SAND2016-7710PE

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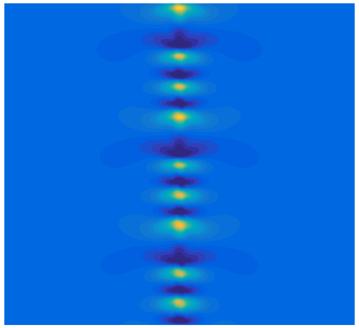
# Interactions of radiation-induced defects with microstructure



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Northwestern University

Supervised by
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Org. 6233

**6220/6230 summer student mini-symposium**
**August, 16th 2016, Sandia Nat'l Labs, Albuquerque NM**

U.S. DEPARTMENT OF ENERGY
NNSA National Nuclear Security Administration
LDRD Laboratory Directed Research & Development

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# Outline

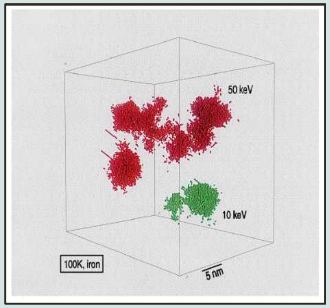
1. Microstructural changes due to irradiation directly lead to a degradation of materials performances

2. Modeling the coupling of radiation damage accumulation with mechanics using a chemo-mechanical numerical framework

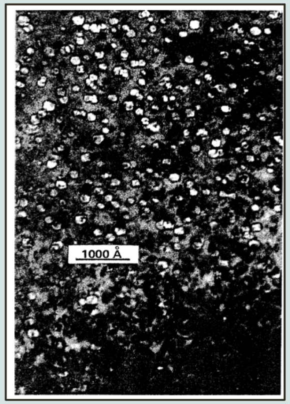
3. Segregation of radiation-induced defects to microstructural defects: dislocations, grain boundaries and triple junctions

4. Conclusion

# Radiation damage and radiation effects in materials

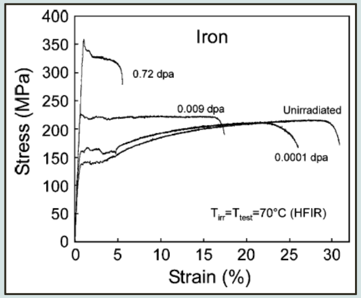


Stoller (2000)

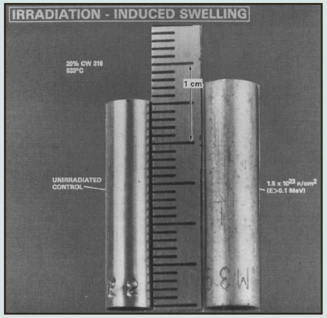


Harkness and Li (1971)

## Radiation Damage



Eldrup et al. (2002)



Mansur (1994)

