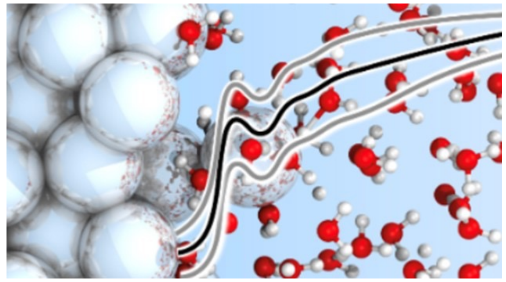


Bridging the Gap: Transitioning from Deterministic to Stochastic Interaction Modeling in Electrochemistry

Phase-Field Modeling of Microstructural Evolution Resulting from Corrosion

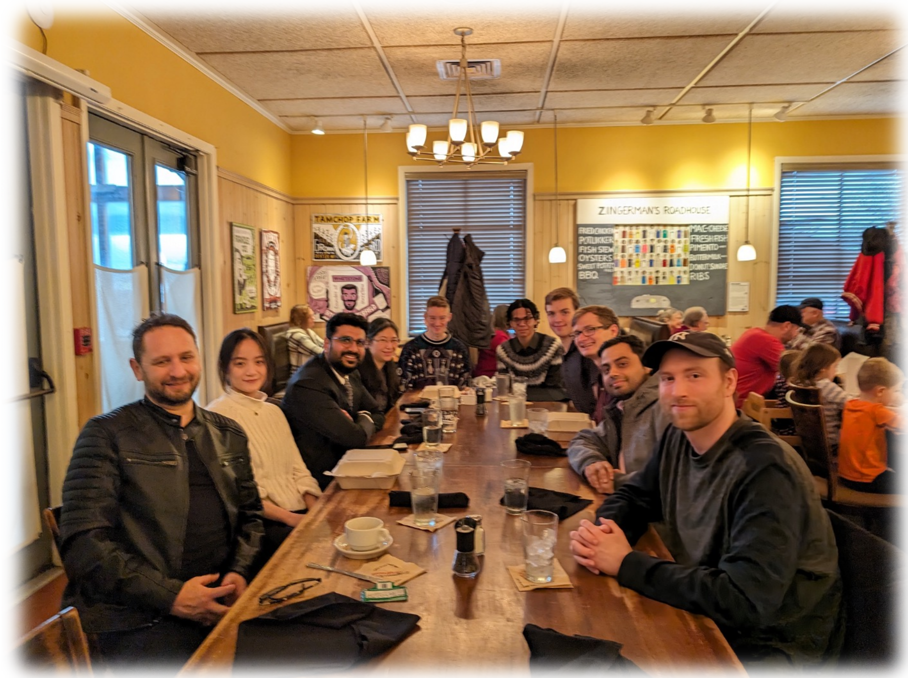
Katsuyo Thornton

University of Michigan

Acknowledgments

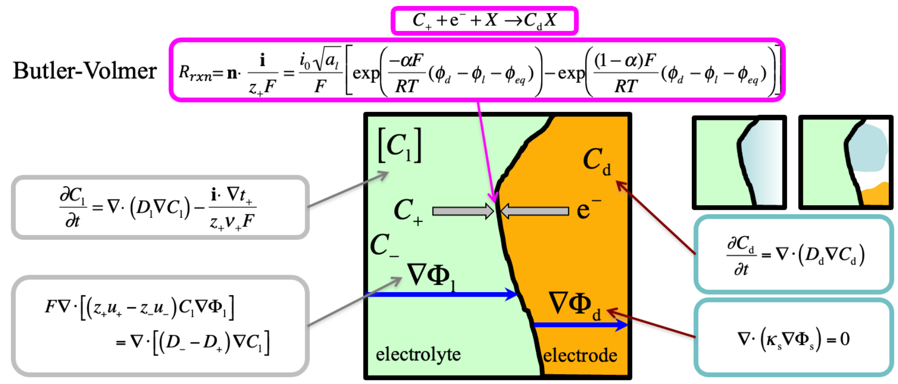
Funding: Molten Salt in Extreme Environment (MSEE) EFRC
Center for PRedictive Integrated Structural Materials Science (PRISMS)
Computational Resources: NSF XSEDE/ACCESS, DOE NERSC, UM ARC

Students & Postdocs (*Alumni):
Beck Andrews, Vishwas Goel (industry)*, Ellery Hendrix, Steve DeWitt (ORNL)*, and Alex Chadwick (NRL)*
Collaborators: David Montiel (PRISMS), Karen Chen-Wiegart (Stony Brook/BNL)

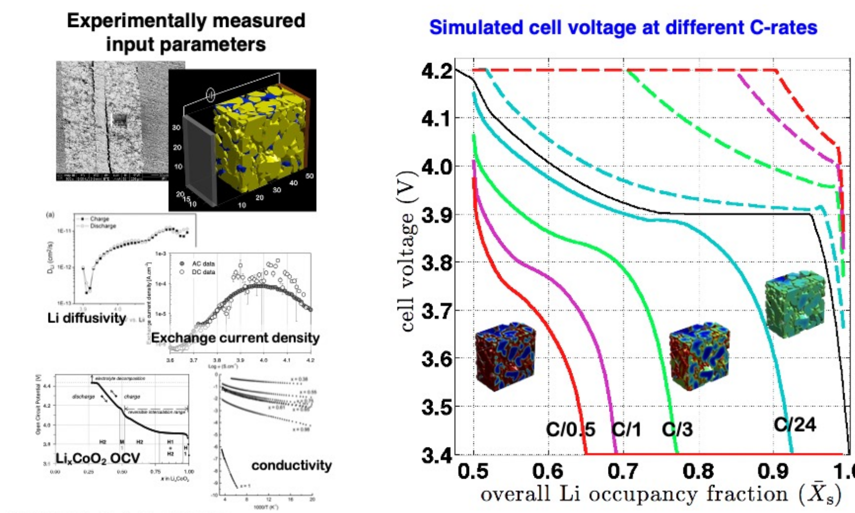


Thornton IPAM Talks So Far

- Tutorial 1: The Role of Materials and Microstructures in Electrochemical Energy Storage Part 1
- Tutorial 2: The Role of Materials and Microstructures in Electrochemical Energy Storage Part 1
- Hands-On Session
- Today: Corrosion & Microstructural Evolution



John Newman and Karen E. Thomas-Alyea. Electrochemical Systems. Wiley Inter-Science, third edition, 2004.



[1] H. Xia *et al.*, *Electrochim Acta* (2007)
[2] P. J. Bouwman, Ph.D. Thesis (2002); [3] D. Carlier *et al.*, *J Electrochem Soc* (2002)

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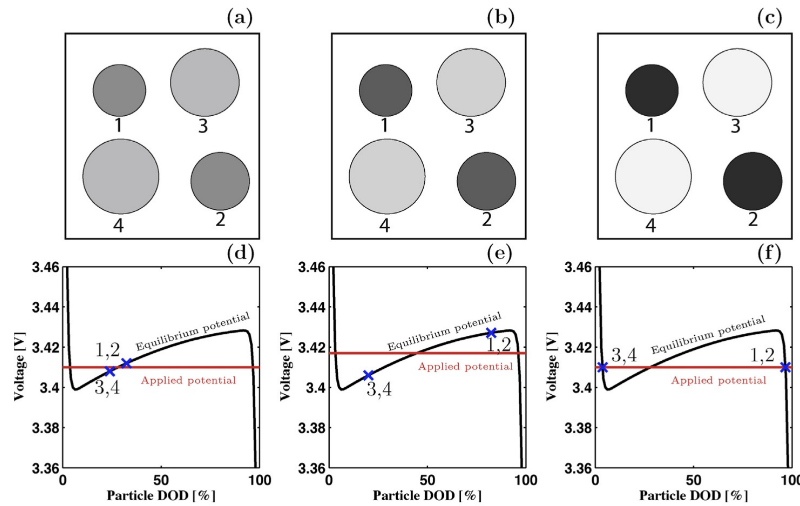

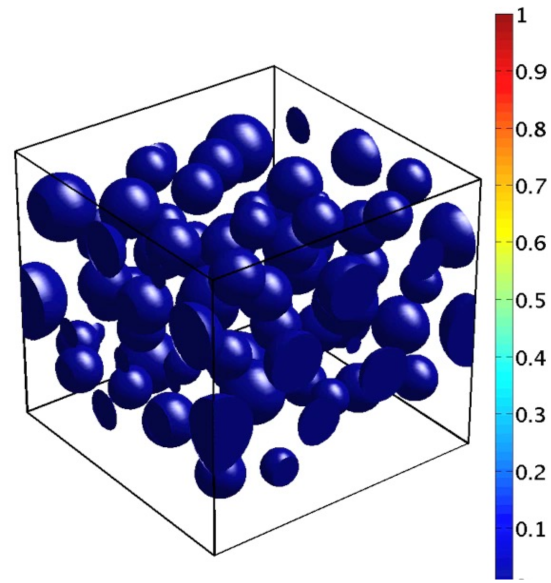

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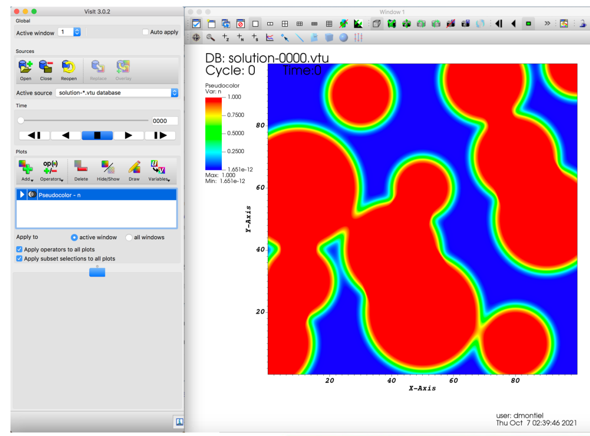
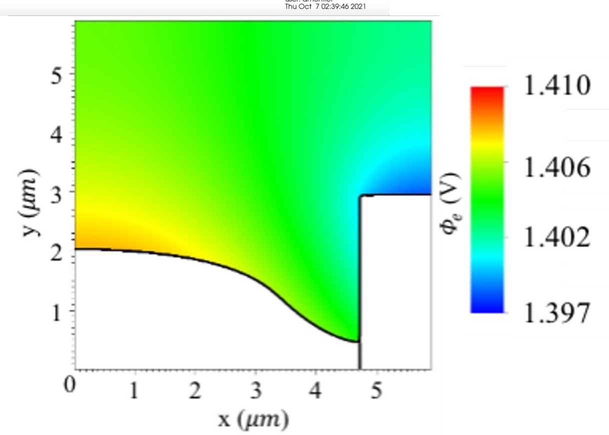
An Open-Source Phase Field Modeling Framework





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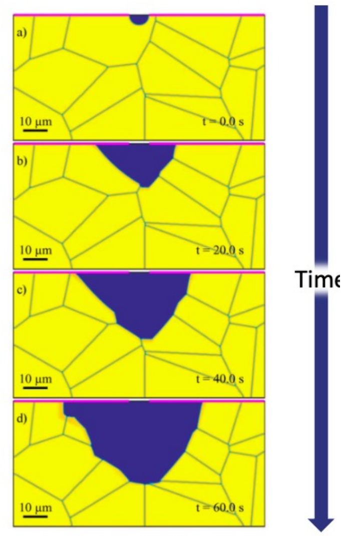

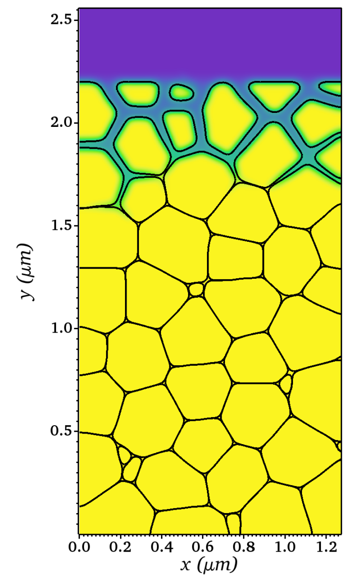

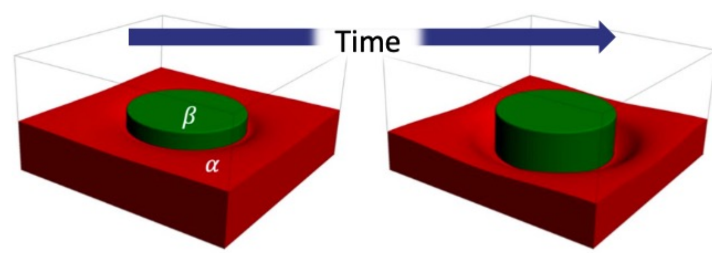

Microgalvanic corrosion

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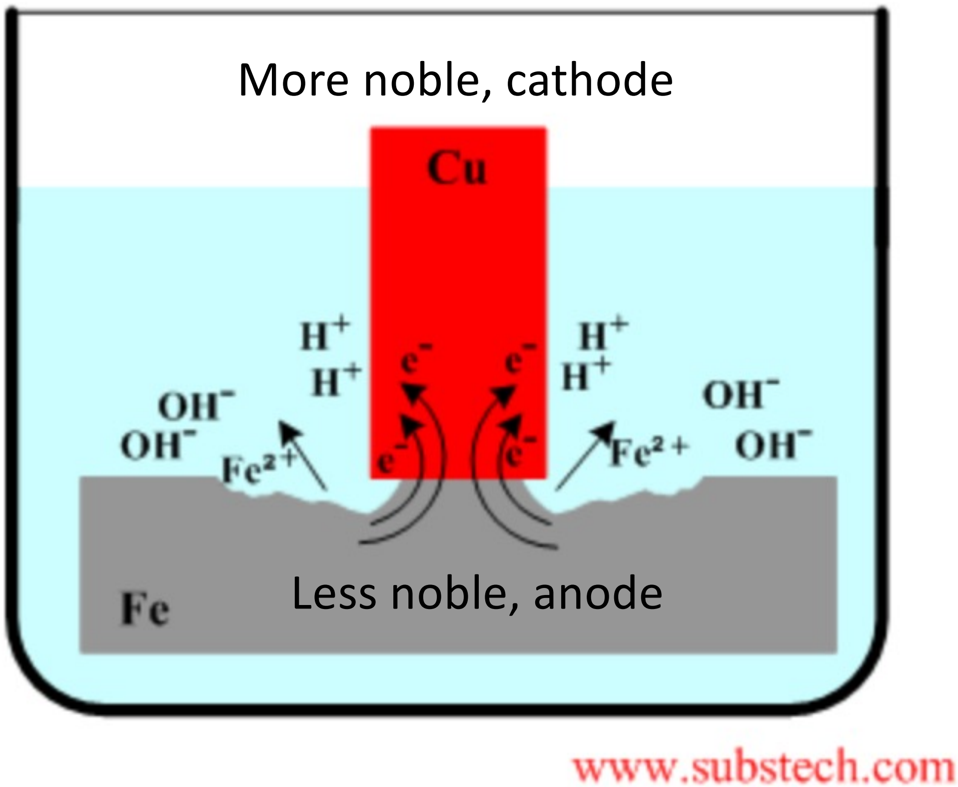
What is Galvanic Corrosion?



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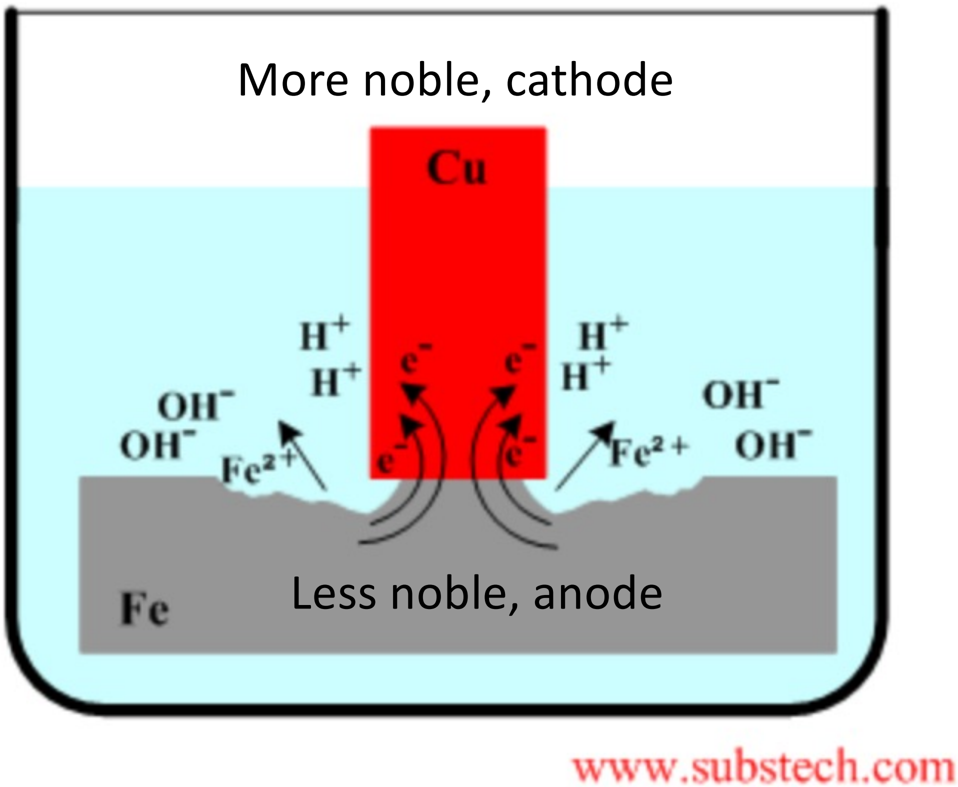
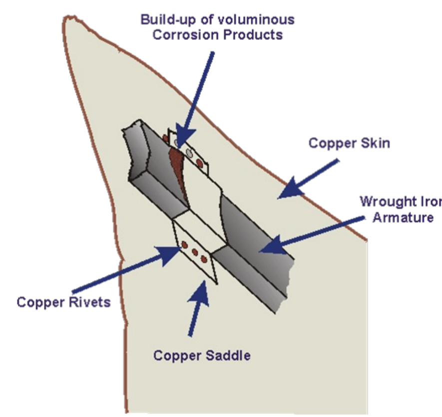
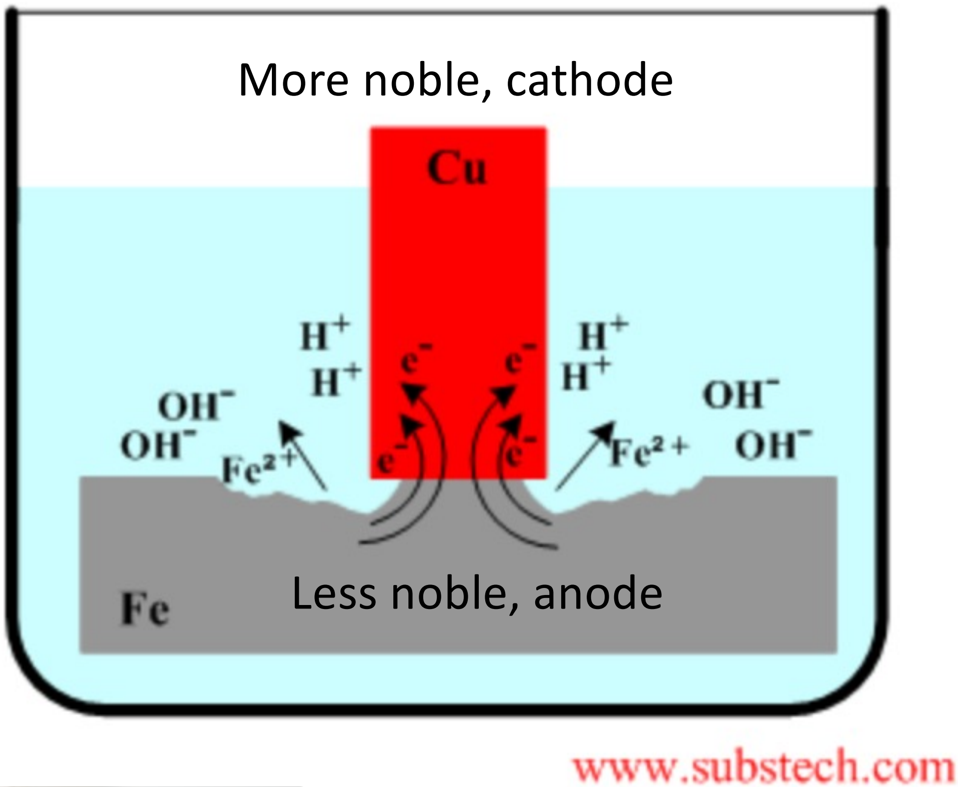


Source: Public domain

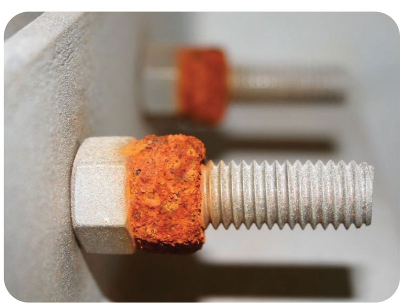


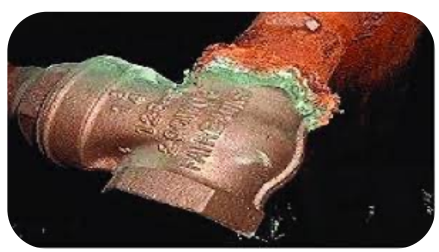
Source: Public domain

What is Galvanic Corrosion?

