SAND2022-2203C

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Dose Rate Effect on Radiation-Induced Segregation

A Phase Field Examination in MEMPHIS

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03/02/2022
TMS 2022 Annual Meeting & Exhibition
Anaheim, California

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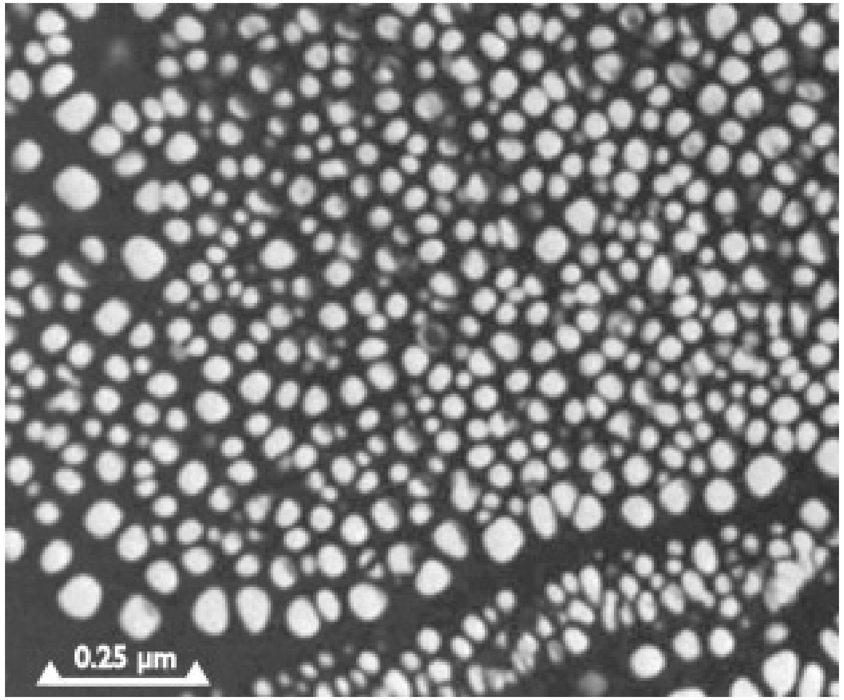
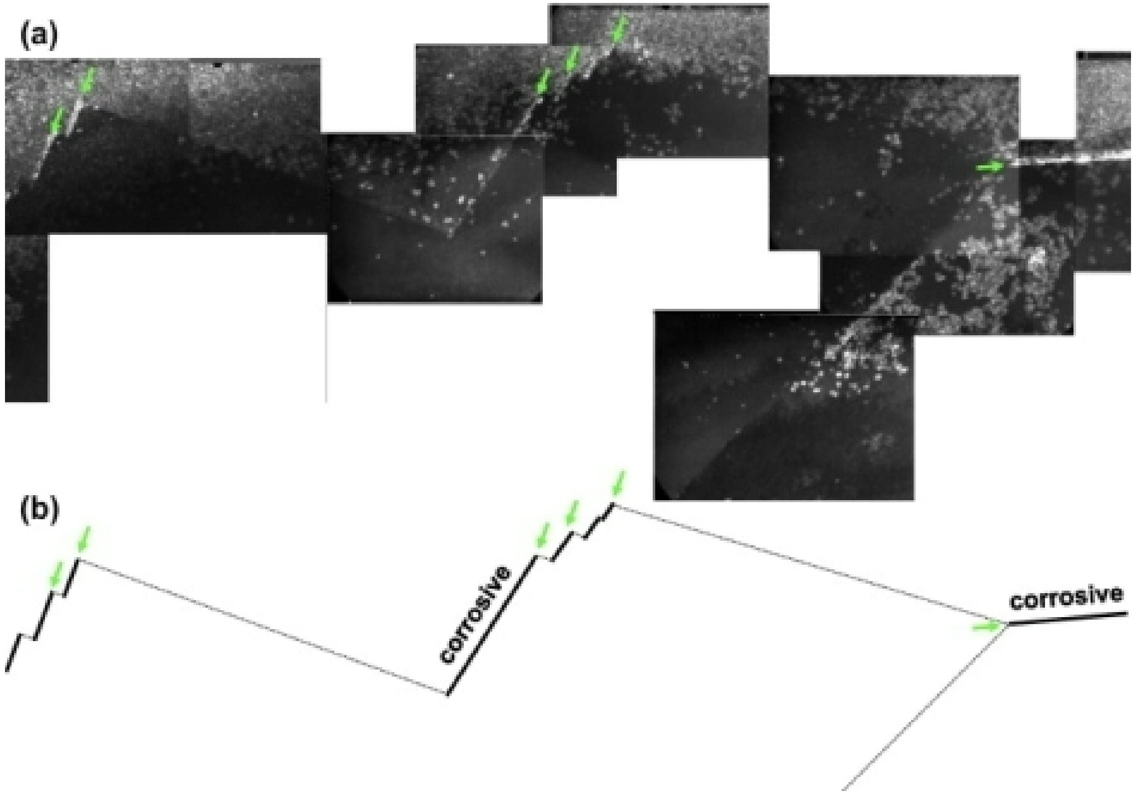
What is Radiation-Induced Segregation (RIS)?



Dark field image showing Ni_3Si precipitation in a Ni-8 at.% Si alloy irradiated at 600°C by 400 keV protons to a dose of 0.25 dpa[1,2].



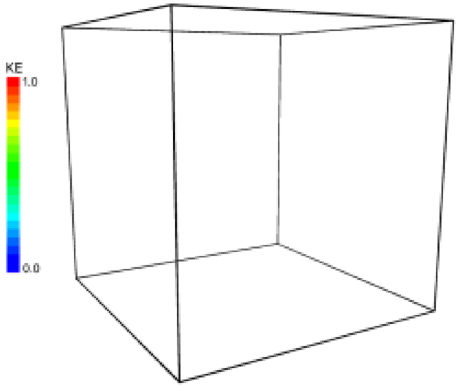
TEM images of proton irradiated 316L stainless steel after electrochemical etching, and a schematic of the grain boundary[3].