## Radiation Effects

**Cascade / Frenkel pair implantation**

**Defect accumulation**

**Hardening, swelling, embrittlement**

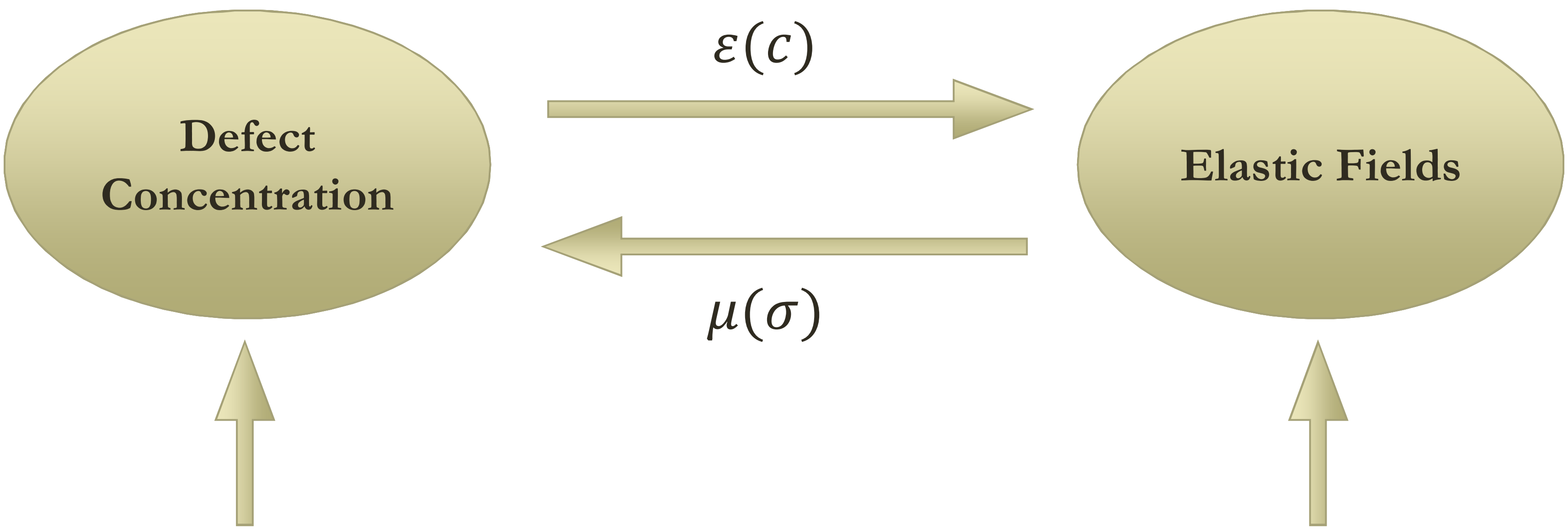
## Time Scale

picoseconds — microseconds - years — seconds - years

tens of nm — hundreds of nm - hundreds of μm — cm - m

## Length Scale

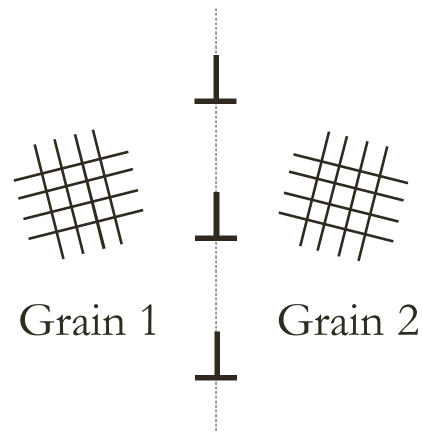
# Modeling of radiation damage accumulation: Cluster Dynamics coupled with mechanics

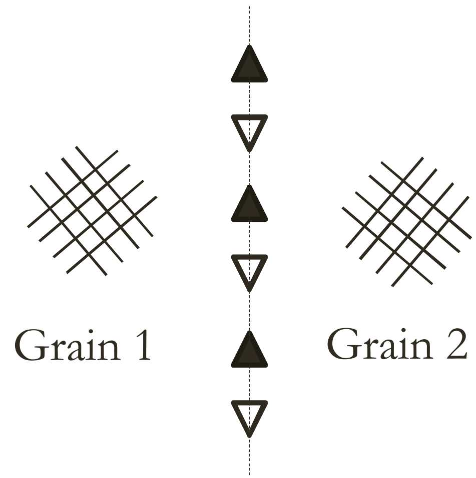



Defects diffuse according to Fick's laws and interact with each other based on mean field rate theory.

Intrinsic stress of the local microstructure is calculated using continuum mechanics.