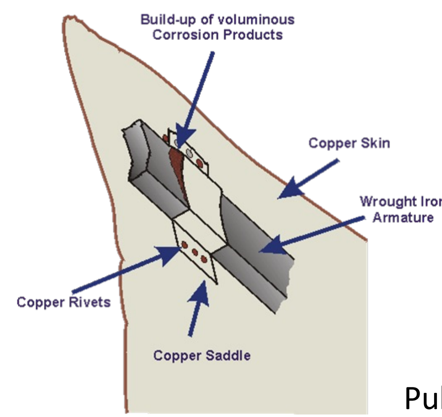


Public domain





Palanisamy, DOI: 10.5772/intechopen.80542



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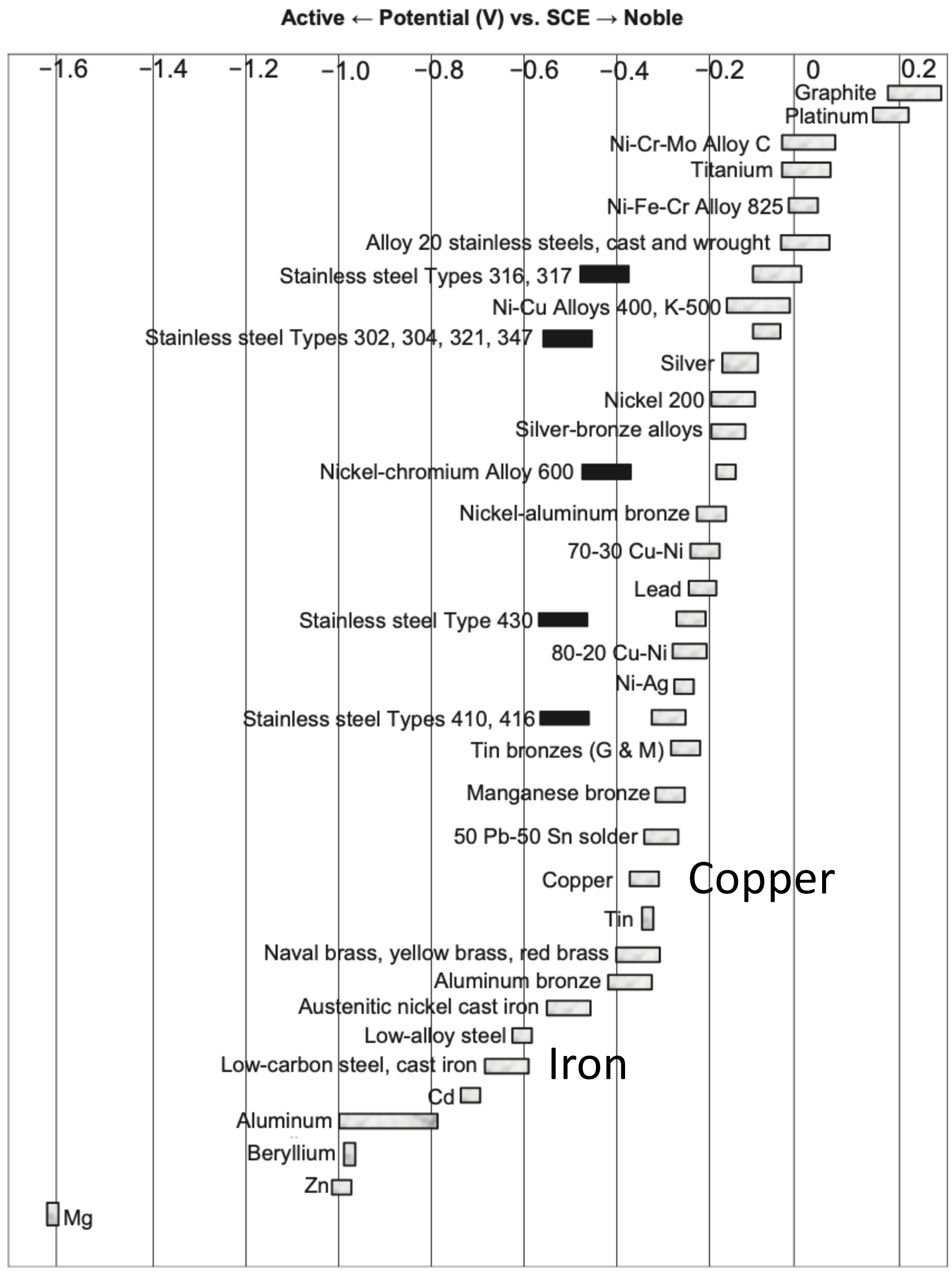
Galvanic Series

H.P. Hack, Evaluating galvanic corrosion, in: Corrosion: Fundamentals, Testing and Protection, 9th ed., vol. 13A, ASM Handbook, Metals Park, OH, 1987, pp. 562–567.



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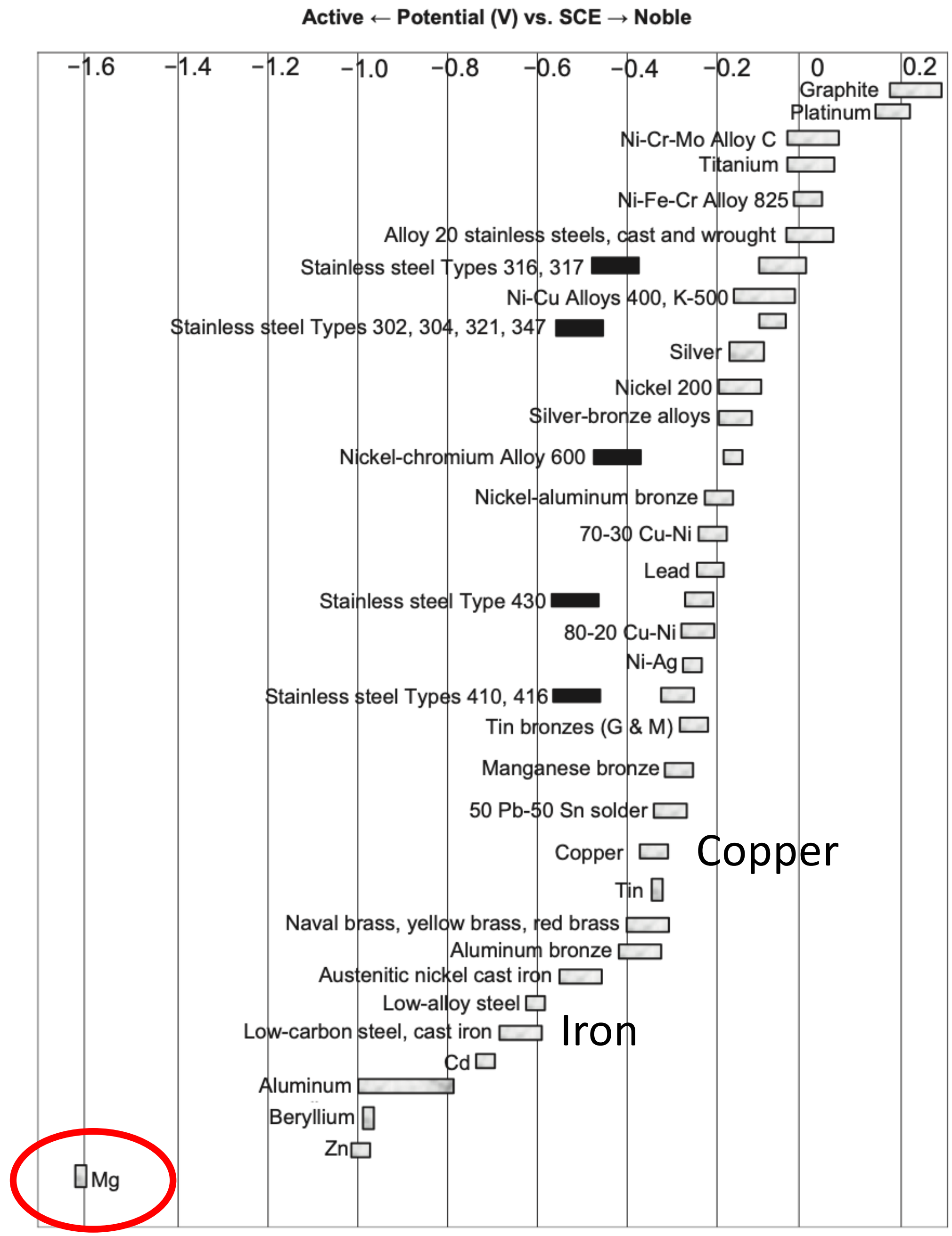
H.P. Hack, Evaluating galvanic corrosion, in: Corrosion: Fundamentals, Testing and Protection, 9th ed., vol. 13A, ASM Handbook, Metals Park, OH, 1987, pp. 562–567.

PRISMS Center focuses on advancing magnesium alloys as lightweight structural materials

Improved mechanical properties can be achieved via alloying

Magnesium



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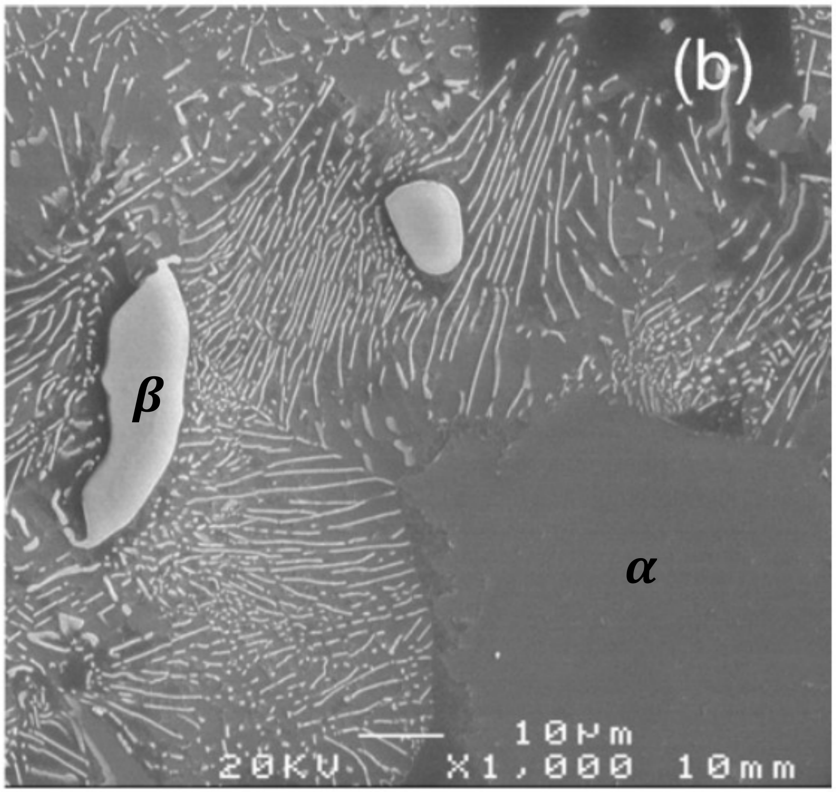
Microgalvanic Corrosion

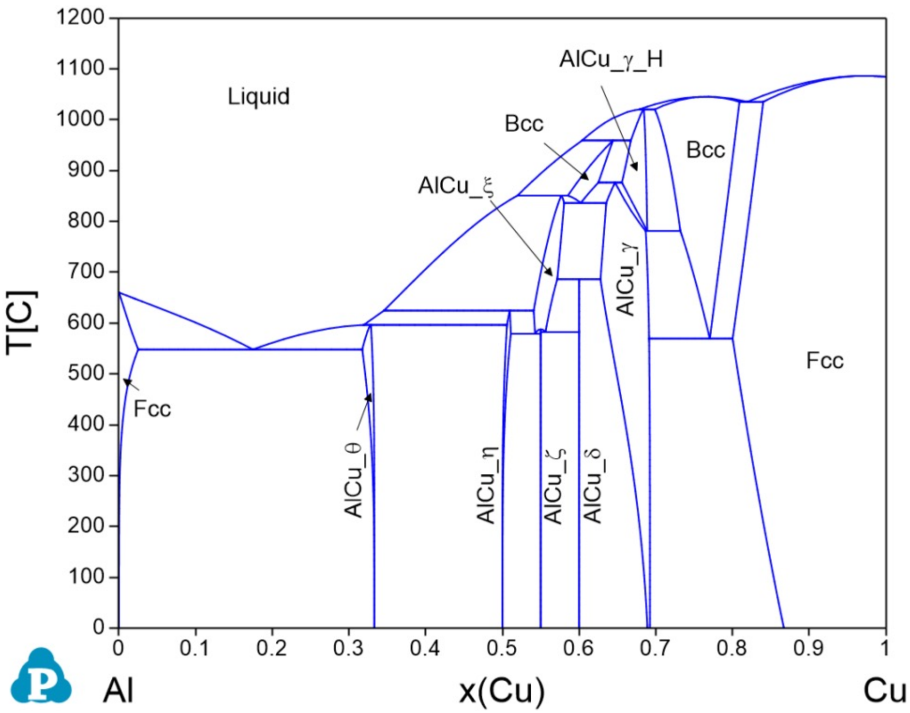
As-cast magnesium alloy (AZ91)

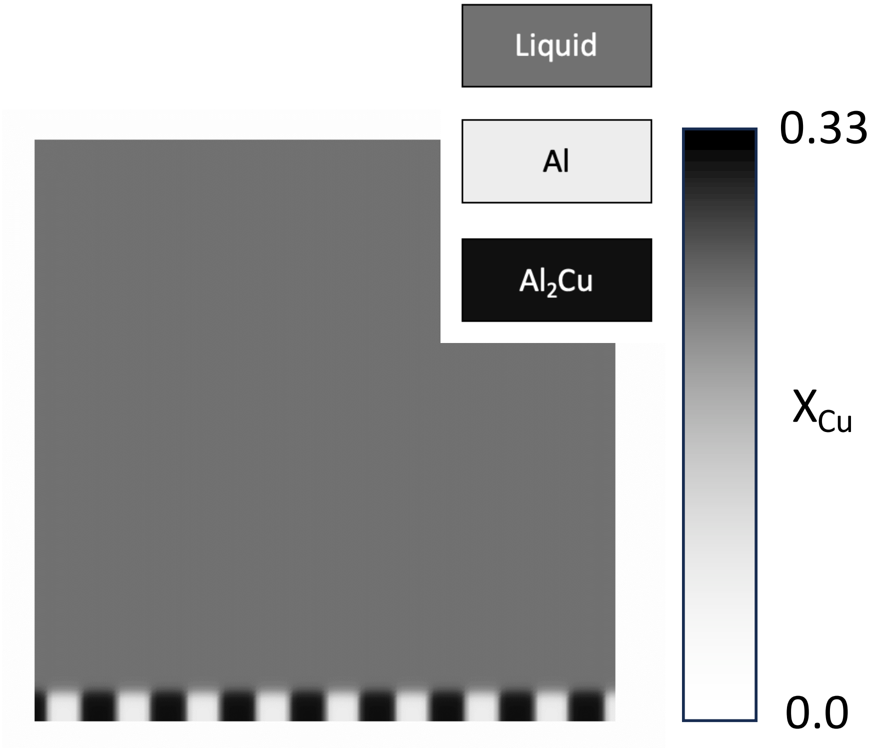


Zhao et al., Corrosion Science 50 (2008) 1939–1953

The presence of multiple phases (regions with different concentrations causes a galvanic effect!