The evolution of radiation damage involves complex processes across scales

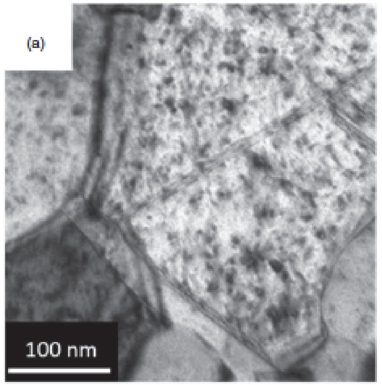
Picoseconds — Microseconds - Days — Seconds - Years

Tens of nm — Hundreds of nm - Hundreds of μm — cm - m

Molecular Dynamics → Kinetic Monte Carlo → Rate Theory



Simulation Courtesy of Elton Chen.



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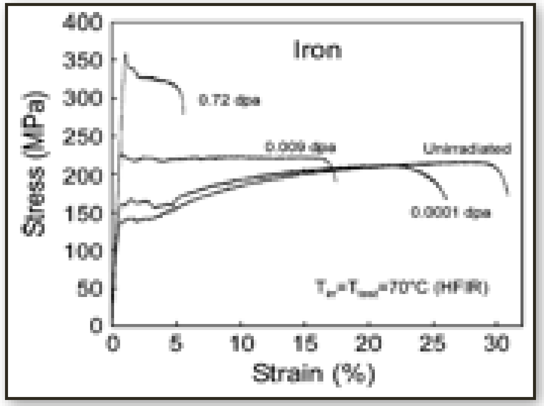


Eldrup (2002) *J. Nucl. Mater.*

"Special" Physics

- keV-energy collision between nuclei
- Energy loss to electronic excitation
- Transition to high P-T
- Long term relaxation

Radiation Damage

- Defect production: Frenkel pairs, Cascade
- Transmutation
- Segregation
- Amorphization
- Sputtering

Radiation Effects

- Hardening
- Swelling
- Embrittlement

What are the microstructural features of interest?

- **Field variables:**
  - Species: X_A and X_B
  - Point Defects: X_V X_{iA} X_{iB}
  - Defect Clusters: X_{VC} X_{iAC} X_{iBC}
- **Interactions:**
  - Diffusion of point defects and species A and B
  - Point defect recombination
  - Point defect-defect cluster interactions
    - In these terms, changes to defect concentrations directly effect the concentrations of the A and B species
  - Point defect and defect cluster evolution at dislocations

Composition evolution

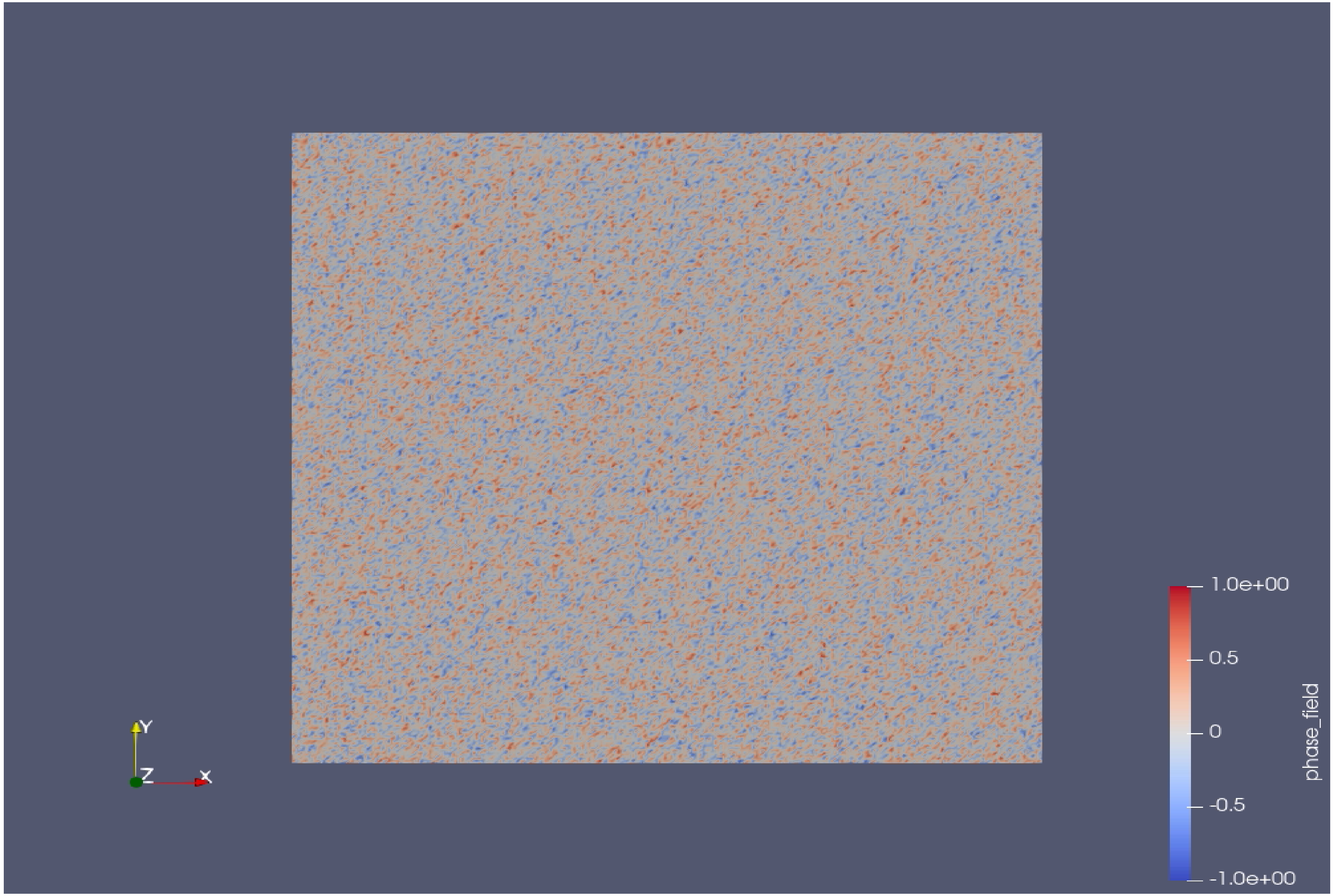
- $\frac{\partial X_\alpha}{\partial t} = \nabla \cdot \left[\sum_d \sum_\beta \frac{\ell^d_{\alpha\beta} X_d}{k_B T} (\nabla \mu_\beta + sign(d) \nabla \mu_d)\right] + R_{V,i\alpha} + R_{VC,i\alpha} + R_{V,i\alpha C}$