# Construction of grain boundaries using dislocations and disclinations

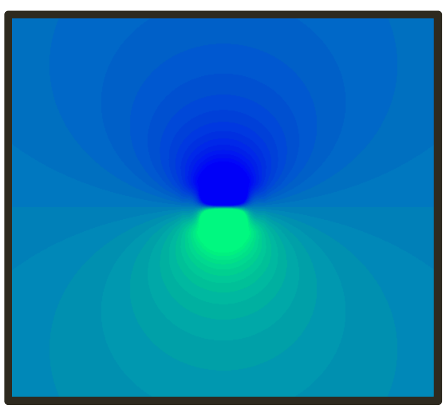


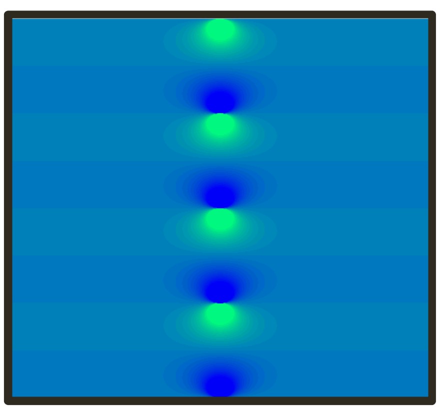



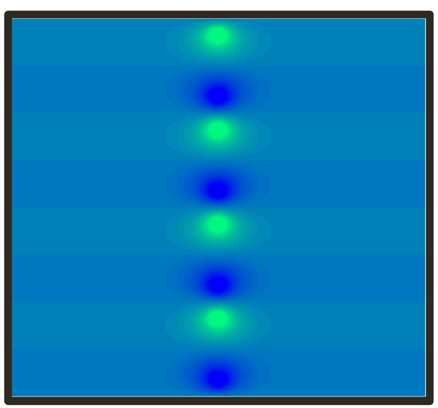

Isolated edge dislocation

Low-angle symmetric tilt grain boundary

High-angle symmetric tilt grain boundary

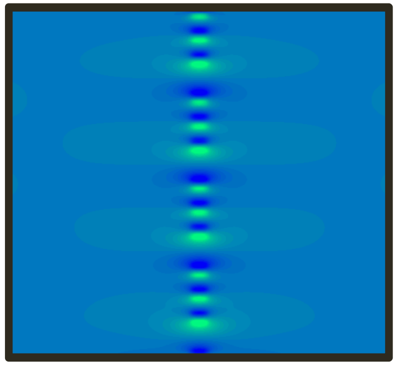




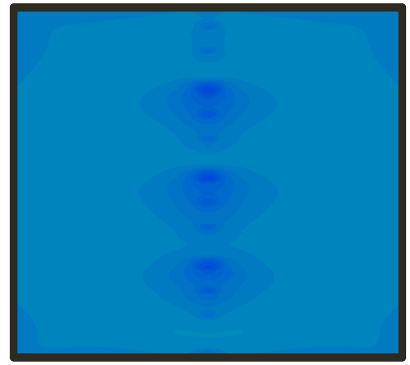


# Simulation flow

Calculate stress field associated with the microstructure.



Stress field $\sigma_{kk}$ with no defects



Relaxed stress field $\sigma_{kk}$ with defects at equilibrium

Two-way coupling leads to relaxation of the stress field.

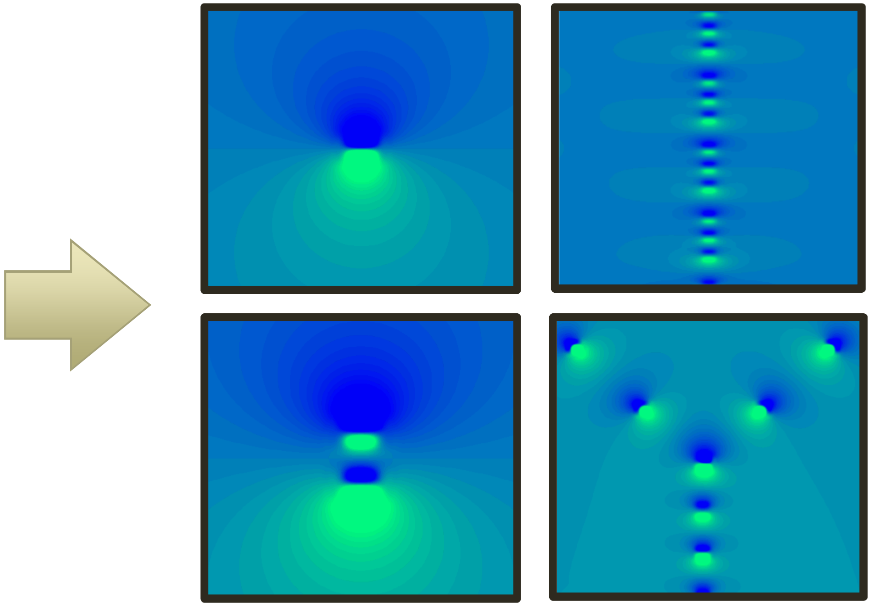
Populate the simulation box with point defects.

Defects diffuse to regions of large hydrostatic tension/compression.

# Methodology overview: benefits and drawbacks

## Benefits

- Can simulate large doses, time scales, and domains.
- Can model different defects by simply changing diffusion and interactions parameters.
- Can represent a wide range of structural features via elastic fields.

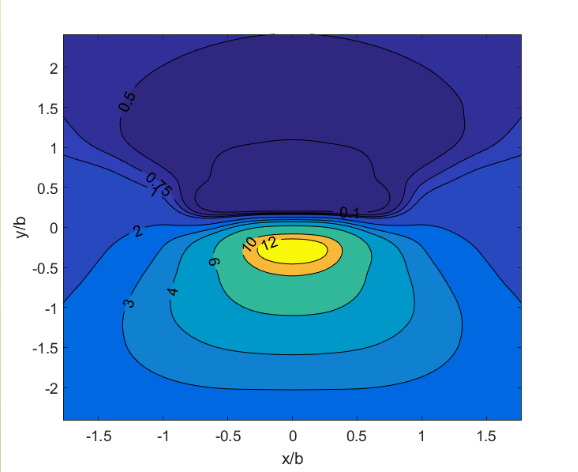


## Drawbacks

- Complexity of defect interactions is limited.
- Alloying elements, precipitates, and other impurities are not currently represented.