Microstructure Example: Eutectic Solidification





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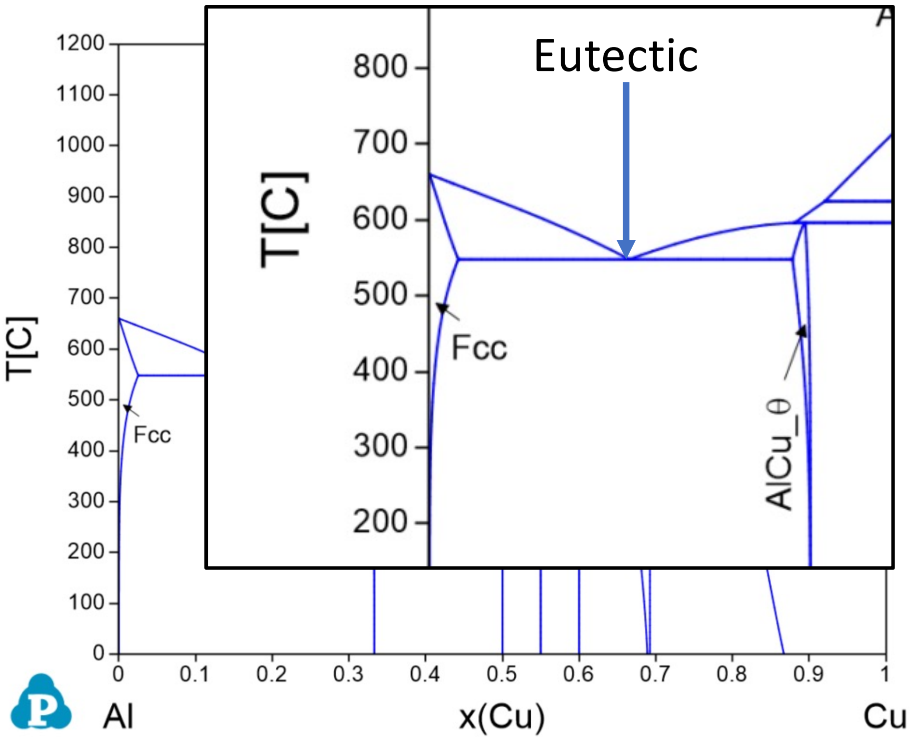
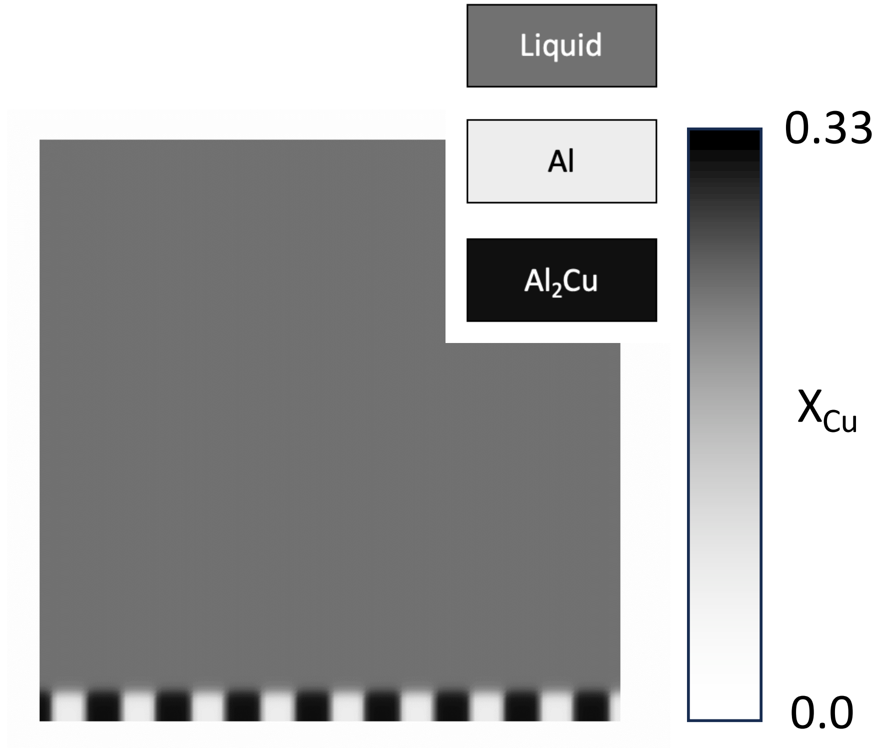
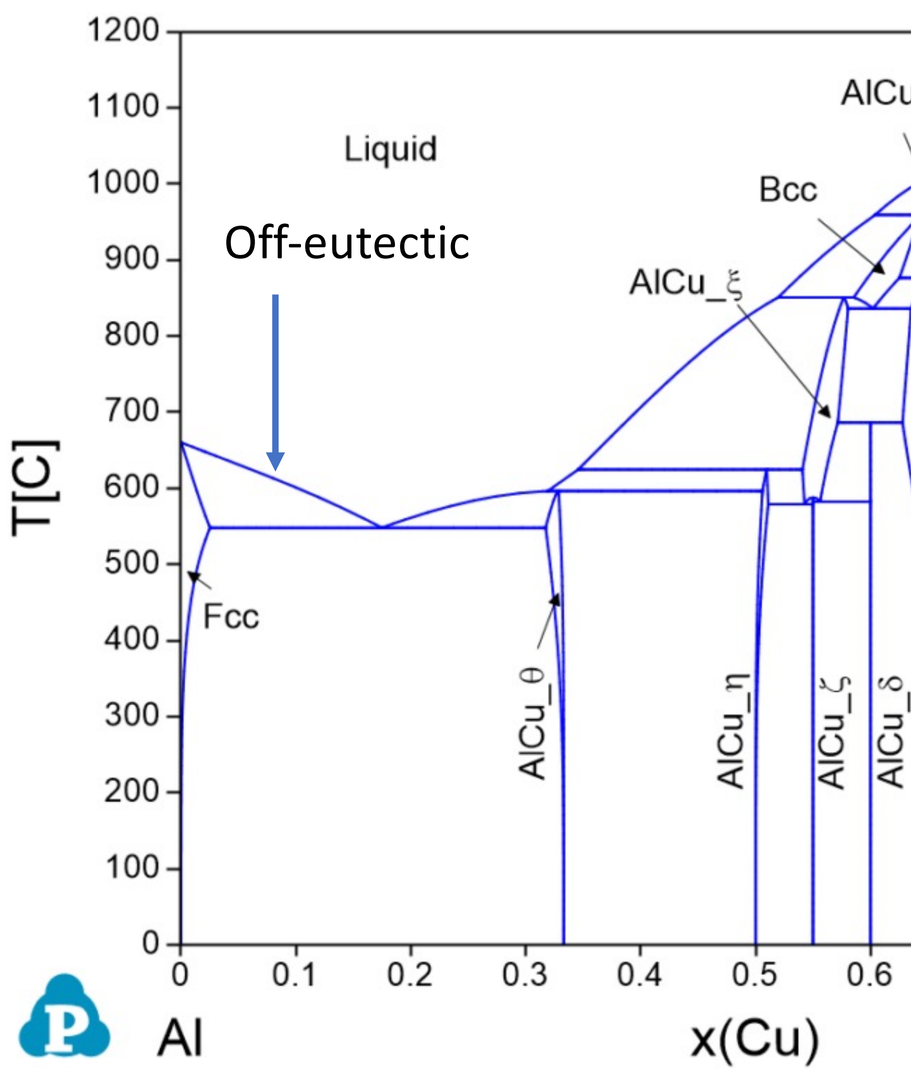


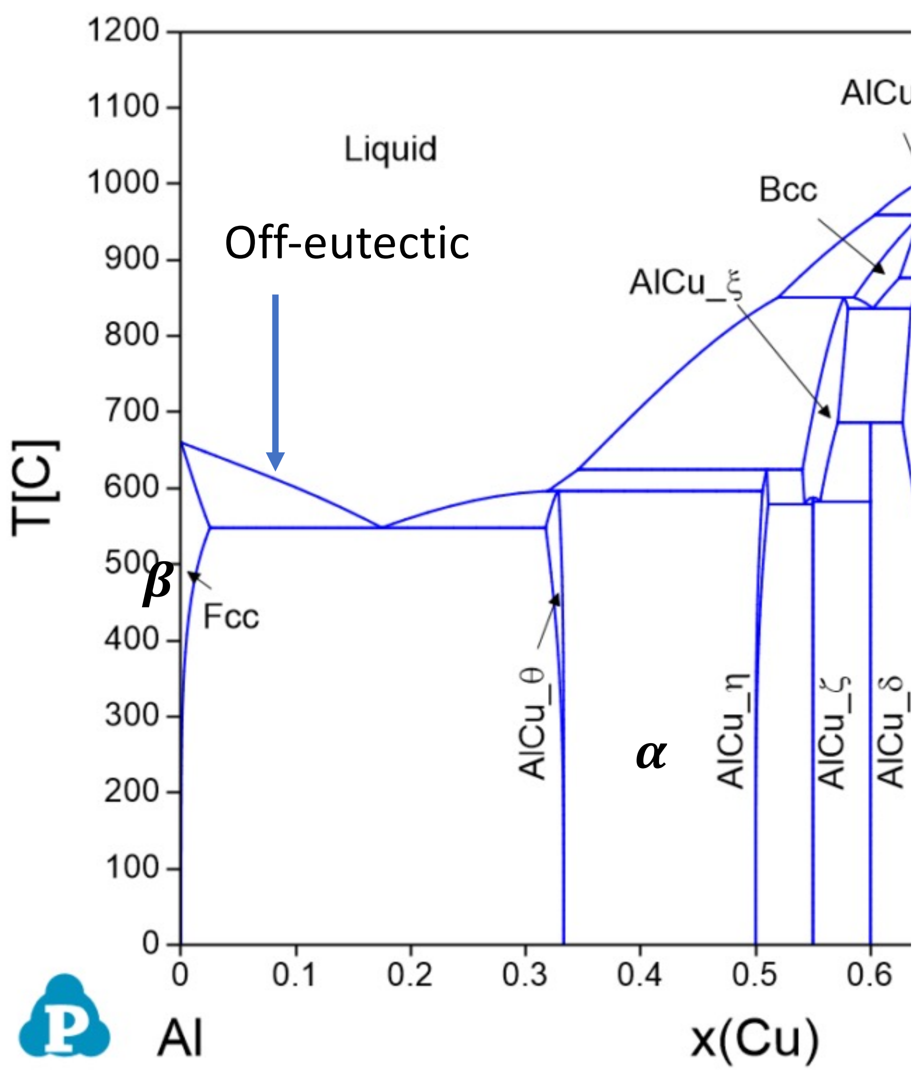


Microstructure Example: Eutectic Solidification



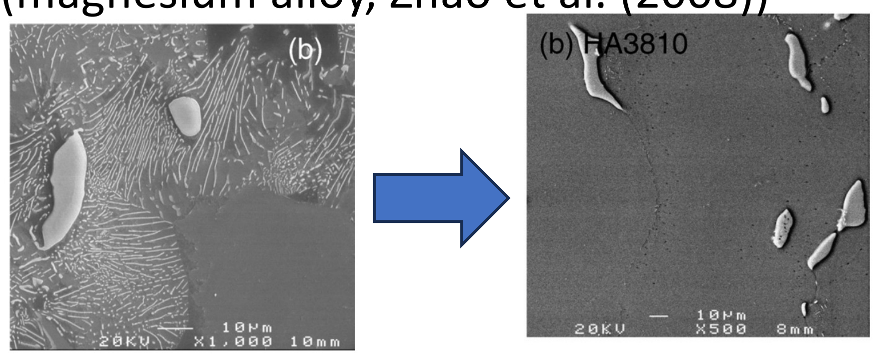
- Formation of “primary”
- Enrichment of Cu in liquid
- Primary grow
- Liquid concentration hits the eutectic value
- Eutectic microstructure forms around the primary

Microstructure Example: Eutectic Solidification



- Formation of "primary"
- Enrichment of Cu in liquid
- Primary grow
- Liquid concentration hits the eutectic value
- Eutectic microstructure forms around the primary
- Subsequent **heat treatment** can alter the microstructure

(magnesium alloy, Zhao et al. (2008))



Phase-Field Model for Localized Corrosion with the Smoothed Boundary Method

Kinetics at the interface: reaction current

$$\frac{i_{rxn}}{i_{corr}} = \left(1 - \frac{i_{rxn}}{i_{max,c}}\right) \exp\left(\frac{z_M (1-\beta) F}{RT}\eta\right)$$

$$\eta = V_s - Ecorr - \Phi$$

Ionic transport within the electrolyte (smooth boundary method)

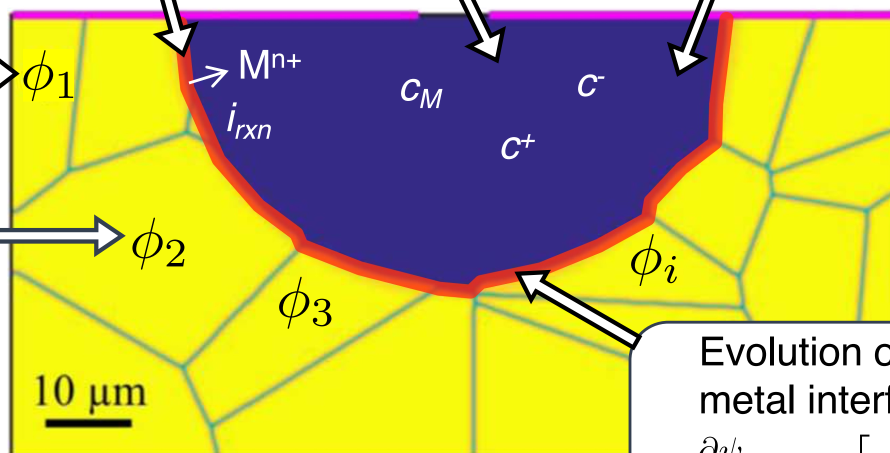
$$\frac{\partial c_i}{\partial t} = \frac{1}{\psi}\nabla\cdot(\psi D_i \nabla c_i) + \frac{1}{\psi}\left(\frac{z_i F}{RT}\nabla\cdot(\psi D_i c_i \nabla\Phi)\right) + \frac{|\nabla\psi|}{\psi}\left(\frac{i_{rxn}}{z_i F}\right)$$

Electrostatic potential

$$\nabla\cdot(\psi\kappa\nabla\Phi) = F\nabla\cdot\left(\psi\sum_{j=1}^{n-1} z_j(D_n - D_j)\nabla c_j\right) - |\nabla\psi| i_{rxn}$$

Evolution of phases in the metal (grains or intermetallic particles)

$$\frac{\partial\phi_i}{\partial t} = \nabla\cdot\left[M(\psi)\nabla\frac{\delta\mathcal{F}}{\delta\phi_i}\right] - \frac{V_M i_{rxn}}{z_M F}|\nabla\psi|$$



Evolution of the electrolyte-metal interface

$$\frac{\partial\psi}{\partial t} = \nabla\cdot\left[M(\psi)\nabla\frac{\delta\mathcal{F}}{\delta\psi}\right] + \frac{V_M i_{rxn}}{z_M F}|\nabla\psi|$$

A. Chadwick, J. Stewart, R. A. Enrique, S. Du, and K. Thornton, *J. Electrochem. Soc.*, 165 (10) C633 (2018).

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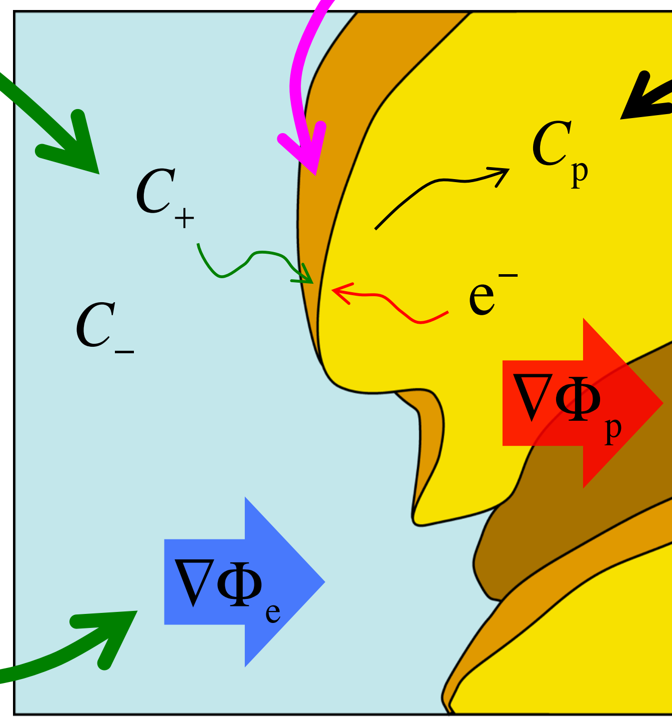
Similarities to Microscale Model of Battery Lithiation/Delithiation

$$i_0(C_p^{surf}, C_e)\left(\exp\left(\frac{0.5F}{RT}\eta\right) - \exp\left(\frac{-0.5F}{RT}\eta\right)\right)$$

$$\frac{\partial C_e}{\partial t} = \nabla\cdot\left(D_e\nabla C_e\right) - \frac{i_e\cdot\nabla t_+}{z_+\nu_+F}$$

$$\nabla\cdot\left[\left(z_+m_+ - z_-m_-\right)FC_e\nabla\Phi_e\right] - \nabla\cdot\left[\left(D_- - D_+\right)\nabla C_e\right] = 0$$



$$\frac{\partial C_p}{\partial t} = \nabla\cdot\left(M_p\nabla\mu_p\right)$$

$$\nabla\cdot\left(\kappa_s\nabla\Phi_s\right) = 0$$

Ref: Doyle et al., Journal of the Electrochemical Society, 140, 6, 1993

Pit Growth within a Single Grain

Chadwick, et al.

- Exposed metal surface (top)

  V_s = 50 mv; E_{corr}=-0.24 vs SCE, i_{corr} = 0.99 mA/cm^2

- Boundary conditions are uniform throughout the top of the domain

  $c_M = 0$ M, $c_+ = 1$ M, and $\Phi = 0$ V vs. SCE

- Motion of the electrolyte/single metal grain interface is tracked

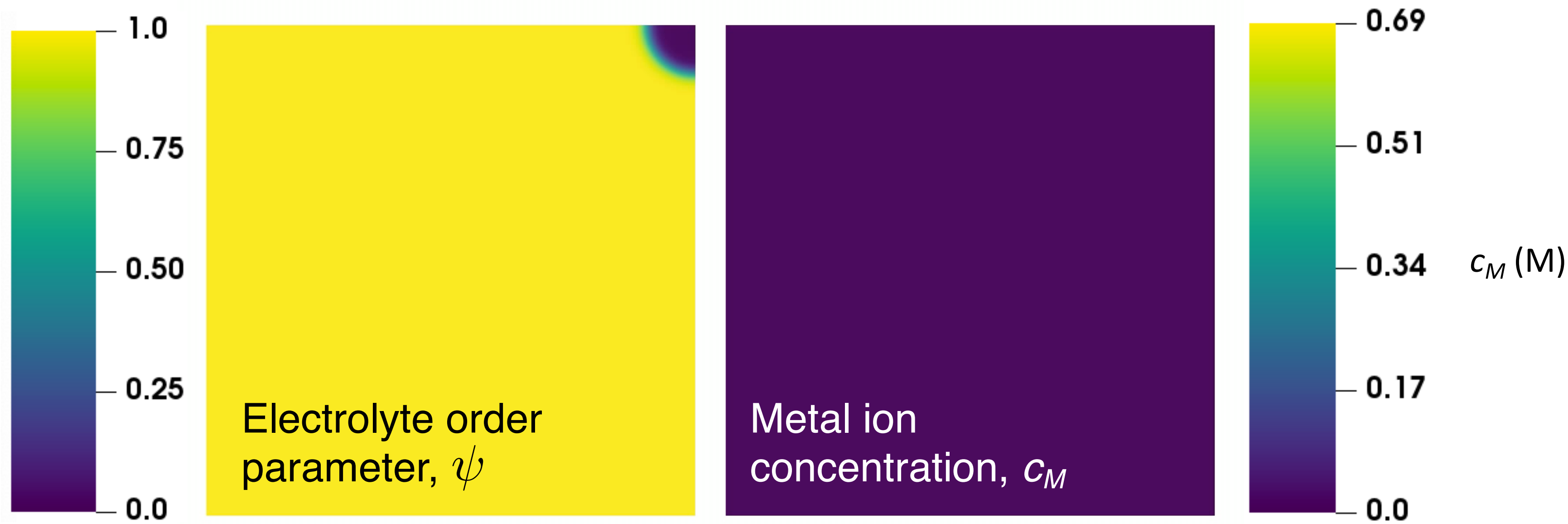
$$\nabla \cdot (\psi \kappa \nabla \Phi) = F \nabla \cdot \left(\psi \sum_{j=1}^{n-1} z_j (D_n - D_j) \nabla c_j \right) - |\nabla \psi| i_{rxn}$$

$$\frac{i_{rxn}}{i_{corr}} = \left(1 - \frac{c_M}{c_{M,sat}}\right) \exp\left(\frac{z_M (1-\beta) F}{RT} \eta\right)$$