Irradiation environment

- $\frac{\partial X_d}{\partial t} = \nabla \cdot \left[\sum_d \sum_\beta \frac{\ell^d_{\alpha\beta} X_d}{k_B T} (sign(d) \nabla \mu_\beta + \nabla \mu_d)\right] + R_{recom} + R_{d,sink}$
- $\frac{\partial X_{VC}}{\partial t} = R_{V,VC} - \sum_\alpha R_{i\alpha,VC}$
- $\frac{\partial X_{i\alpha C}}{\partial t} = (R_{i\alpha,iAC} + R_{i\alpha,iBC}) - R_{V,i\alpha C}$

Radiation damage evolution

Phase-field method to track the spatio-temporal evolution of both radiation damage and local composition evolution

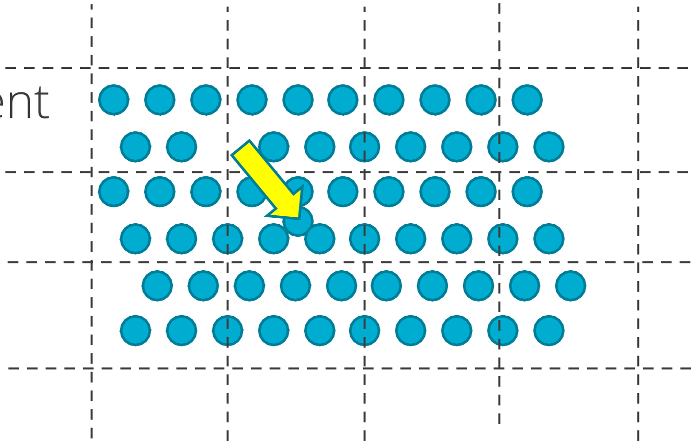


Methodology: Damage insertion mechanisms

Higher Event Rate

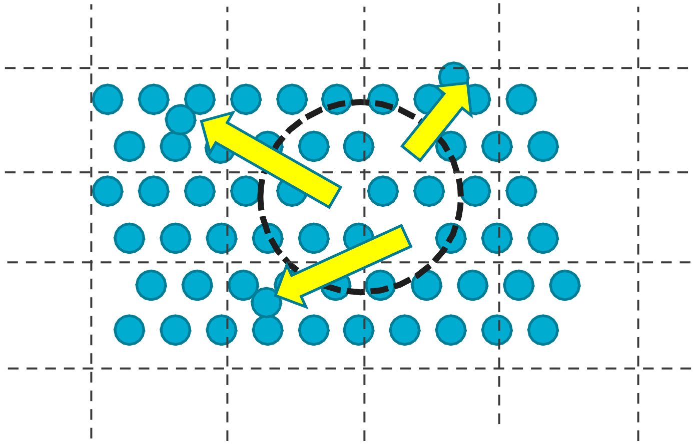
Lower Event Rate

Frenkel Pair Insertion



Defects per Event
1 Vacancy
1 Interstitial

Cascade-like Insertion*



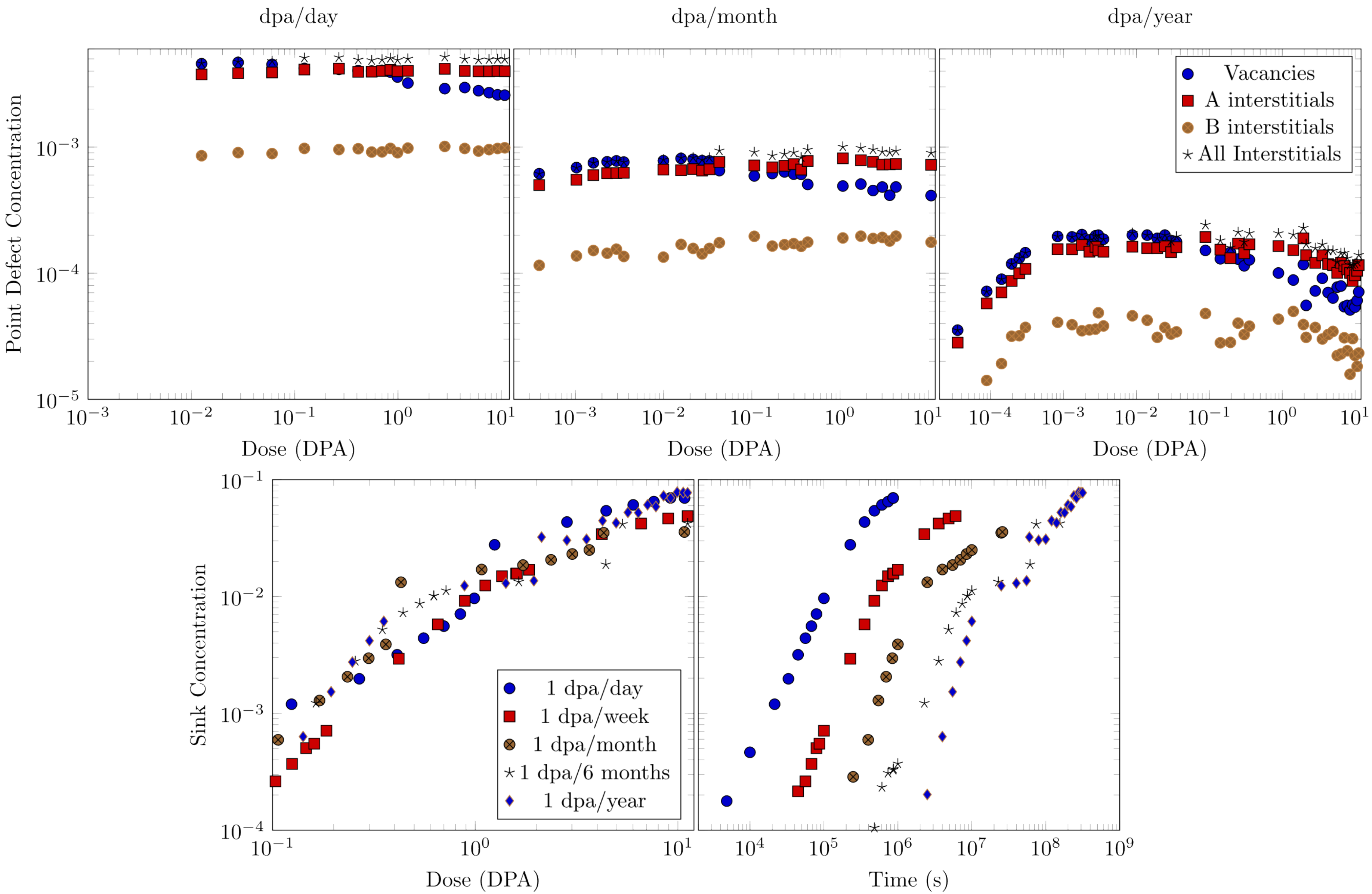
Defects per Event
N_{dpa} Vacancies
N_{dpa} Interstitials

Less Local Mixing

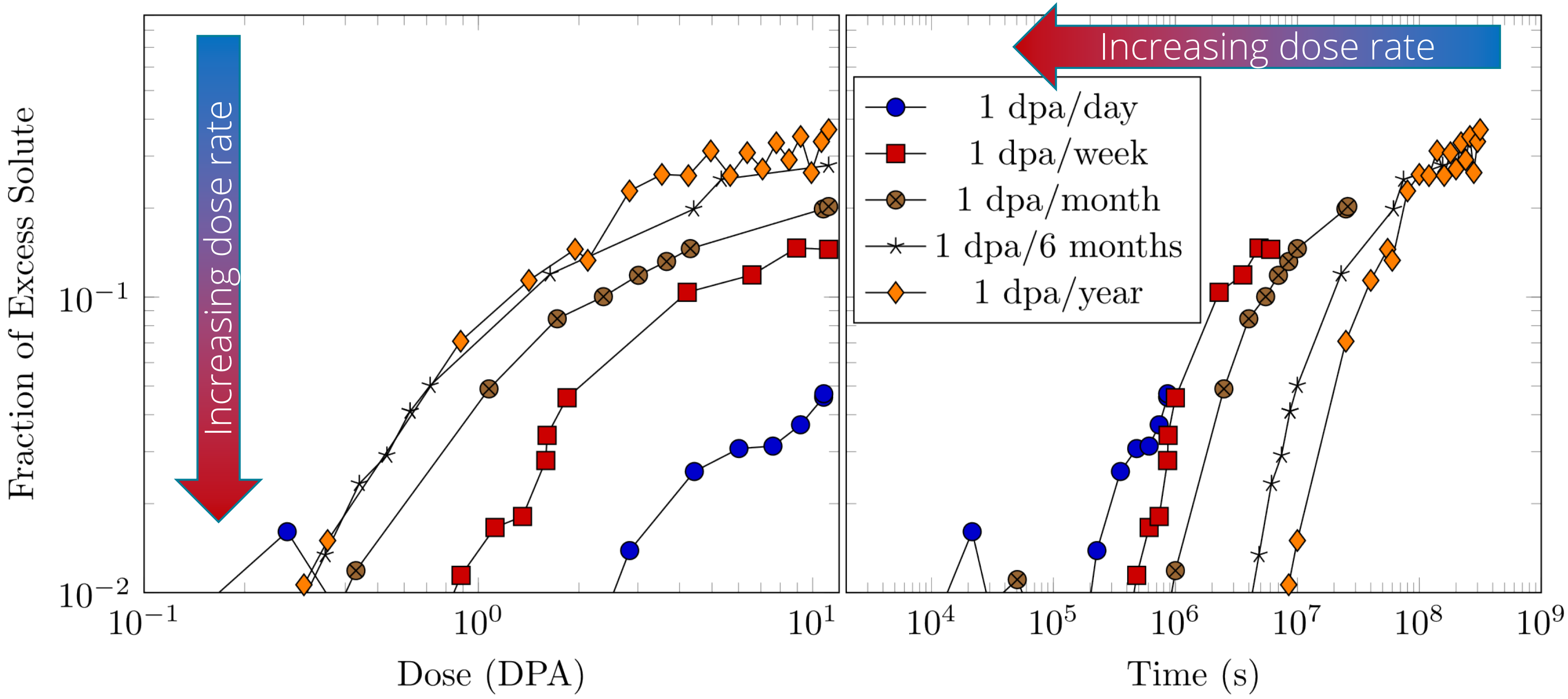
More Local Mixing

*: modeled after [4]

