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Project # 213006 / Phase Field Modeling of Radiation-Induced Segregation

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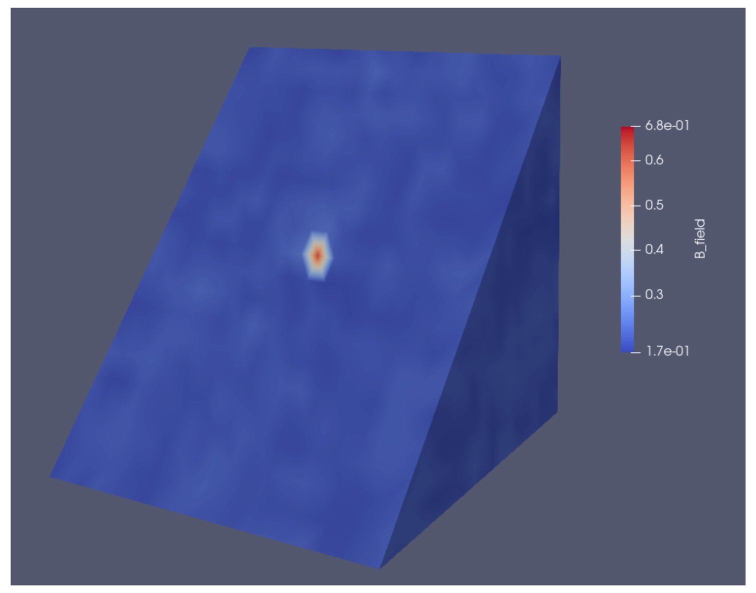
Introduction / Motivation

- **Radiation-induced segregation (RIS)** is a degradation process where defects created in radiation damage events accelerate the diffusion of alloying elements in metals, disrupting the random distribution of alloys.
- RIS can lead to the **formation of precipitates or segregation at microstructural defects** such as grain boundaries, which can change the mechanical properties of the material and potentially lead to premature failure.
- The length-scale and time-scale of radiation-induced segregation is too large and too long to use conventional quantum mechanics or atomistic simulation techniques.
- Here we developed and used a phase field model **simulate RIS in binary alloy systems allowing for very long simulated times and high dose rates.**