$$\eta = V_s - Ecorr - \Phi$$

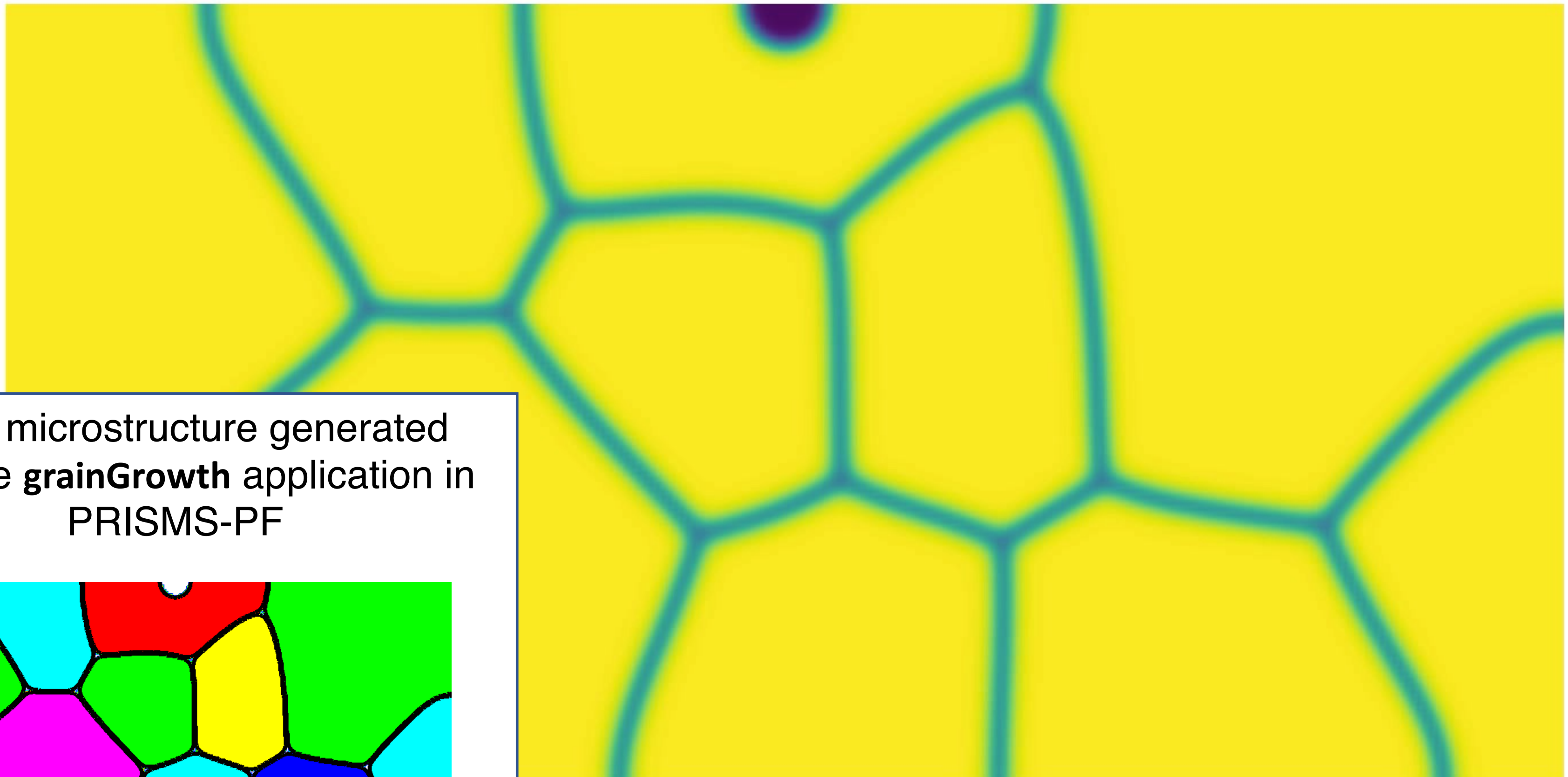
$$\text{system size} = 18.75\,\mu\text{m} \times 18.75\,\mu\text{m}$$

$$\text{time} = 4\text{ s}$$



Pit Growth into a Polycrystal

Chadwick, et al.



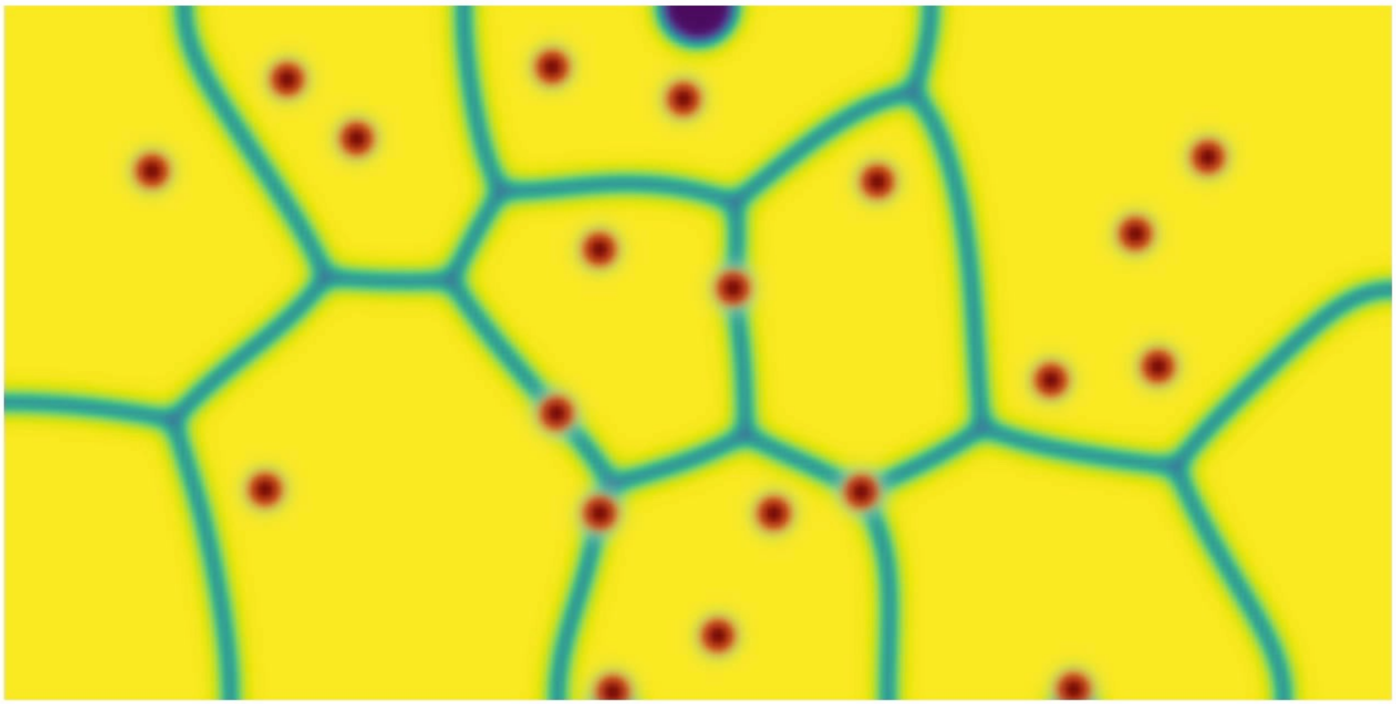
Initial microstructure generated with the **grainGrowth** application in PRISMS-PF

Polycrystal with Precipitates

Chadwick, et al.

$$\frac{i_{rxn}}{i_{corr}} = \left(1 - \frac{c_M}{c_{M,sat}}\right) \exp\left(\frac{z_M(1-\beta)F}{RT}\eta\right)$$

$$i_{corr,prec} = 5 \times i_{corr,matrix}$$



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PRISMS-PF: An Open-Source Parallel Phase-Field Modeling Framework

prisms-center.github.io/phaseField

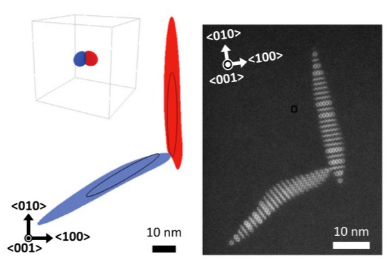
DeWitt et al., npj Comput. Mater. 6, 29 (2020)

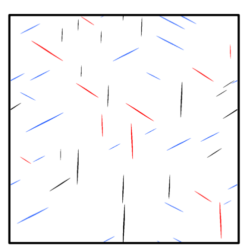
Advanced capabilities

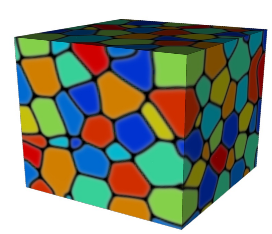
Based on the deal.II finite element library
Matrix-free finite element approach
Solution of an arbitrary number of coupled PDEs
Up to 6th order elements
Multi-level parallelism
Adaptive meshing
Explicit nucleus placement
Grain-remapping
Newton/Picard nonlinear solver

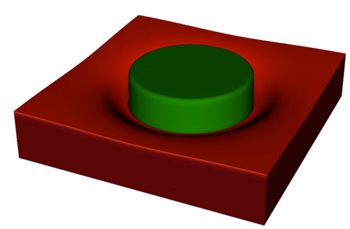
Functionalities / Ease of Use

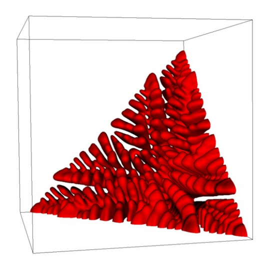
Simple interface
Detailed online user guide
30 pre-built applications
Simple Docker-based installation
nanoHUB tool w/ GUI for educational use
Integrated with Materials Commons
Postprocessing scripts for results analysis
YouTube video tutorials
Virtual Machine
Troubleshooting/FAQ page











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PRISMS-PF Application to Mg Corrosion

MRS Communications (2022) 12:1050–1059

https://doi.org/10.1557/s43579-022-00266-6

MRS Communications

Computational Approaches for Materials Discovery and Development Prospective

Check for updates

Simulating microgalvanic corrosion in alloys using the PRISMS phase-field framework

Vishwas Goel, Yanjun Lyu, Stephen DeWitt, David Montiel, Katsuyo Thornton, Department of Materials Science and Engineering, University of Michigan, Ann Arbor, MI 48150, USA

Address all correspondence to Katsuyo Thornton at **kthorn@umich.edu**

(Received 6 May 2022; accepted 2 September 2022; published online: 17 October 2022)

Journal of The Electrochemical Society, 2023 **170** 101502

CrossMark

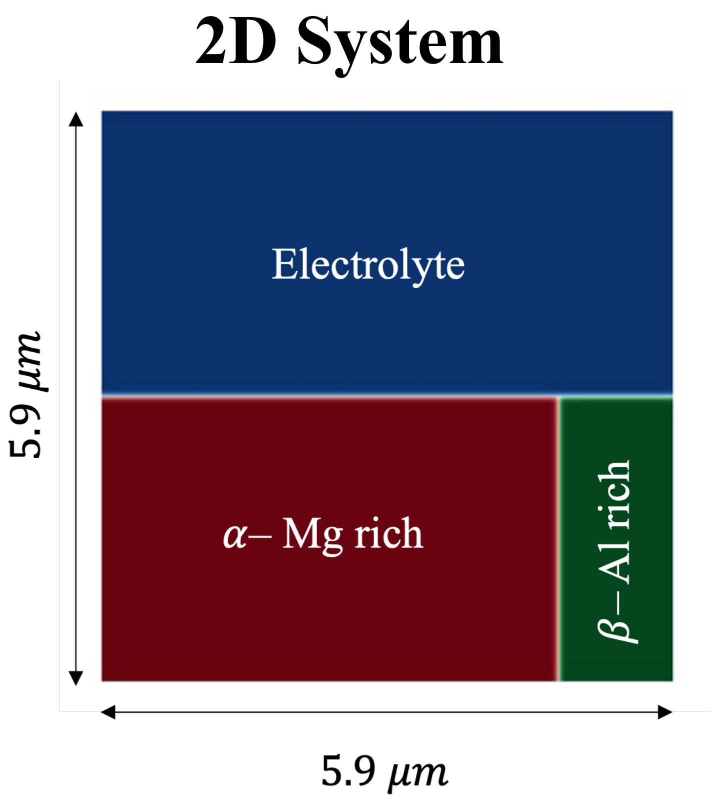
Understanding the Effect of Electrochemical Properties and Microstructure on the Microgalvanic Corrosion of Mg Alloys via Phase-Field Simulations

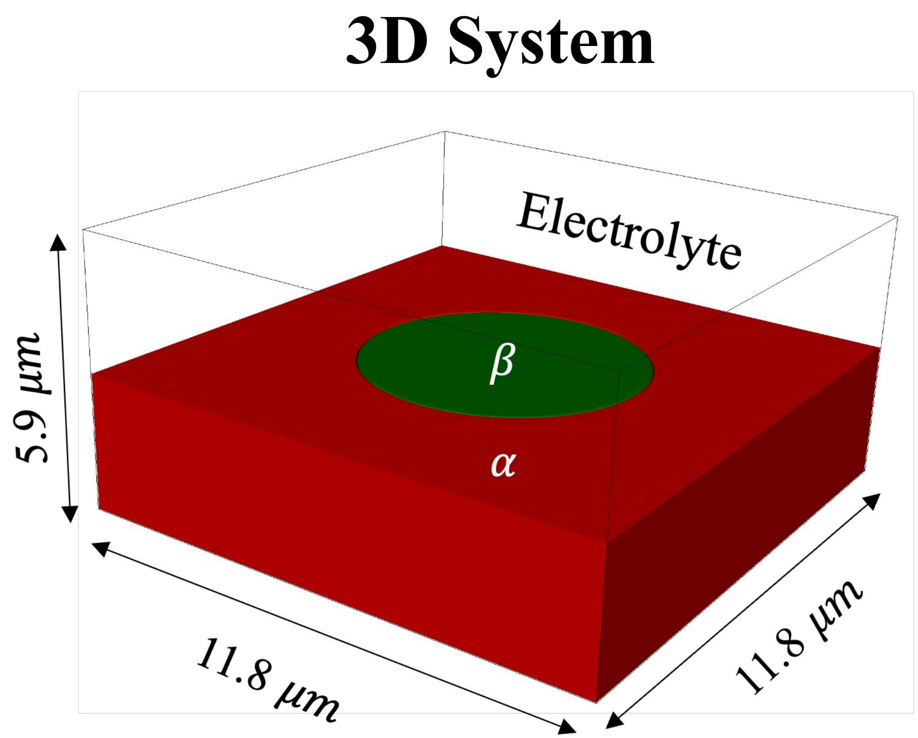
Vishwas Goel, David Montiel, and Katsuyo Thornton[z]

Department of Materials Science and Engineering, University of Michigan, Ann Arbor, United States of America

Simulation Setup

Effects of microstructures, as well as material properties were examined





Goel et al., MRS Communications, 2022; Goel et al., J. ECS, 2023.

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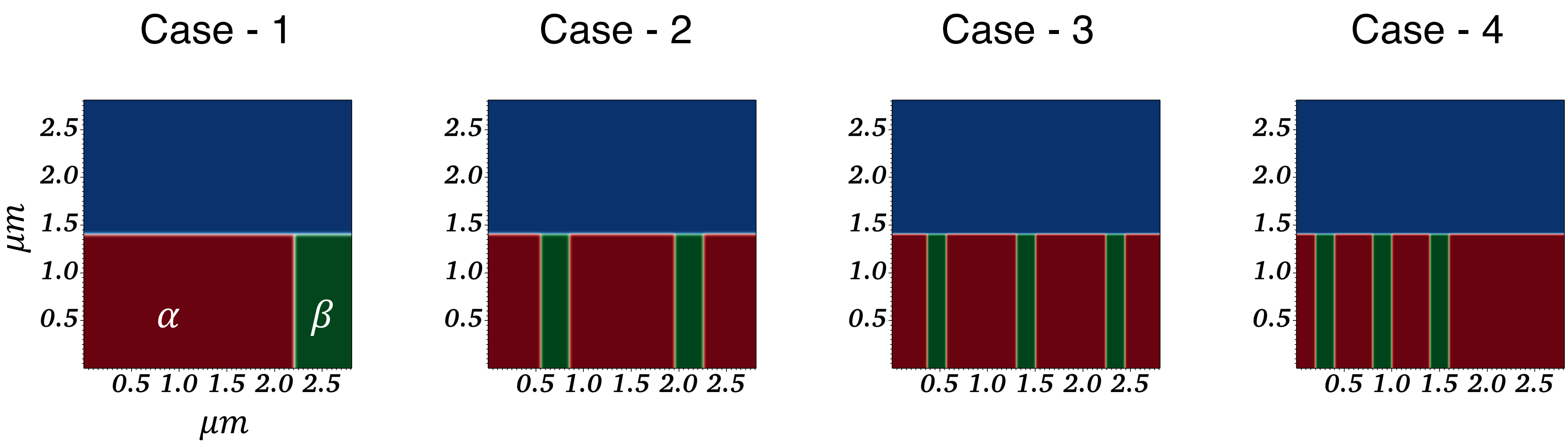
Effect of lamellae on the microgalvanic corrosion rate – 4 different 2D microstructures, 21% β



- Wide lamellar
- Medium lamellar
- Narrow lamellar
- Lamellar region next to a larger α region

Goel et al., J. ECS, 2023.