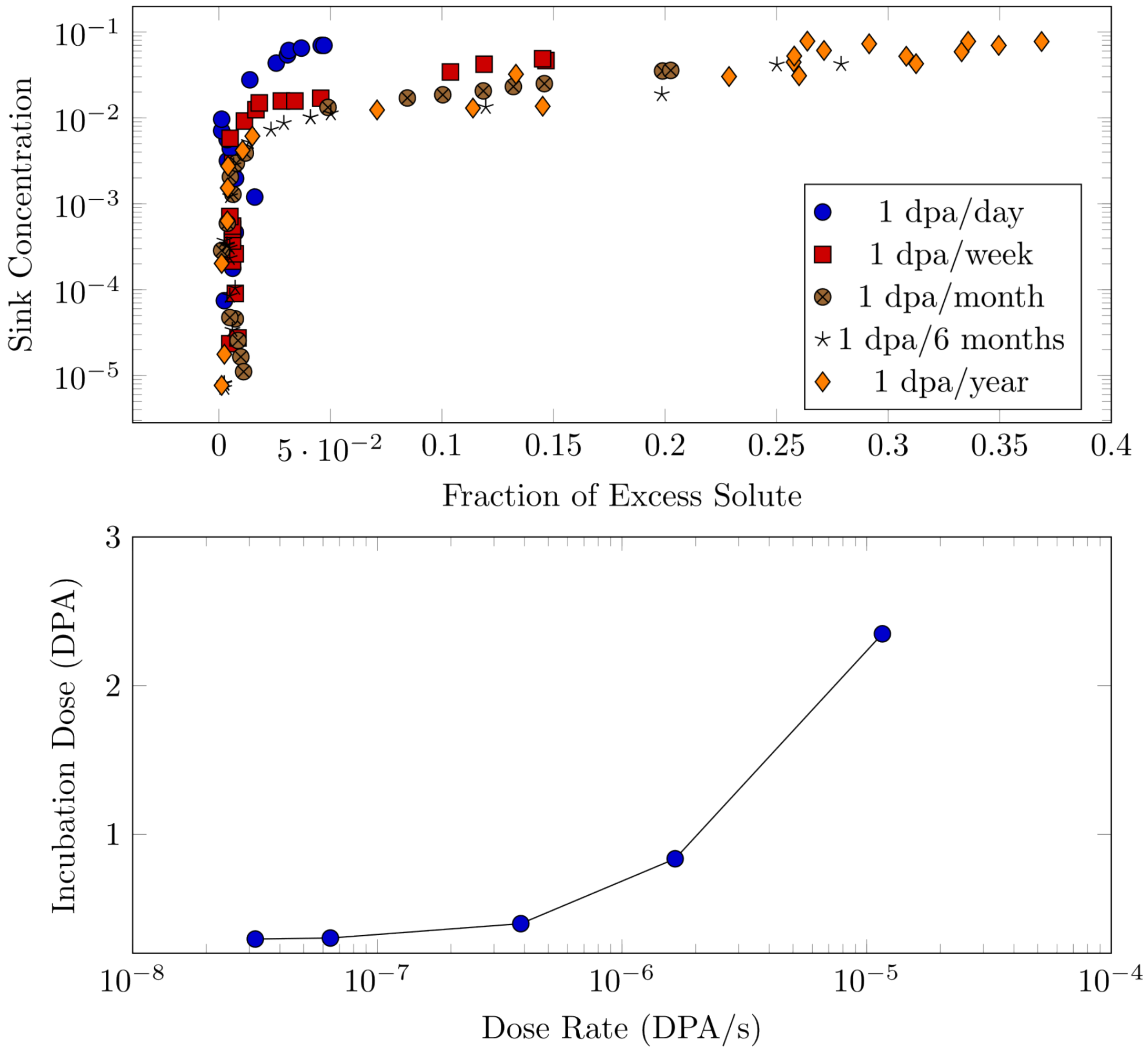
Low dose rates result in lower defect densities



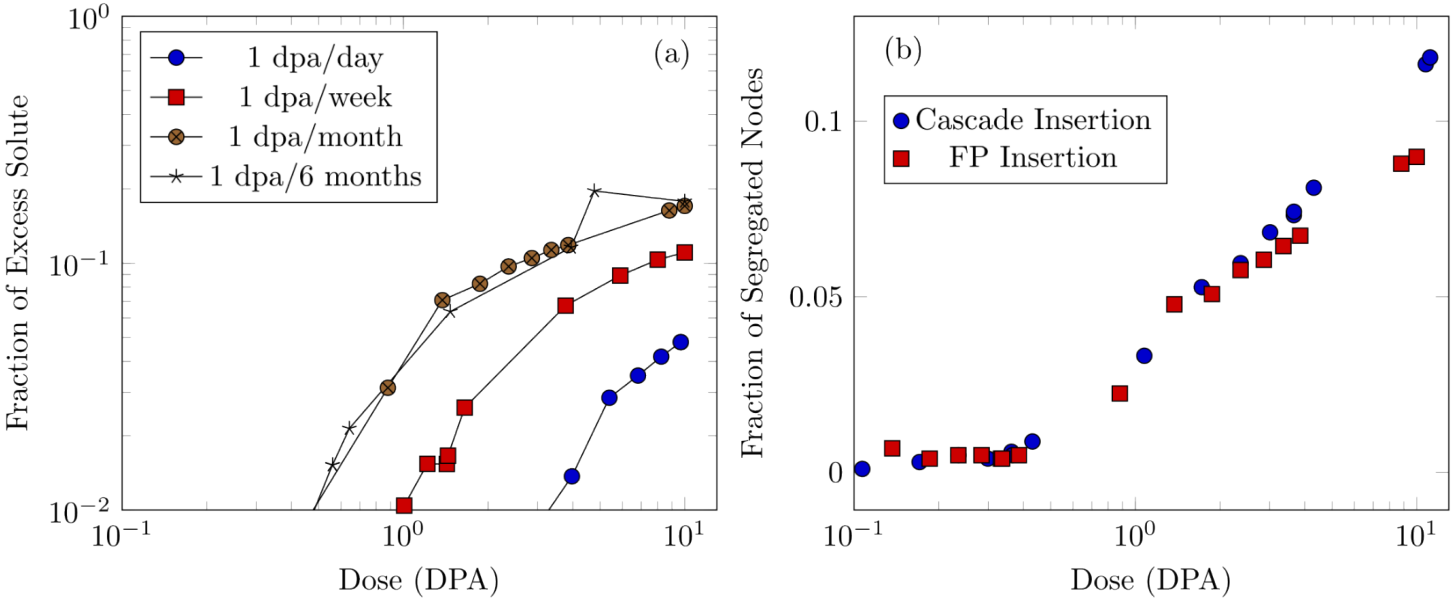
Increasing dose rate results in a reduction in RIS