Approach

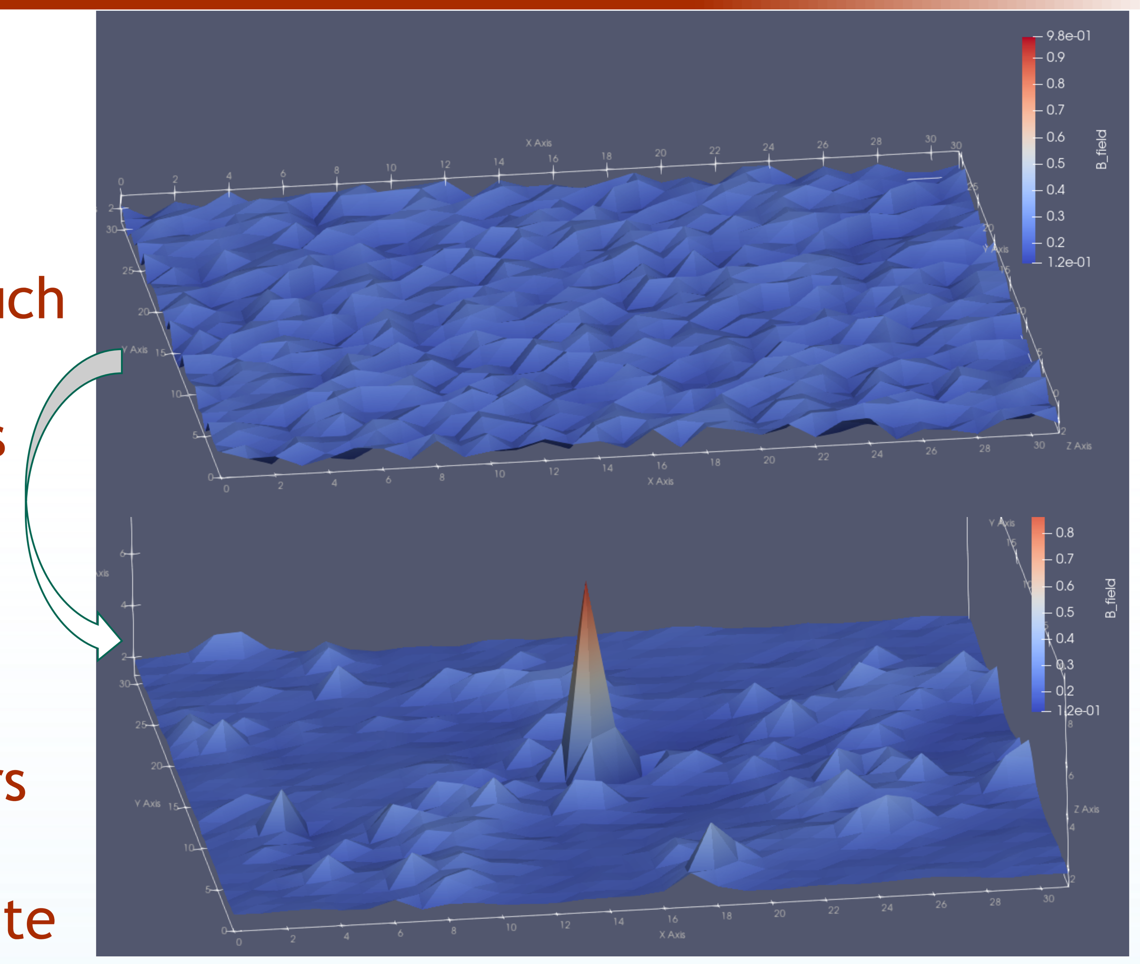
- Phase field models use coupled partial differential equations (PDEs) to model the evolution over time of as many species as you have equations.
- This model uses eight unique PDEs to model RIS.
- **Electron vs. ion irradiation:** Defects can be introduced into the system via two different methods: Frenkel pair insertion or cascade-like insertion.
- **Point defects** are allowed diffuse through the system and recombine with each other.
- **Defect clusters** are created by damage events and can either grow or shrink in size by interacting with point defects.
- **Segregation and/or phase separation** can occur via direct migration of the alloy species or via diffusion and annihilation of point defects.
- This model also includes dislocations as defect sinks and considers the elastic effects of dislocations as well as radiation-induced defects on the chemical potentials of the mobile species.



Render of the B species concentration after 1 day at 10^{-7} dpa/s .

Current Status/ Results

- Implementation into SNL's phase-field simulation framework MEMPHIS.
- **Result 1 - Effect of pre-existing defects:** segregation begins to occur at defect sinks such as dislocations and defect clusters.
- **Result 2 - Effect of defect type:** Dislocations are the most efficient sinks for initiating RIS, with vacancy and interstitial clusters also working but on a substantially longer time-scale.
- **Result 3 - Effect of radiation type:** RIS occurs sooner with cascade-like damage insertion, although this could also be related to dose rate and temperature.



B-species evolution in an 80-20 alloy irradiated at 10^{-7} dpa/s. Segregation at the dislocation is complete after one month.

Challenges

- **Calibration:** The equations for this model are highly sensitive to small changes in the constants used to define the material behavior, some of which are abstracted from real material constants.
- **Time-integration:** The behavior of the model is also highly temperature dependent, with large temperature changes requiring either changes to the constants used or a decrease in the size of the timestep used.

Next Steps/ Future Work

- Benchmarking.
- **Molten-Salt Corrosion:** Integration of the radiation-induced segregation model in MEMPHIS with a corrosion model.
- **Aging of microstructures:** Possible integration of this model with a grain growth model to examine RIS in polycrystalline systems.
- Publication in preparation.