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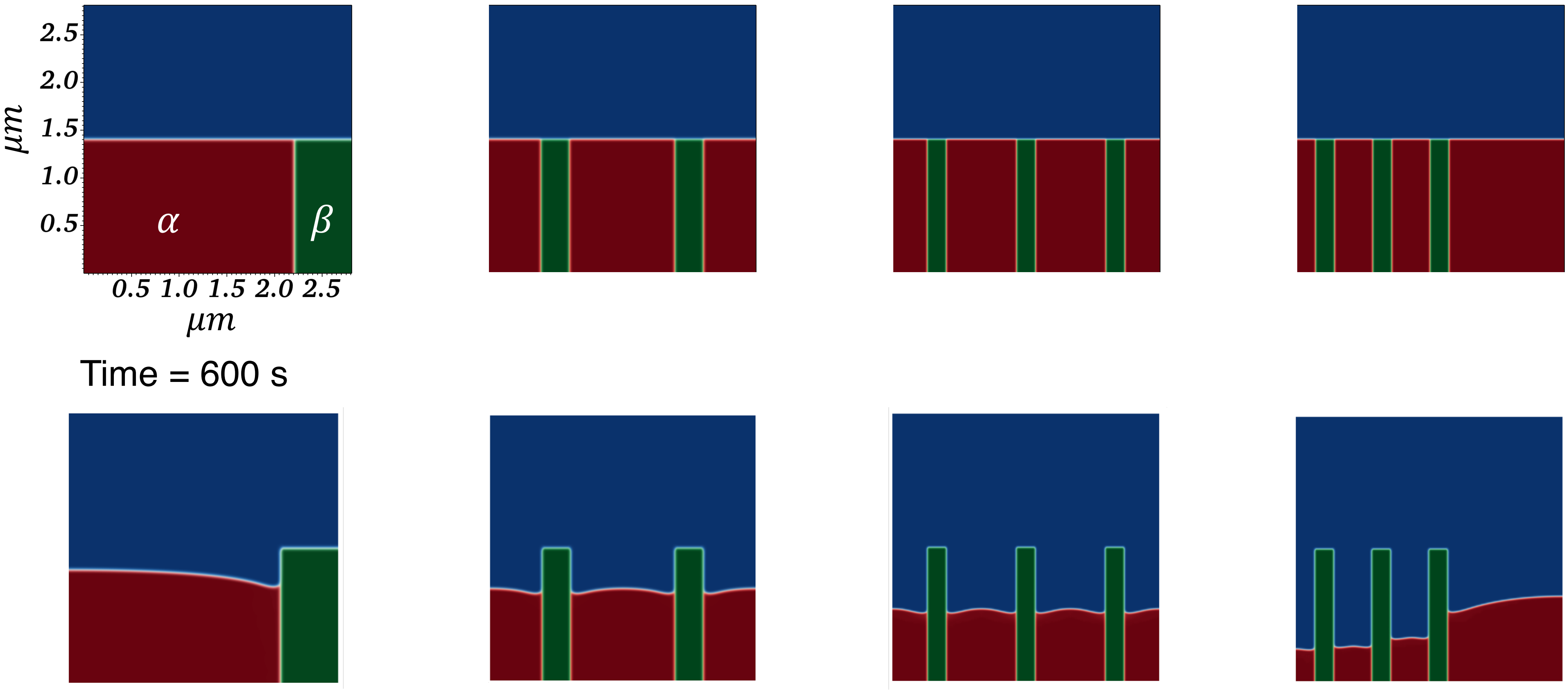
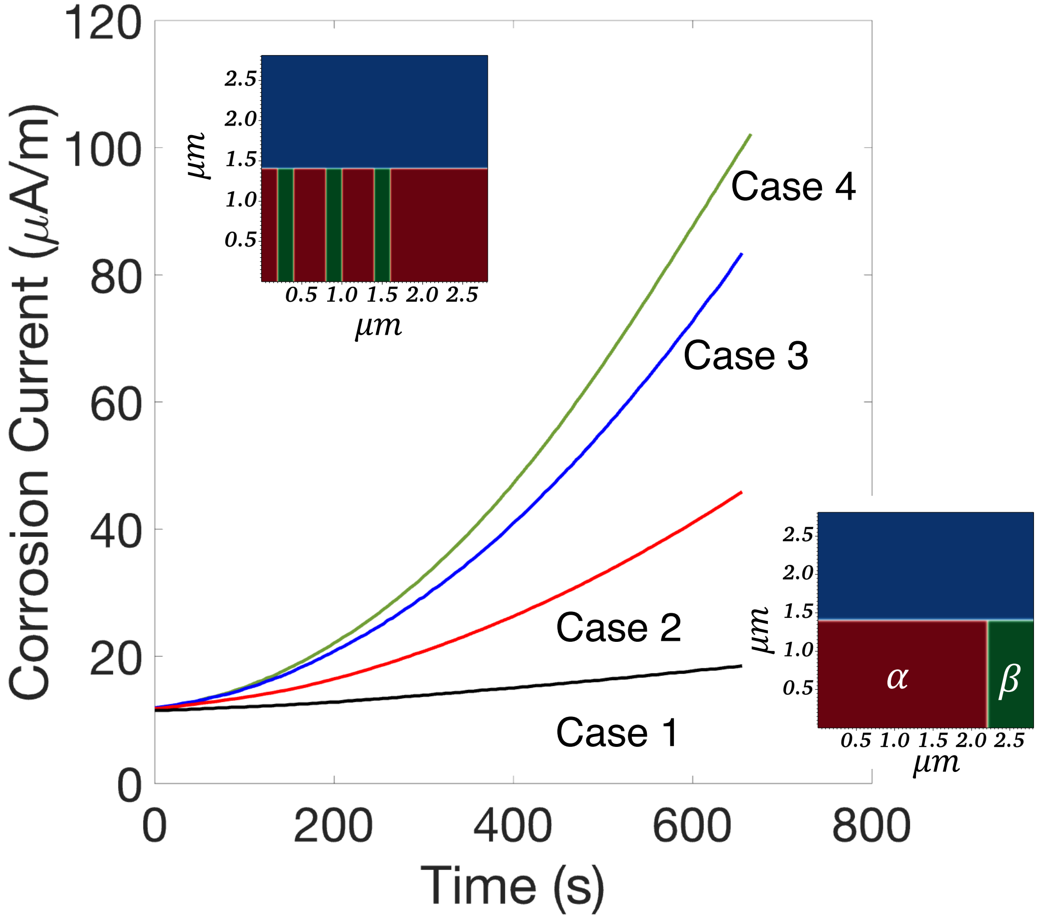
Goel et al., J. ECS, 2023.



Less corrosion ⟷ More corrosion

Presence of the lamellar region is detrimental to the corrosion resistance

- Quantification via corrosion current
- In all cases, the rate increases
- Finer lamellar structure show the largest corrosion rate
- Why?



Goel et al., J. ECS, 2023.

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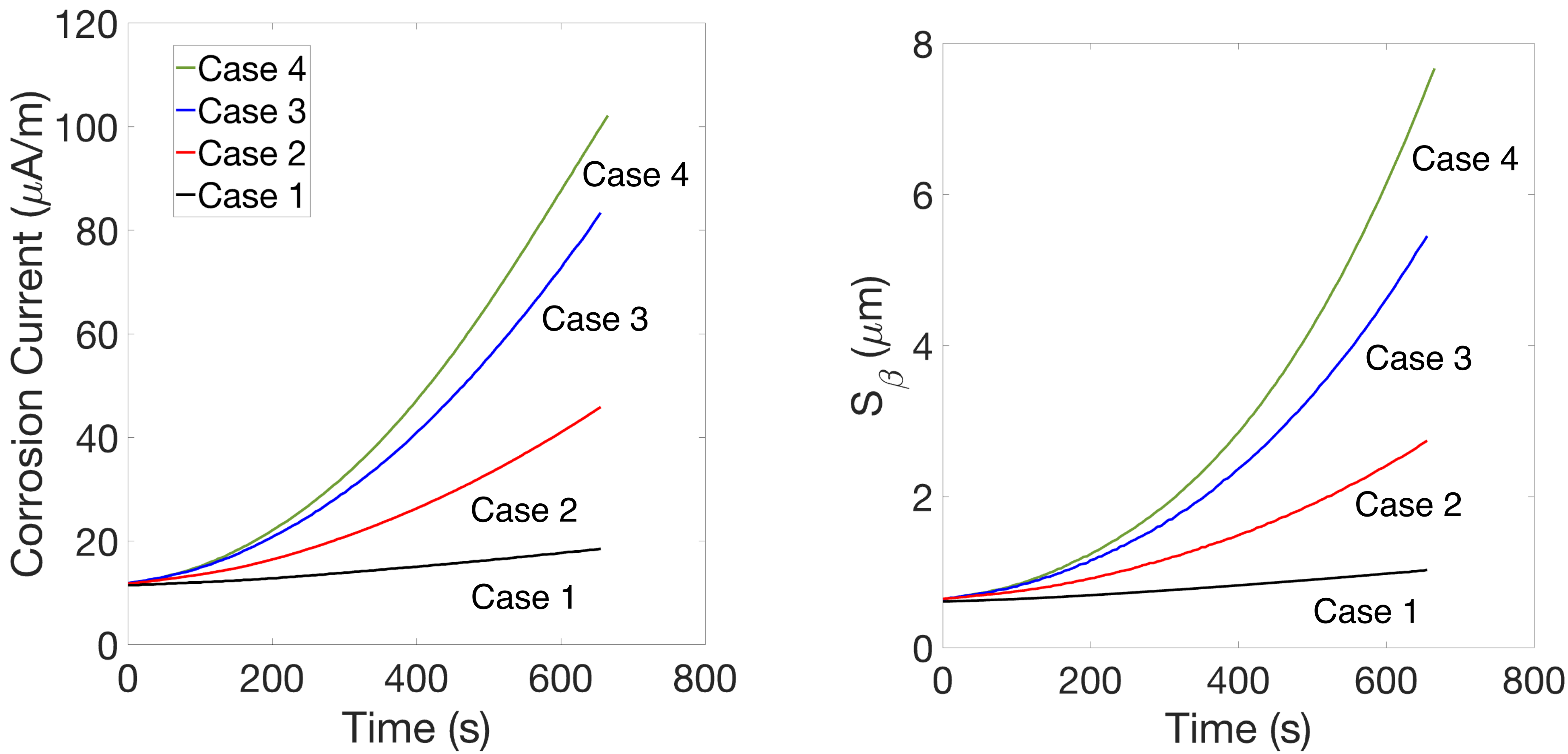
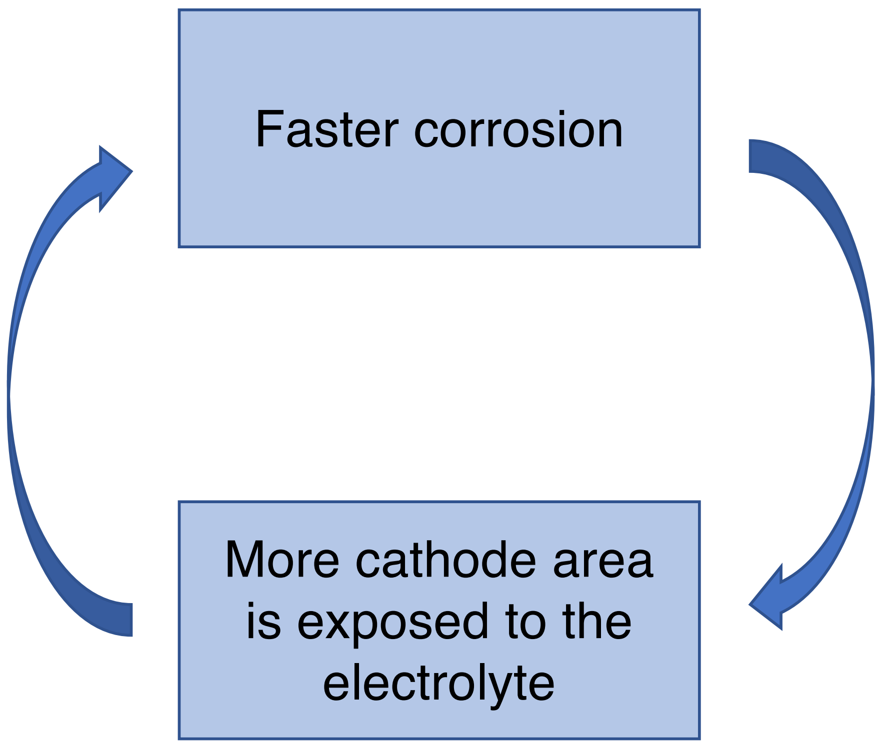
Because it increases the cathode area exposed to the electrolyte with the progression of corrosion



Goel et al., J. ECS, 2023.

And thereby establishes a positive feedback loop



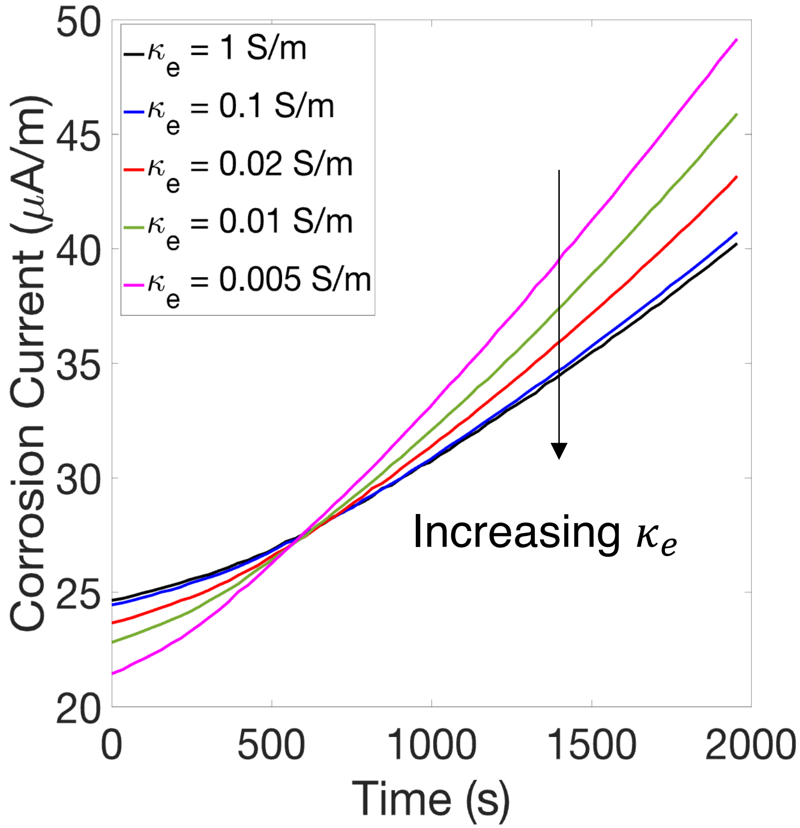
Also, the results highlight that it is NOT the volume of the cathodic component, but ***<u>the area that matters.</u>***

Goel et al., J. ECS, 2023.

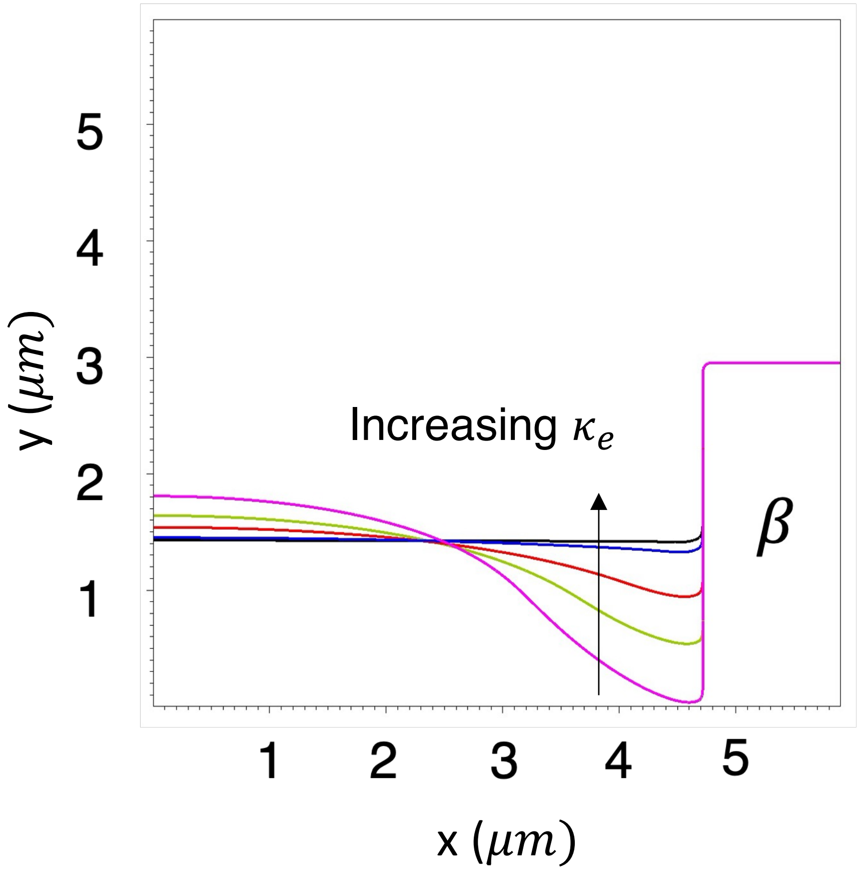
High ionic conductivity improves the corrosion performance at later times due to the improved homogeneity of corrosion

Goel et al., J. ECS, 2023.

κ_e:the ionic conductivity of the electrolyte



Interface location
t = 2825 s



Low κ_e initially has a lower rate of corrosion, but it then accelerates!

Wagner Length to Predicts the Nonuniformity in Corrosion

$$W_\alpha = \kappa_e \frac{\partial \eta_\alpha}{\partial i_{rxn,\alpha}}$$

Wagner et al., J. Electrochem. Soc., 98, 116 (1951)

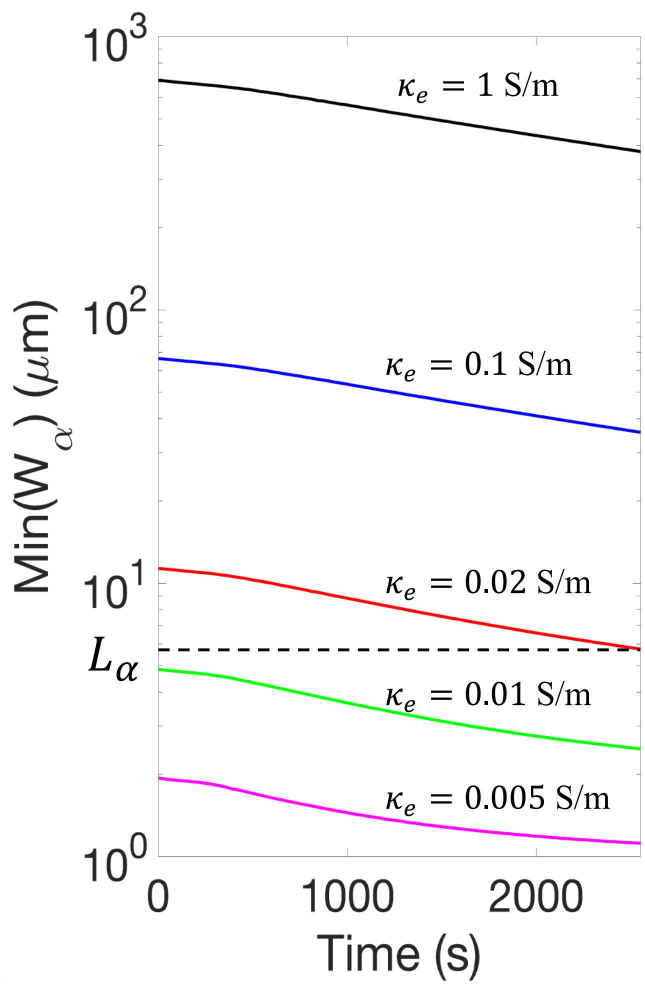
- $W_\alpha \gg L_\alpha$ – Uniform corrosion
- $W_\alpha \ll L_\alpha$ – Nonuniform corrosion

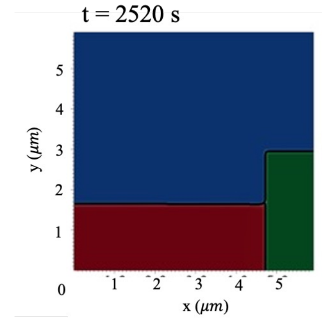
Affected by the material properties and microstructure