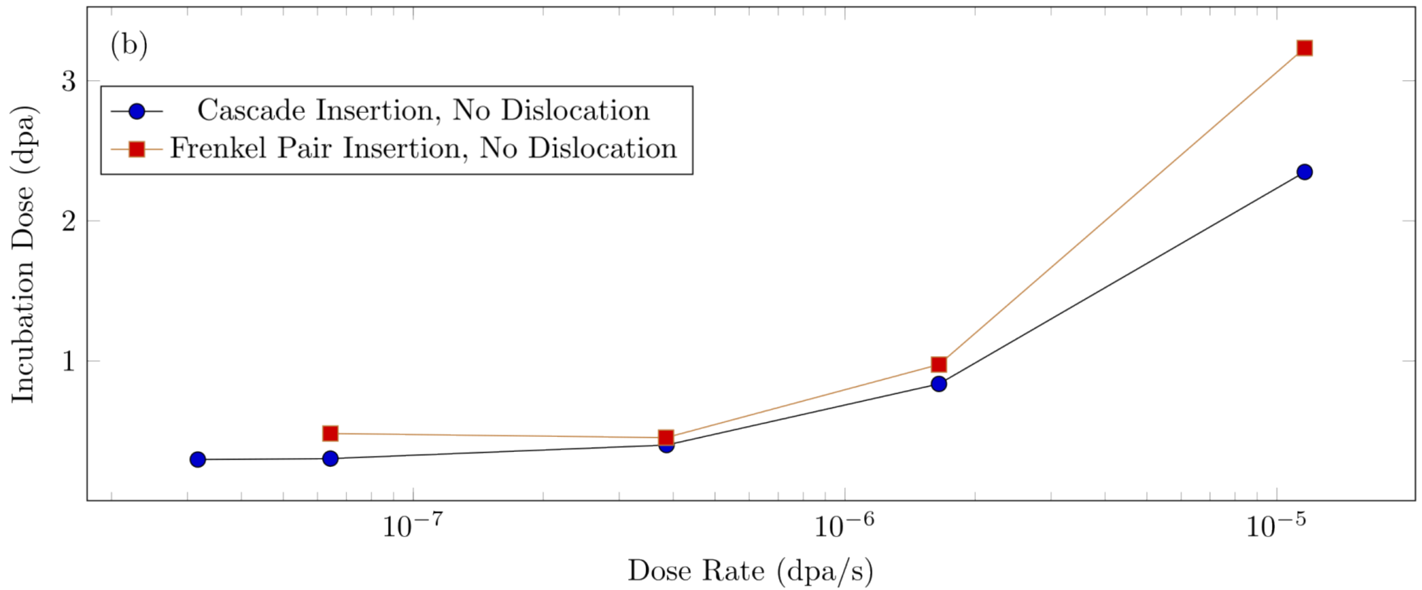


Increasing dose rate increases incubation dose

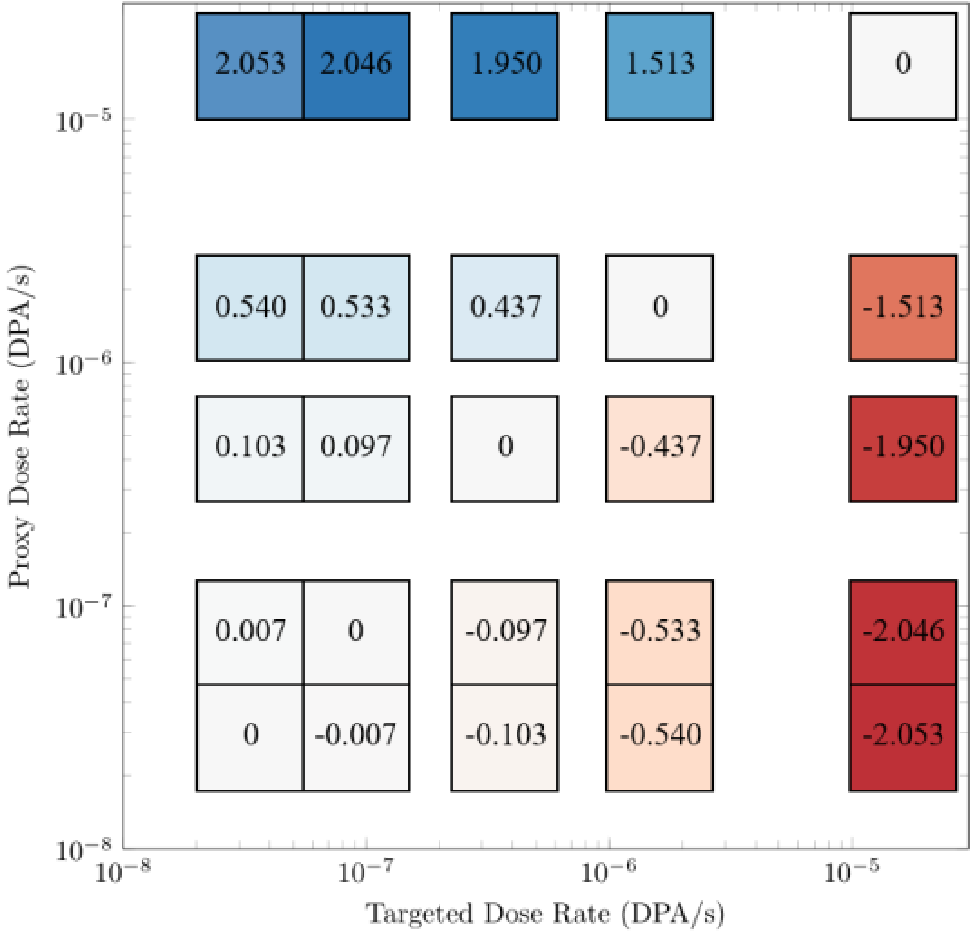


The effect of incident particle type:
FP vs. Cascade-like insertion has a dose rate dependent effect

