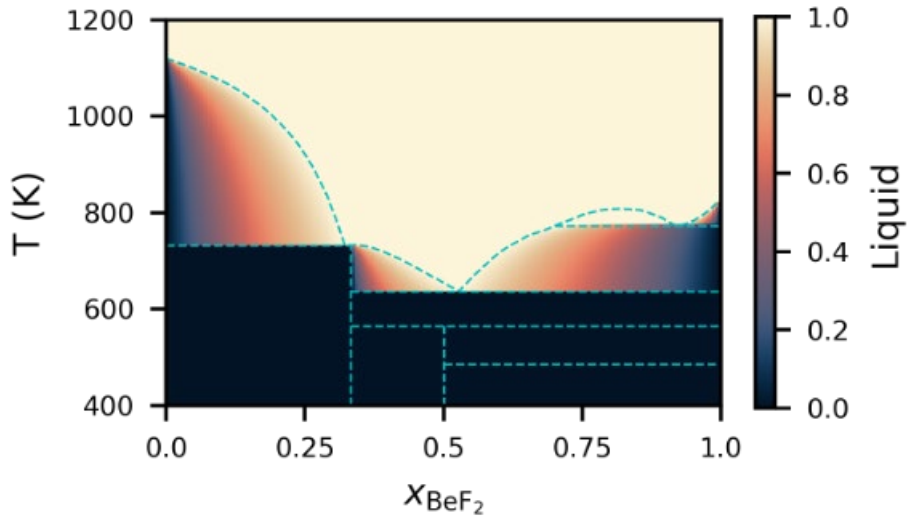
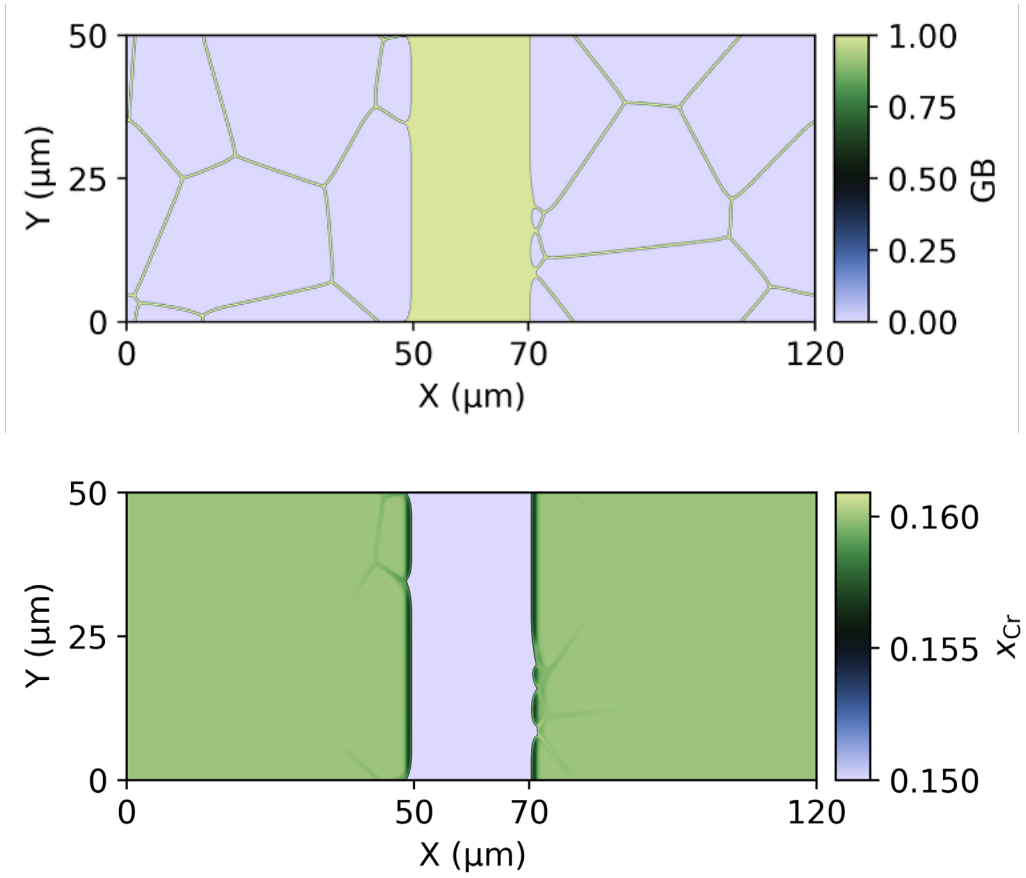
How do we model engineering alloys?

- Moving models towards large multicomponent systems
  - Started with ternary systems last year
- Coupling with MSTDB-TC for thermodynamics



ML surrogate for rapid evaluation of thermodynamics



Cr depletion in Fe-Ni-Cr alloy phase-field model

Summary and outlook

What we have achieved

- **Validated phase-field framework** for molten salt corrosion in Ni-Cr alloys, with direct comparison to experimental mass loss and Cr depletion profiles
- **2D and 3D microstructure-faithful simulations** using EBSD-characterized grain structures, capturing grain boundary-enhanced diffusion
- **Ni-coating barrier model** with Latin Hypercube Sampling sensitivity study quantifying coating thickness and composition effects
- **Ternary Fe-Ni-Cr extension** with MSTDB-TC thermodynamic coupling, moving toward engineering alloy compositions

Future directions

- Extend beyond ternary to quaternary and commercial alloy compositions (Hastelloy N, 316SS) with automated CALPHAD coupling via MSTDB-TC
- Deploy trained ML surrogate to replace costly CALPHAD calls, enabling high-throughput parametric sweeps across composition space
- Broader validation campaign with full uncertainty quantification (UQ) of models

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