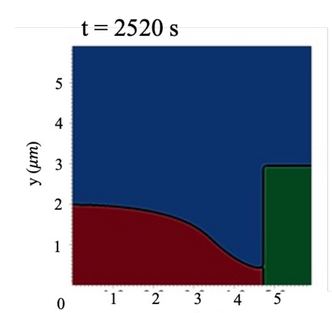
Effect of κ_e on the Wagner length

$W_\alpha \gg L_\alpha$ – Uniform corrosion

$W_\alpha \ll L_\alpha$ – Nonuniform corrosion

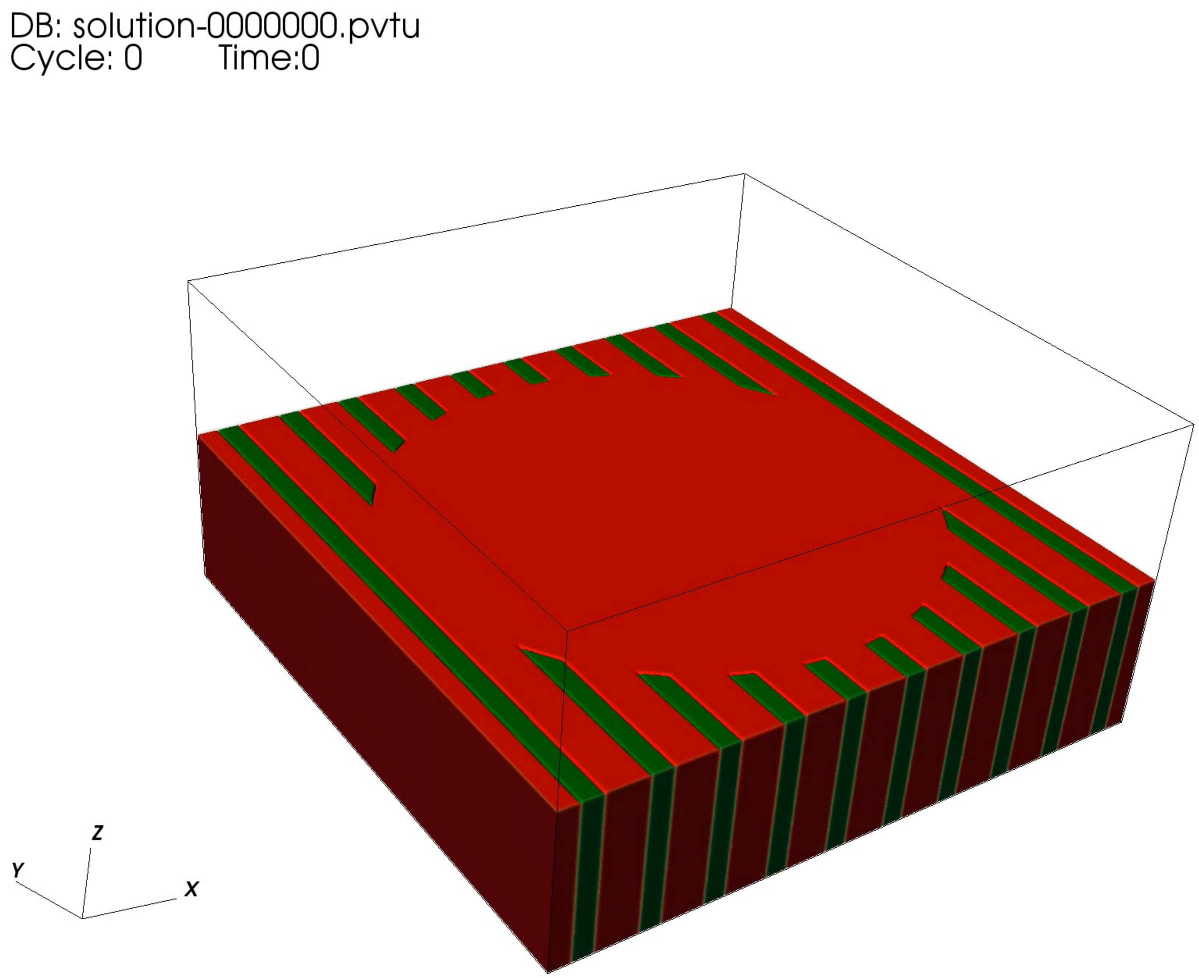






Goel et al., J. ECS, 2023.

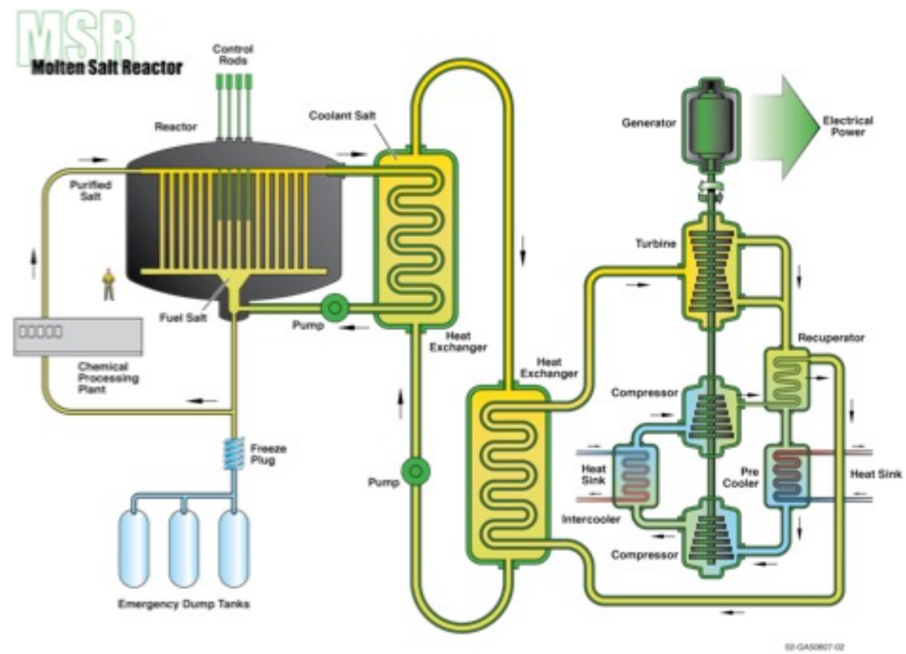
Similar behavior is also observed in 3D

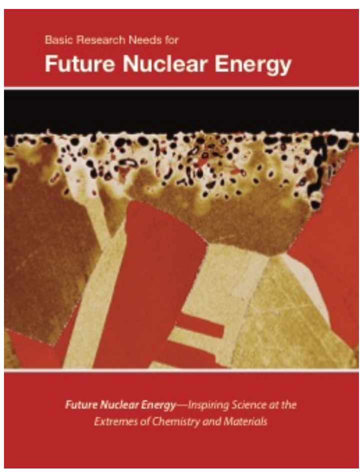


Goel et al., J. ECS, 2023.

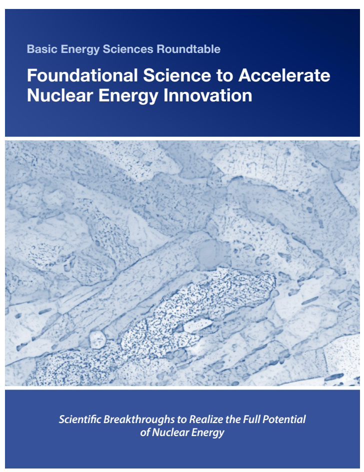
Motivation for the MSEE EFRC: Molten Salt Reactors

- Leading candidates for next-generation nuclear reactors;
- Potential game-changing technology;
- Cost-competitive, safe, and more sustainable commercial nuclear power option.





2017 BES Workshop on Basic Research Needs for Future Nuclear Energy



2022 BES Roundtable on Foundational Science to Accelerate Nuclear Energy Innovation

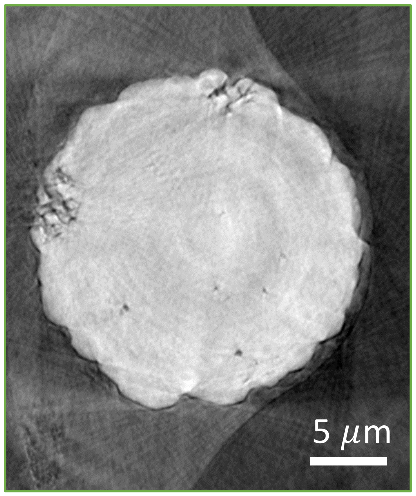
Development of new MSR concepts requires fundamental understanding of, and development of predictive models for:

- the physics and chemistry of molten salts
- interactions with solutes (actinides, fission products, corrosion products) and radiation
- their interactions with, and degradation of, reactor materials.

Morphology in Ni-20Cr at 600°C vs 800°C

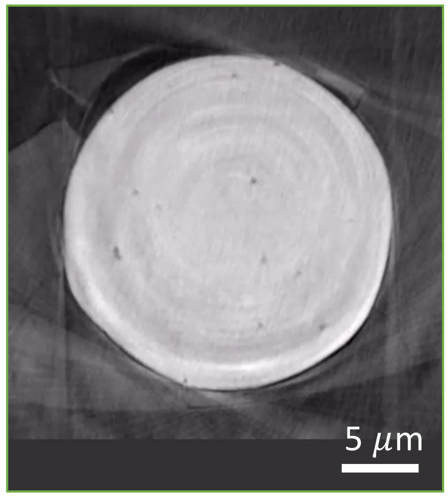
Liu et al. *Nat Commun* **12**, 3441 (2021)
Liu et al. *ACS Appl. Mater. Interfaces*, **15**, 13772–13782 (2023

600 ºC

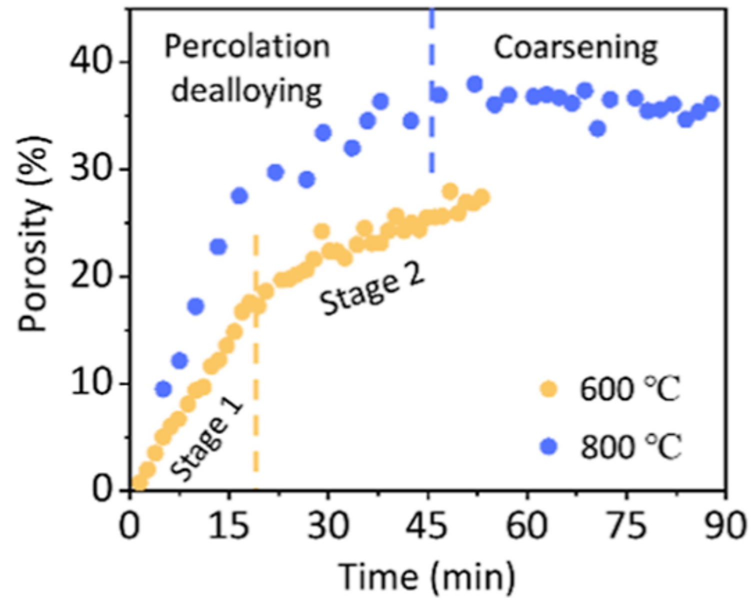


Intergranular Corrosion

800 ºC



Percolation Dealloying



- Ni-20Cr wire in $MgCl_2$-KCl salt
- Several mechanisms affect morphological evolution
  - Surface corrosion
  - Intergranular corrosion
  - Percolation dealloying
  - Surface diffusion

- Use the coarsening regime data to identify the dominant transport mechanism
- Simulate the corrosion regime with a parameterized model (ongoing)

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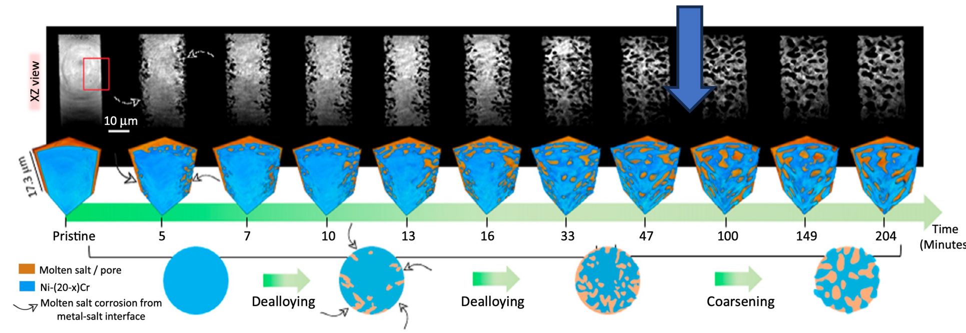
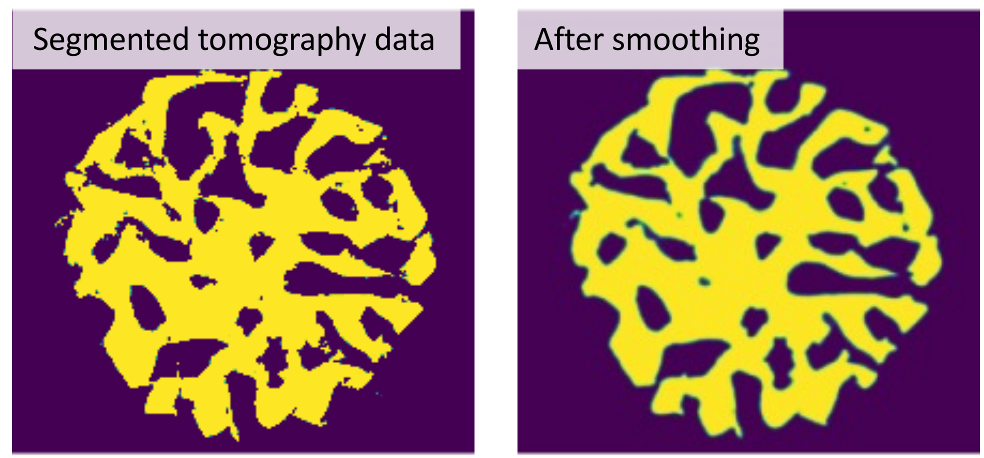
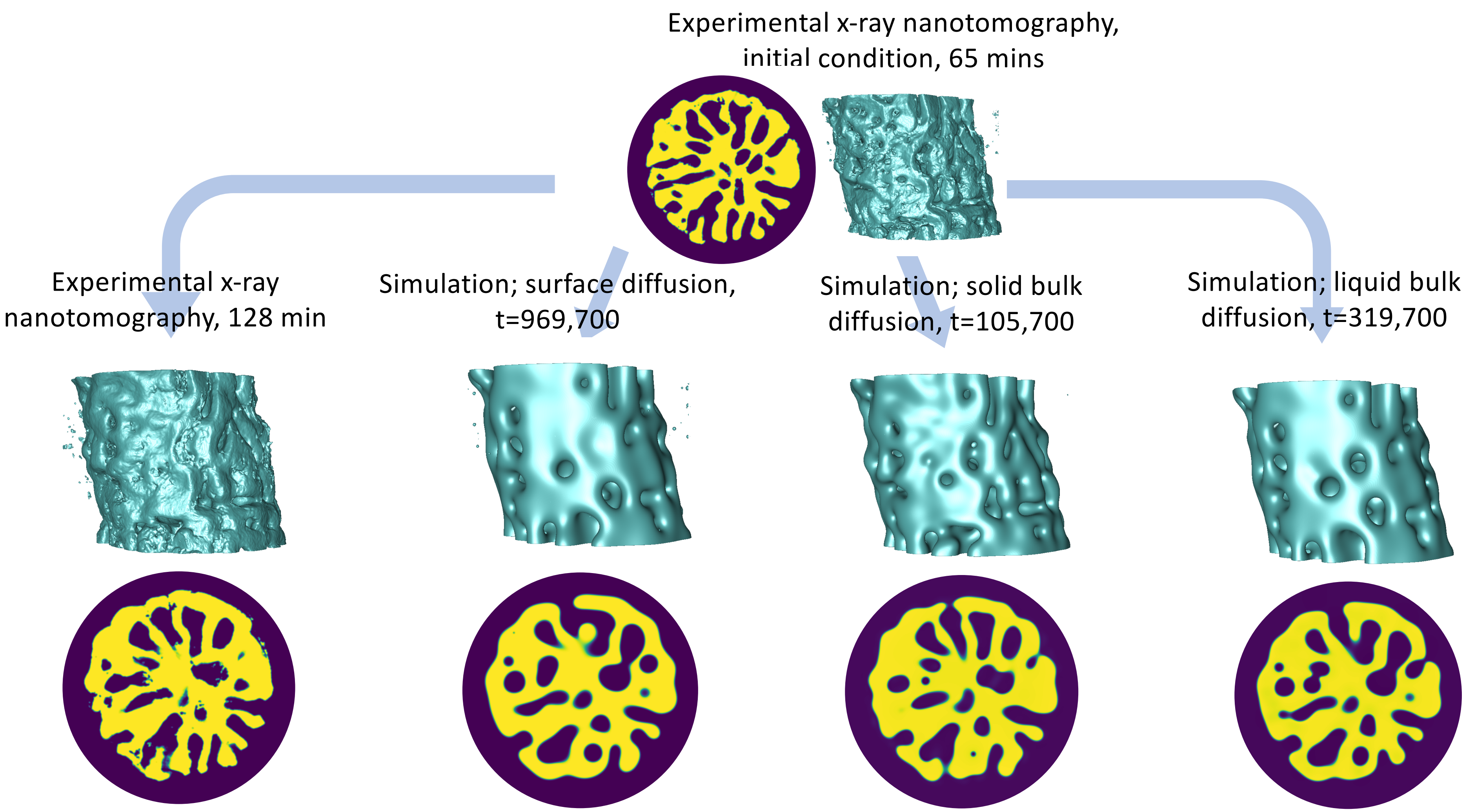
3D Coarsening Simulations

1. Initial condition from X-ray nanotomography experiment at the beginning of the coarsening stage
2. Smooth tomography data
3. Coarsen via…
   - Bulk diffusion through solid
   - Bulk diffusion through liquid
   - Surface diffusion