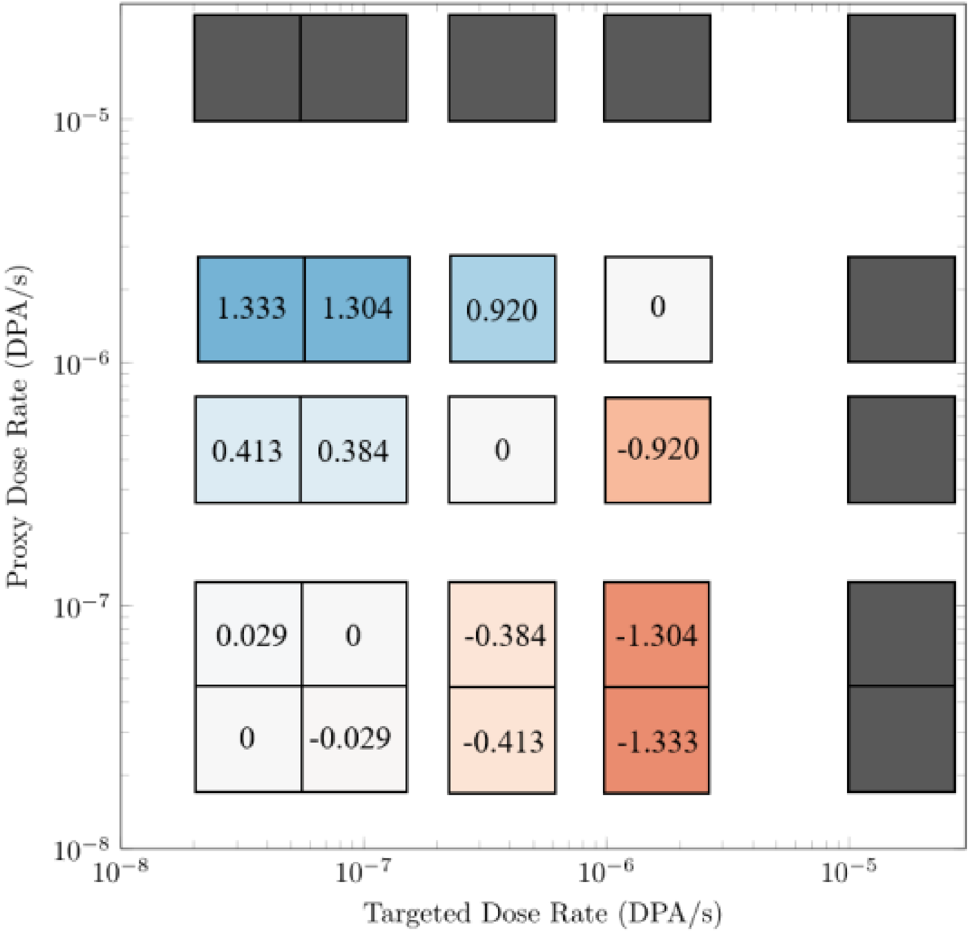




Matching segregation statistics between different dose rates

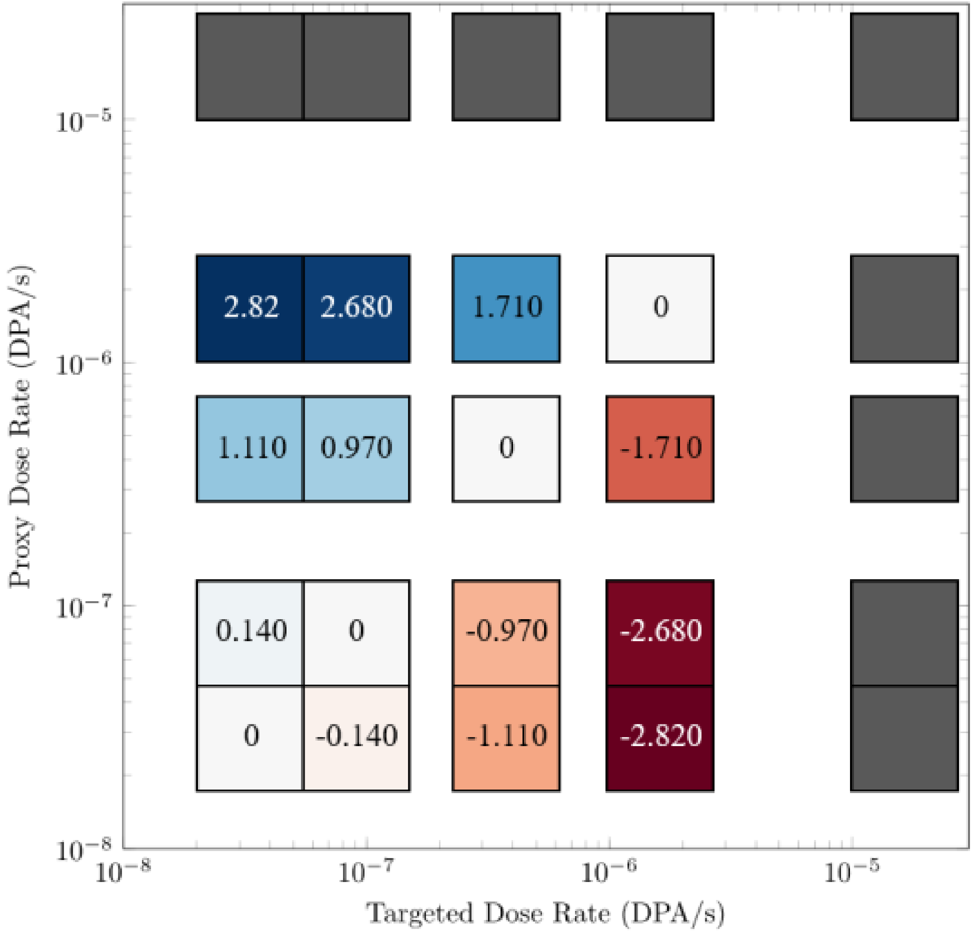


1% RIS

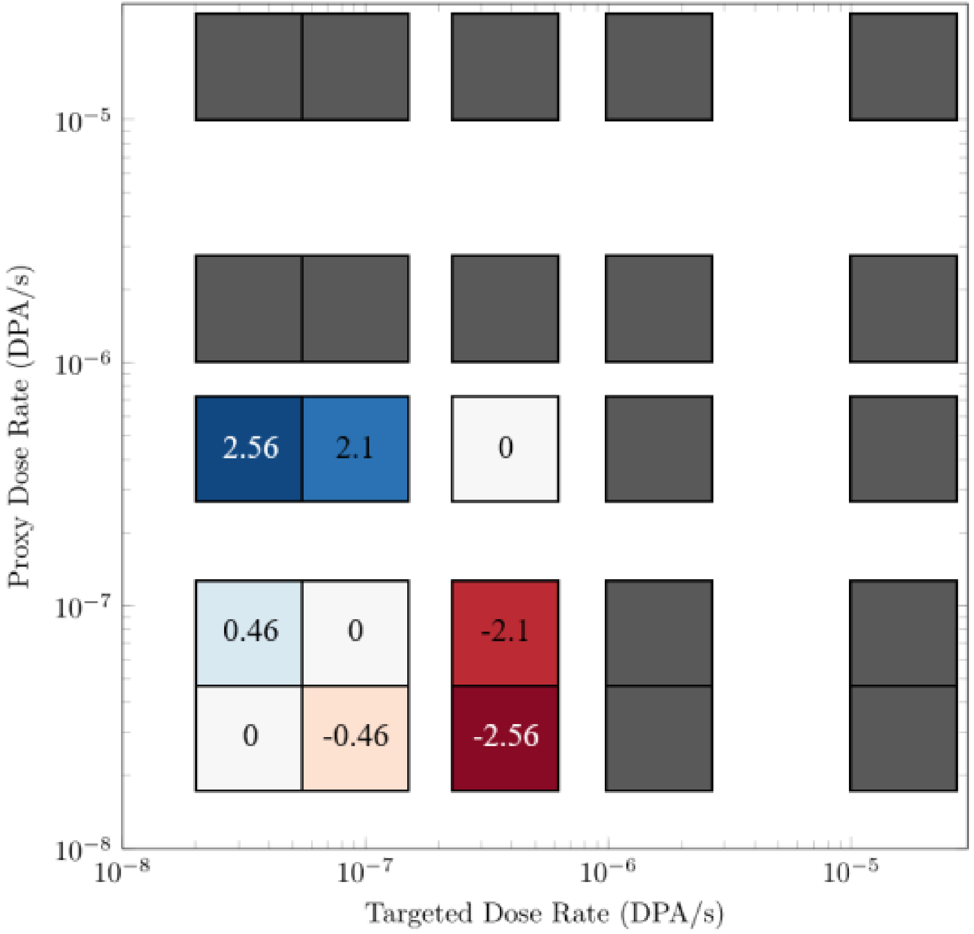


5% RIS

Matching segregation statistics between different dose rates



10% RIS



15% RIS

Conclusions

- We have illustrated the strong dependence of RIS on the presence of defect sinks to serve as nucleation sites for segregation.
- A reduction in dose rate results in a reduction of the incubation dose and an increase in the progression of RIS at equivalent doses.
- Different damage insertion techniques result in measurable differences in RIS behavior, with FP insertion enhancing RIS development at very high dose rates and cascade-like insertion enhancing RIS development at lower dose rates.
- The effect of compensating for changes in dose rate can be achieved in part by shifting the dose at which a specific RIS behavior is observed in a proxy condition to that in a targeted environment.

Funding sources and collaborators

Special thanks to:

- Elton Chen
- James Stewart

Acknowledgements:

R.D. is supported by the United States (U.S.) Department of Energy (DOE) Office of Basic Energy Sciences (BES), Department of Materials Science and Engineering.

D.V. and C.D. are supported through the Sandia Academic Alliance (SAA) Program.

The phase-field framework is supported by the Center for Integrated Nanotechnologies, an Office of Science user facility operated for the U.S. Department of Energy

Questions?

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