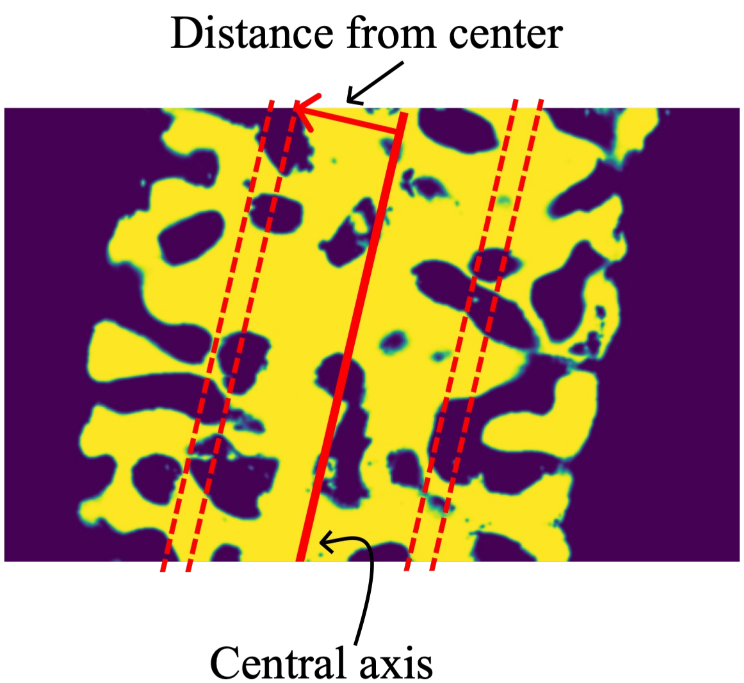




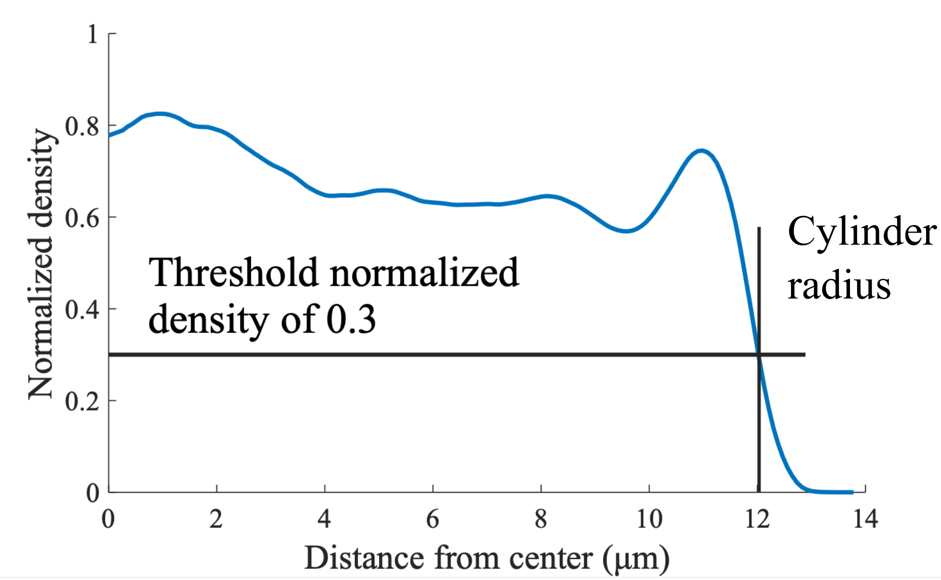
Morphological Evolution



Quantifying Morphological Evolution: Radial Density Functions



Comparison is not trivial due to drift and noise in the experimental data

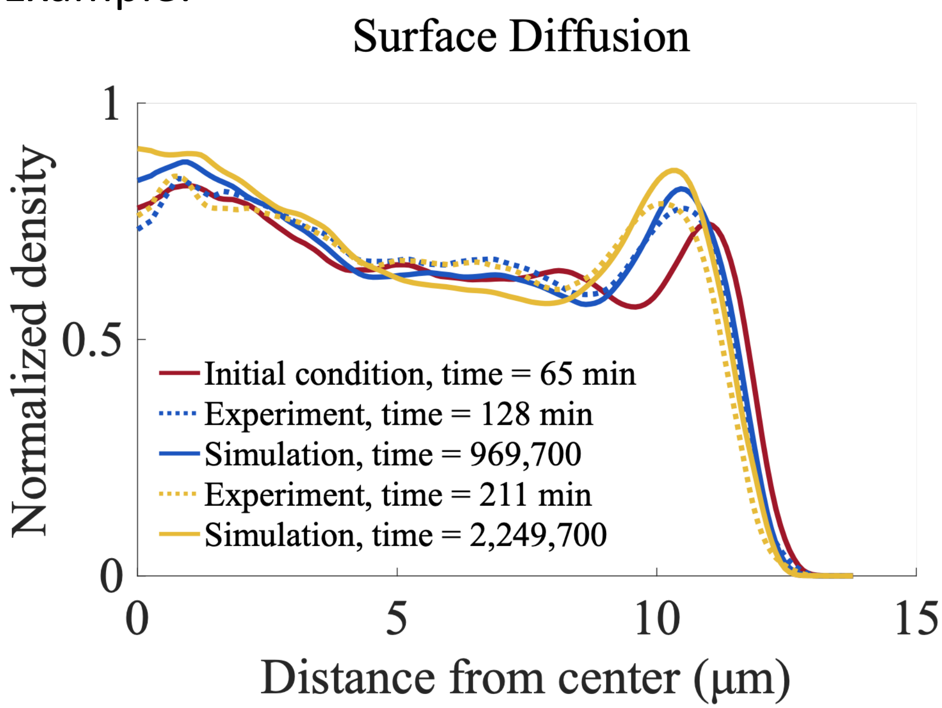


Radial density function

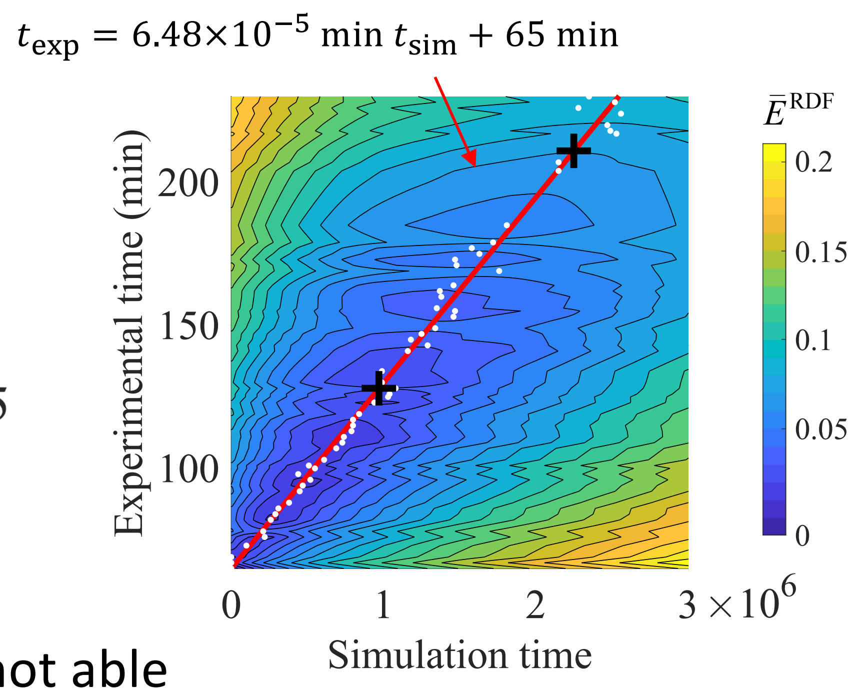
Note the schematics are in 2D, but the actual analyses are in 3D!

Matching the Timescales: Comparing Simulated and Experimental Morphologies

Example:



Relative error between experimental and simulated radial density functions



Key Result: The comparison alone was not able to rule out bulk diffusion or surface diffusion.

Extracted Time Scaling Constant Can Be Used to Infer Diffusivities

	Cylinder radius	RDF	Best match from the literature
Surface diffusion (m^4/s)	1.80×10^{-28}	1.51×10^{-28}	1.69×10^{-29}
Solid bulk diffusion (m^3/s)	7.72×10^{-23}	7.50×10^{-23}	9.40×10^{-27}
Liquid bulk diffusion (m^3/s)	3.63×10^{-22}	2.26×10^{-22}	1.38×10^{-34}

Literature values can be found in Hendrix et al. *Acta Mater.* 297 (2025) 121299

Bulk diffusion

$$\frac{\gamma\Omega x_\infty}{k_B T} D = \frac{\ell^3}{30\tau}$$

literature   simulation

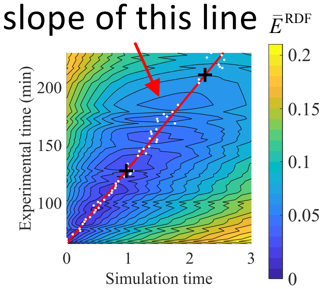
Surface diffusion

$$\frac{\gamma\Omega}{k_B T} D_s = \frac{\ell^4}{6\tau}$$

literature   simulation

ℓ is set by the spatial resolution of the simulation

τ is the slope of this line



Key Result: Surface diffusion is most likely the dominant mechanism, unless dealloying injects a large number of vacancies into the bulk.

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Modeling Corrosion in Molten Salt

Experimentally observed mechanisms

- Surface corrosion
- Intergranular corrosion (enhanced corrosion on grain boundaries)
- Dealloying (involves bulk diffusion)

Other possible processes

- Grain boundary diffusion
- Grain growth
- Stress effect/cracking

Modeling Corrosion in Molten Salt

Experimentally observed mechanisms

✓Surface corrosion

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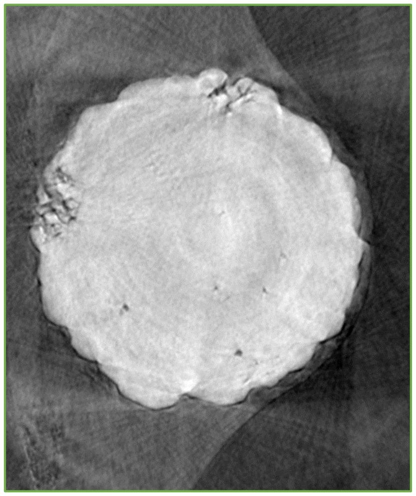

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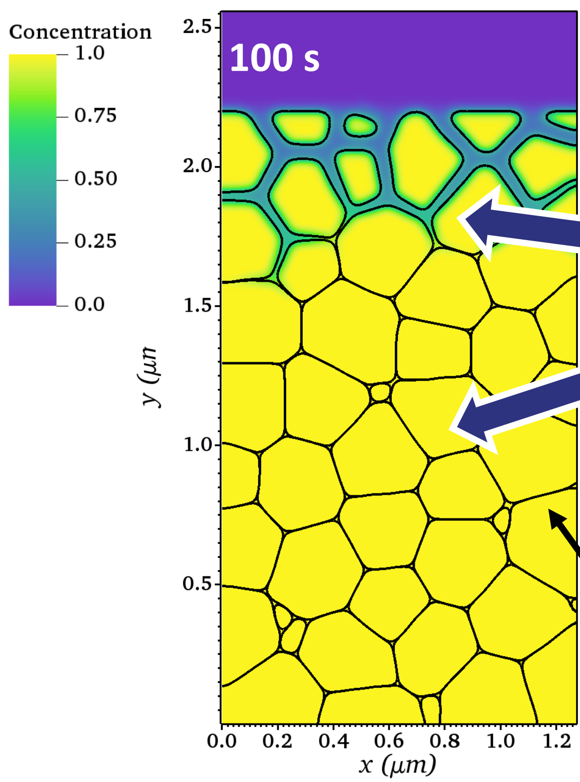
Intergranular Corrosion in a Pure Metal

Grain interfaces controlled by Allen-Cahn equation



$$\frac{\partial \eta_i}{\partial t} = -L \frac{\delta \mathcal{F}}{\delta \eta_i}$$

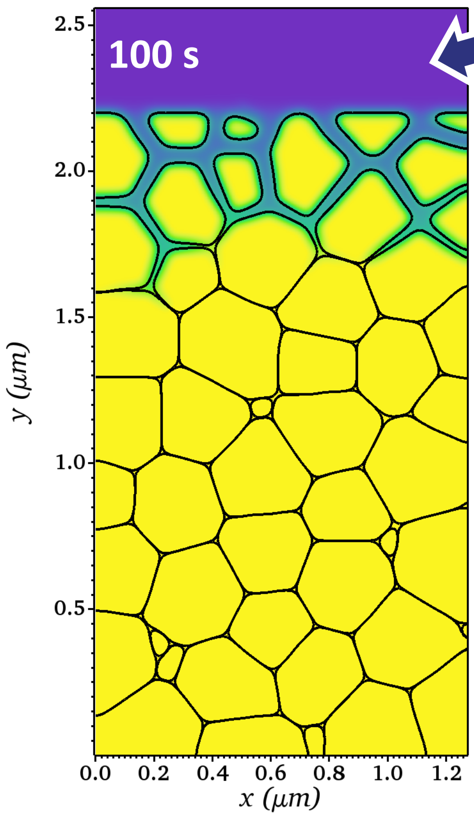
- Consider case of 100% Cr ($c_{\mathrm{Cr}} = \sum_i \eta_i$)
- Assume well-stirred and well-supported limit for the electrolyte

Lines mark $\eta_i = 0.5$ contours or grain boundaries

- The initial condition is a 2D slice from a structure generated in Dream3D

Groeber and Jackson. *Integr Mater Manuf Innov* **3**, 56–72 (2014)

Intergranular Corrosion in a Pure Metal



Metal/electrolyte interface evolution controlled by

$$\frac{\partial \psi_l}{\partial t} = \underbrace{\nabla \cdot \left[M(\psi_l) \frac{\delta \mathcal{F}}{\delta \psi_l} \right]}_{\text{Cahn-Hilliard evolution}} - \underbrace{v |\nabla \psi_l|}_{\text{Interfacial velocity}}$$

$$v = -\left(\frac{V_M}{z_M F} \right) i_{rxn}$$

Reaction current governed by Butler-Volmer equation

$$i_{rxn} = \sum_{j=1}^{N} \left[i_{corr,j} \exp\left(\frac{z_M (1-\beta) F}{RT} \eta \right) \left(\xi_j + 16\alpha \sum_{k>j}^{N} \xi_j^2 \xi_k^2 \right) \right]$$

α controls the enhancement of GB corrosion

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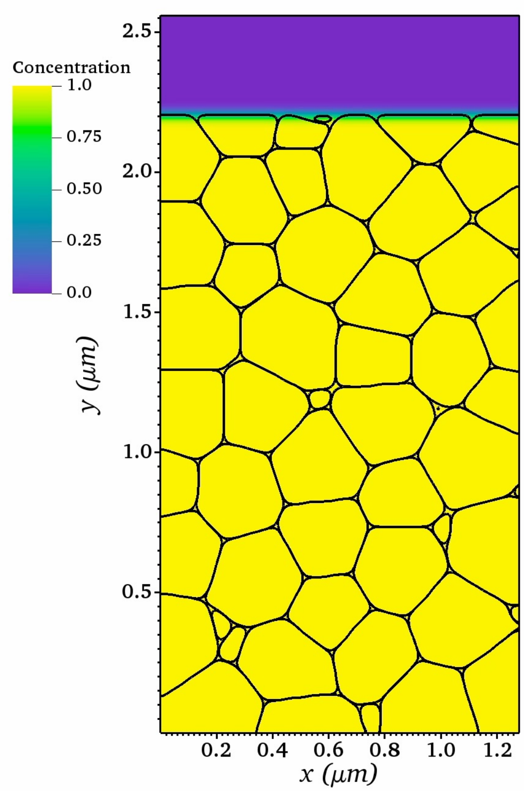
Intergranular Corrosion in a Pure Metal

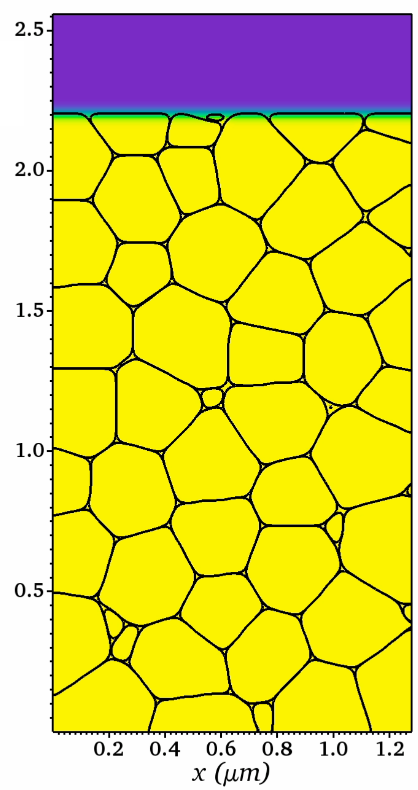
Surface corrosion only

$\alpha = 0$



With GB corrosion

$\alpha = 5$



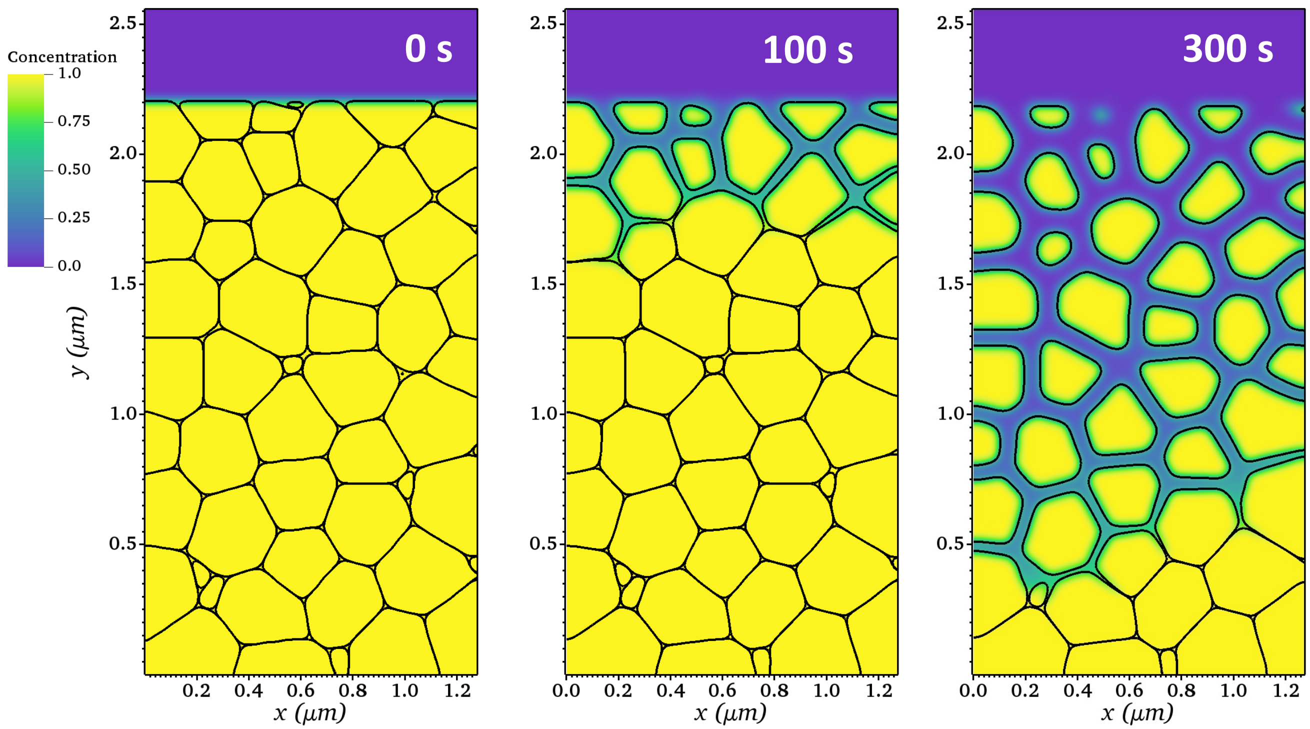
Left:

- Surface recedes nearly uniformly.
- Grain growth is observed

Right:

- Rapid corrosion along grain boundaries leads to potential detachment of grain remnants

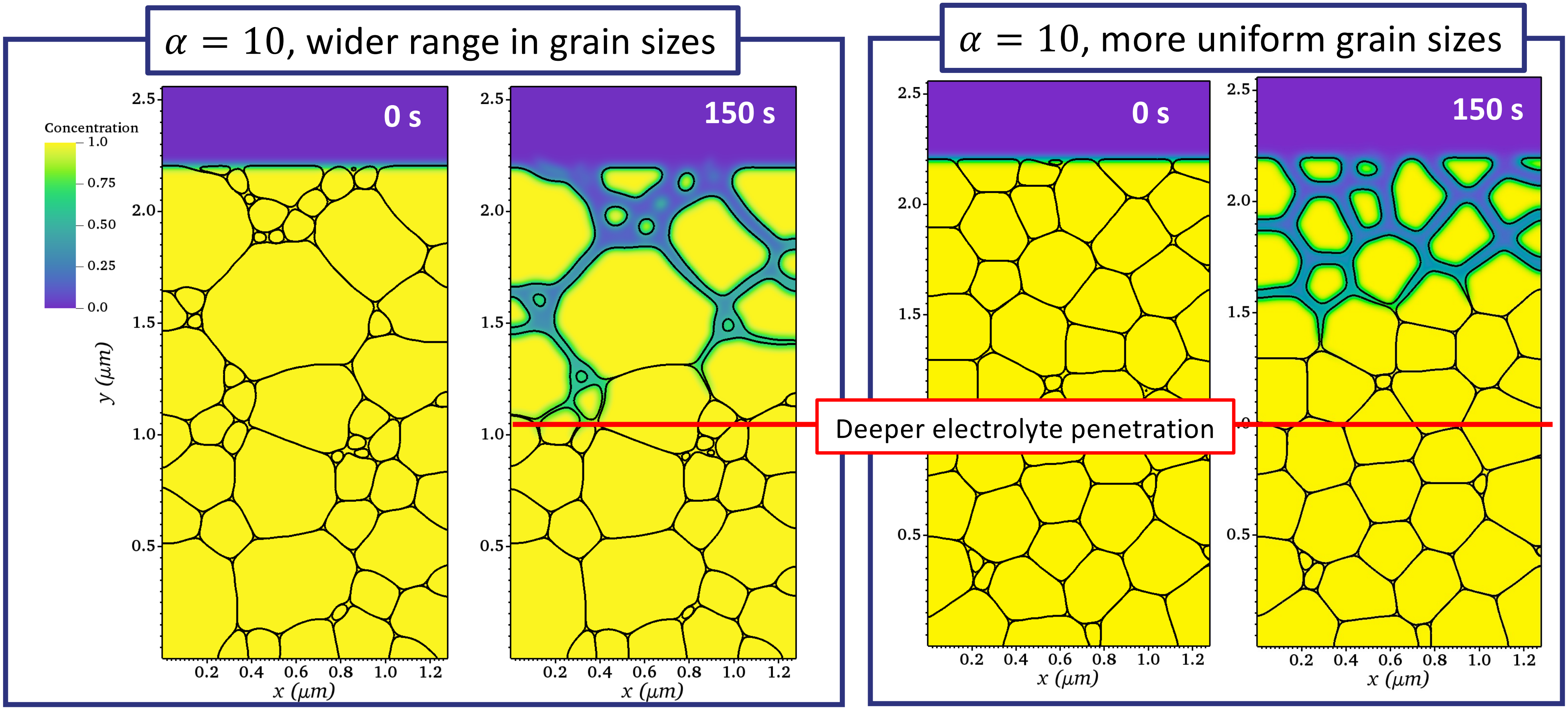
Intergranular Corrosion in a Pure Metal



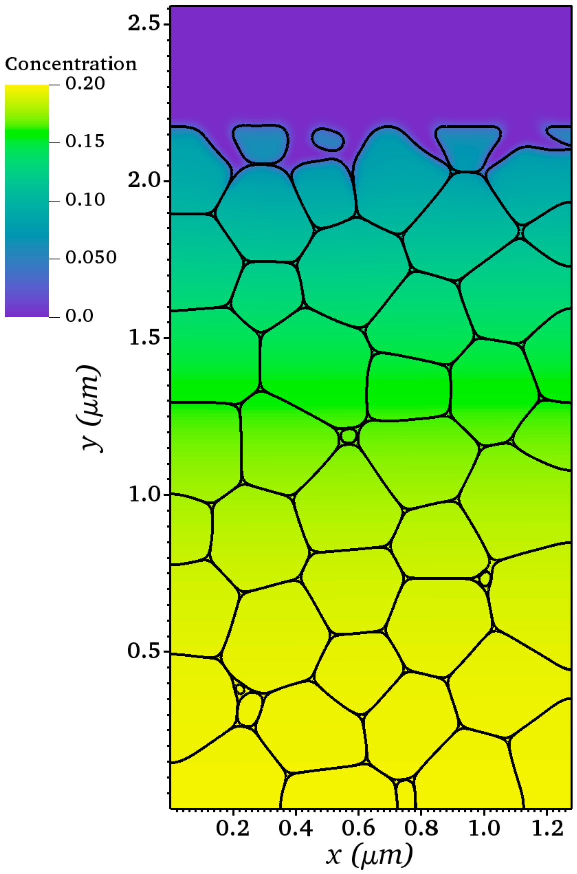
- We demonstrated that intergranular corrosion can be modeled along with grain growth
- While the detachment is exaggerated in 2D, nanoparticle formation is experimentally observed

Effect of Microstructure on Corrosion Behavior

Wider grain size distribution leads to faster corrosion because of the dissolution of small grains and larger ion diffusion path!



Intergranular Corrosion in an Alloy



We track the Cr concentration in the alloy using the smoothed boundary method (SBM):

$$\frac{\partial c_{\mathrm{Cr}}}{\partial t} = \frac{1}{\psi_{\mathrm{s}}} \nabla \cdot (\psi_{\mathrm{s}} D \nabla c_{\mathrm{Cr}}) - \frac{|\nabla \psi_{\mathrm{s}}|}{\psi_{\mathrm{s}}} \left(\frac{i_{\mathrm{rxn}}}{zF} \right)$$

$\psi_{\mathrm{s}} = 1 - \psi_{\mathrm{l}}$ is the domain parameter for the solid phase
Restricts concentration of Cr to the solid phase

We calculate the overpotential from the chemical potential of Cr in molten chloride salt

$$i_{\mathrm{rxn}} = \sum_{j=1}^{N} \left[i_{\mathrm{corr},j} \exp\left(\frac{z_{\mathrm{M}}(1-\beta)F}{RT} (\mu_{\mathrm{Cr}} - \mu_{\mathrm{Cr,eq}}) \right) \left(\xi_j + 16\alpha \sum_{k>j}^{N} \xi_j^2 \xi_k^2 \right) \right]$$

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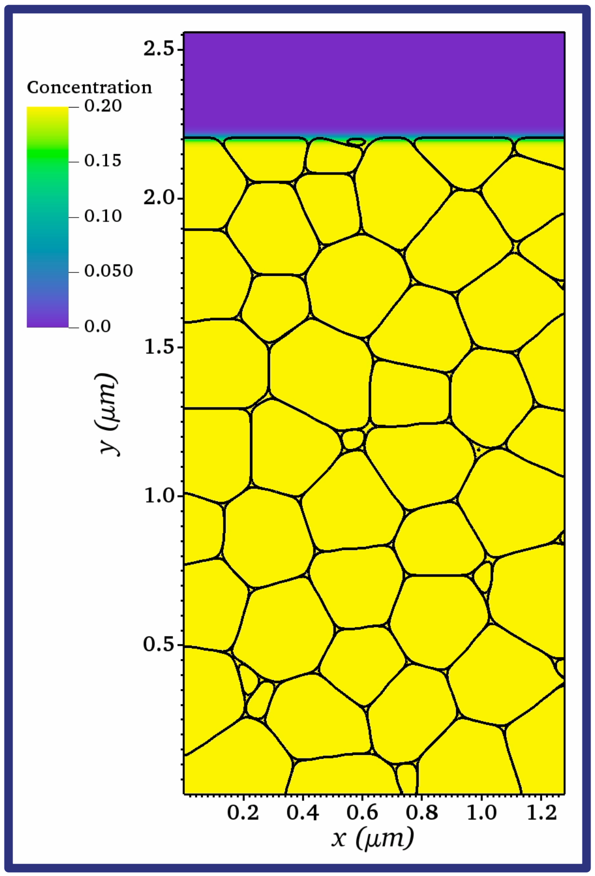
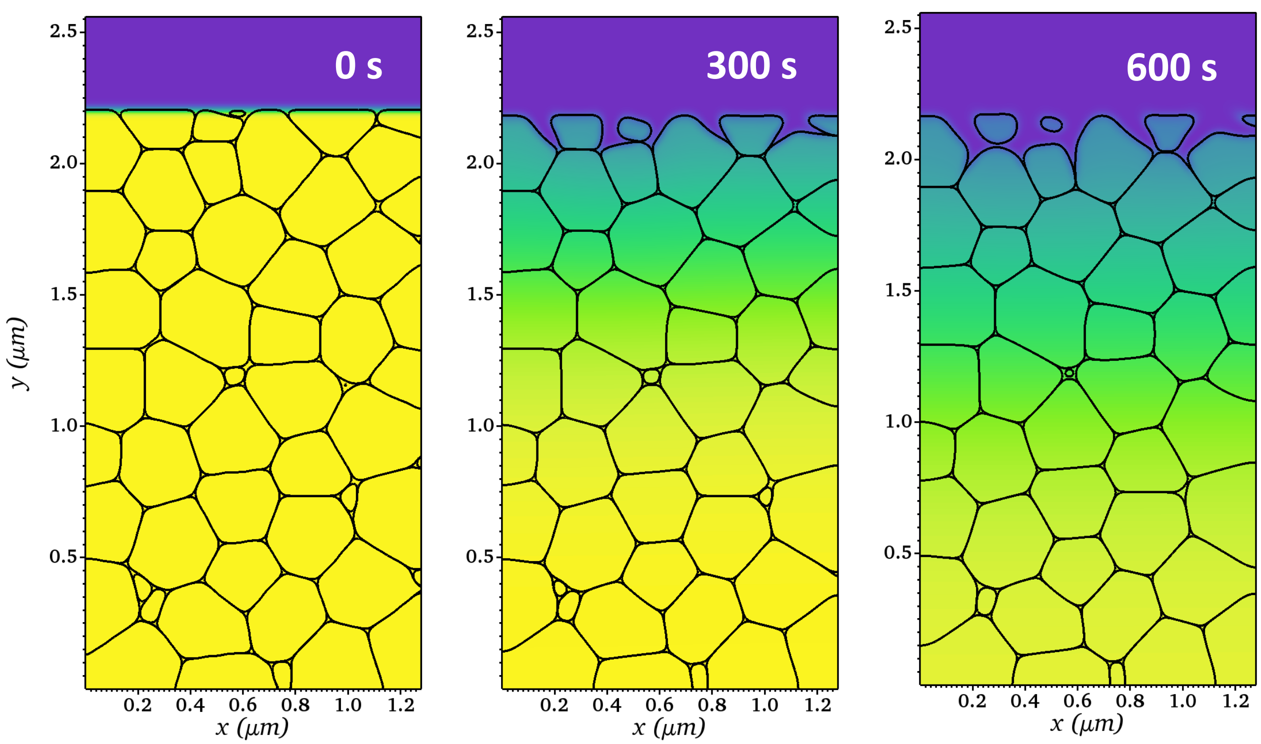
Intergranular Corrosion in an Alloy

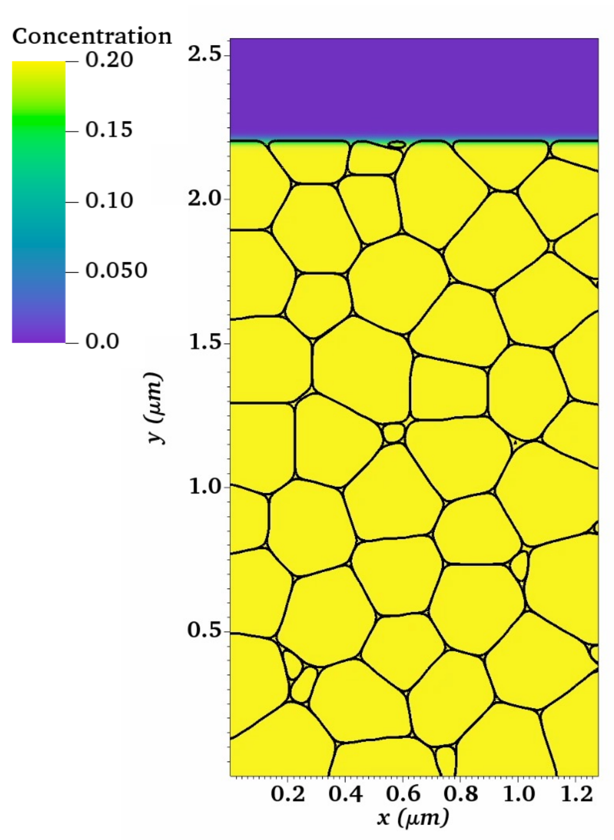
Simply changing the model to a two-component system did not yield a result similar to the experiment! – What's missing?



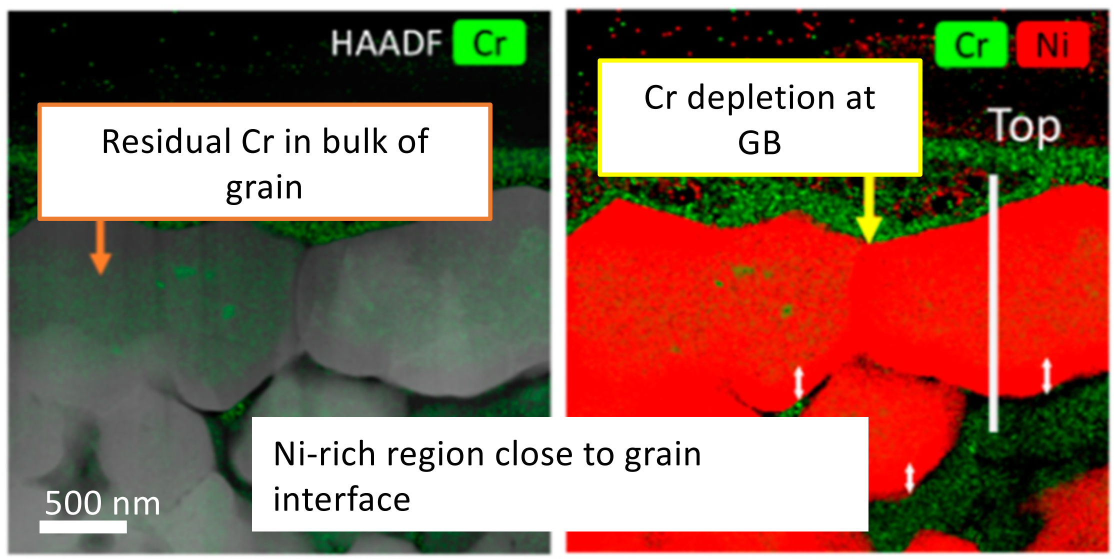
$\alpha = 10$



Enhanced Diffusivity at the Grain Boundary



$$D = \sum_{j=1}^{N}\left[\xi_j D_{\mathrm{bulk}} + 16 D_{\mathrm{GB}} \sum_{k>j}^{N} \xi_j^2 \xi_k^2\right]$$



EDS analysis of Ni-20Cr sample after intergranular corrosion

Liu et al. *ACS Appl. Mater. Interfaces*, **15**, 13772−13782 (2023)

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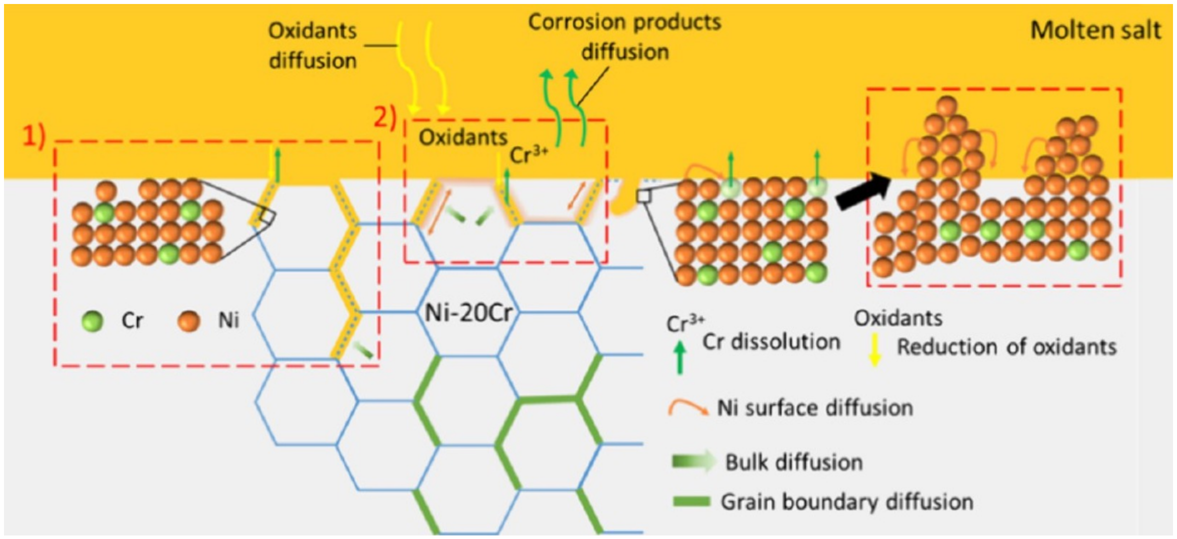
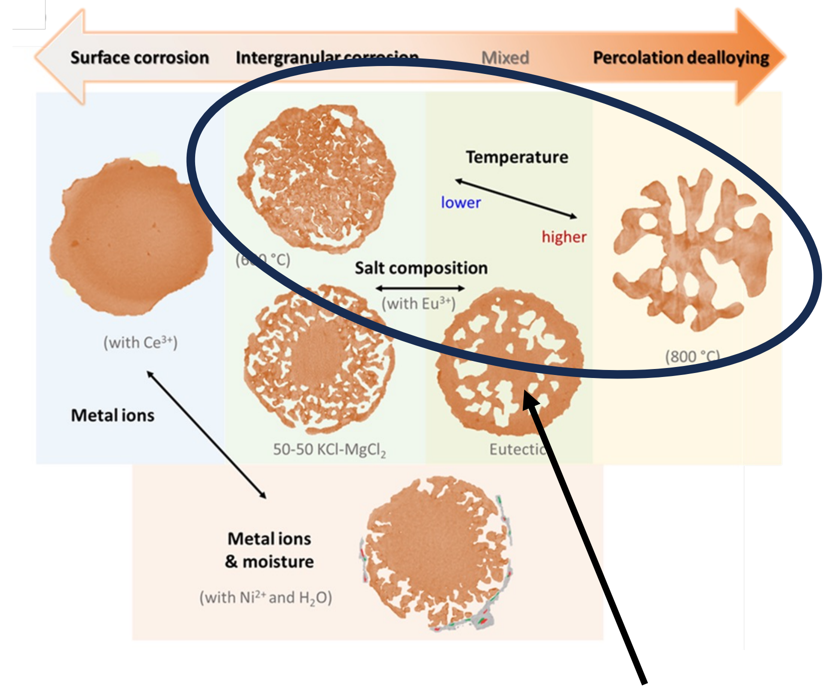
Working Towards the Morphological "Phase Diagrams"



Liu et al. *ACS Appl. Mater. Interfaces*, **16** (34) 45606–45618 (2024)
Liu et al. *ACS Appl. Mater. Interfaces*, **15**, 13772–13782 (2023)



How does this transition occur?

- Challenge: Parameterization of the model
- We need to link electronic structure/atomistic simulations to model parameters!

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Take-Aways

- We developed an open-source software application in PRISMS-PF for the materials science community to simulate corrosion.
- Presented two example applications:
  - Corrosion in magnesium alloys
  - Corrosion in molten salt informed by experiments
- Microstructural effects:
  - The surface area of the cathodic material has a strong effect on how corrosion is accelerated
  - Grain size distribution has an important consequence on the grain boundary corrosion
  - Grain boundary diffusion may be important in molten salt corrosion
  - Electrochemical processes can amplify the stochastic nature of the microstructure; **how can we take this into account on a coarse-grained model?**

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Thank you!

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