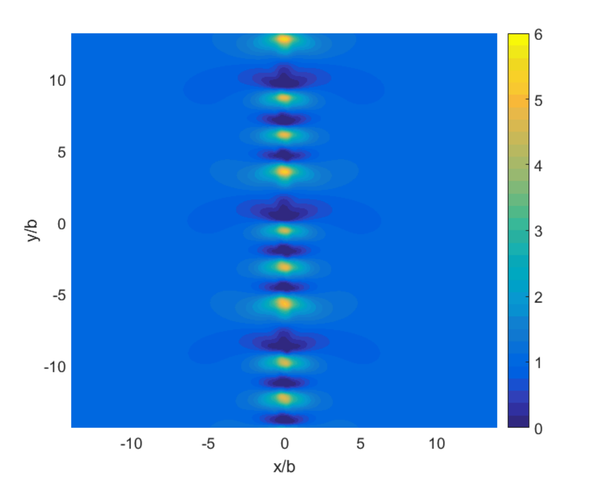
# Segregation of radiation-induced defects

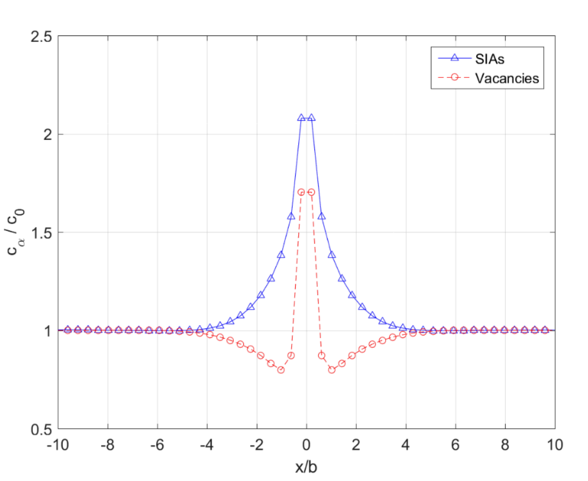
## Segregation to dislocation




SIAs segregate to the region of large hydrostatic tension under an edge dislocation. This agrees with the literature. They are also depleted in the region of hydrostatic compression above.

## Segregation to grain boundaries



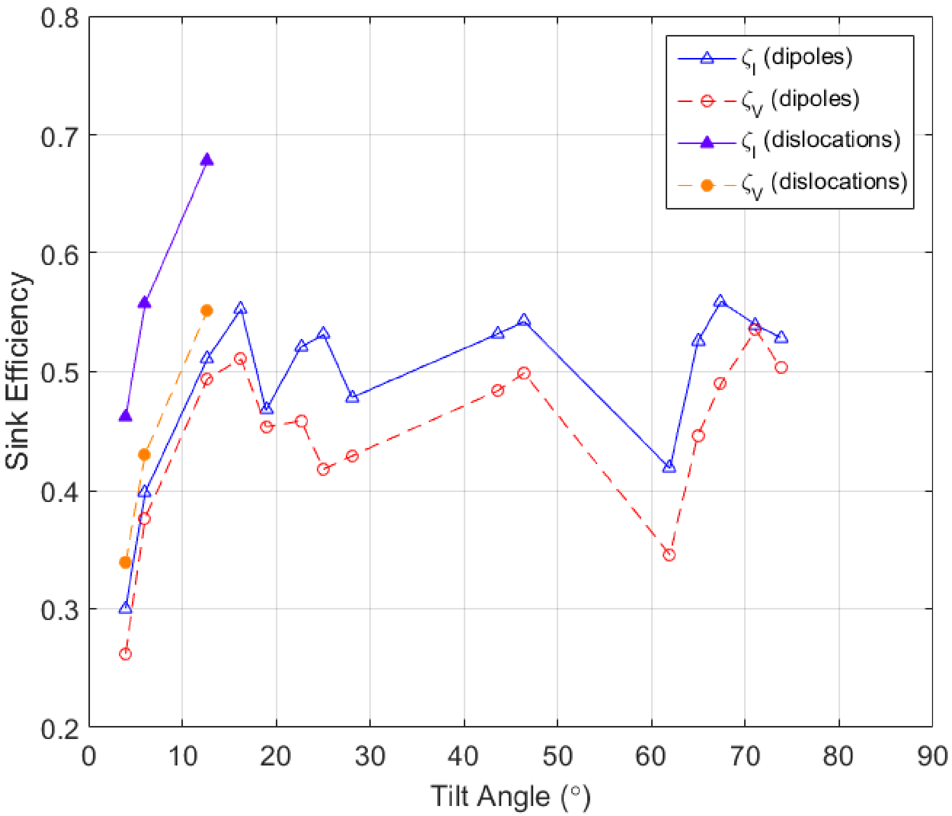




SIAs near a $\Sigma 85, 25.06°$ GB follow the same trend, showing alternating regions of accumulation and depletion corresponding to the disclination dipole arrangement.

Average concentrations along the length of the same GB reveal SIA enrichment and vacancy depletion in nearby areas. This vacancy depletion reflects the void denuded zones sometimes seen near GBs in experiments.

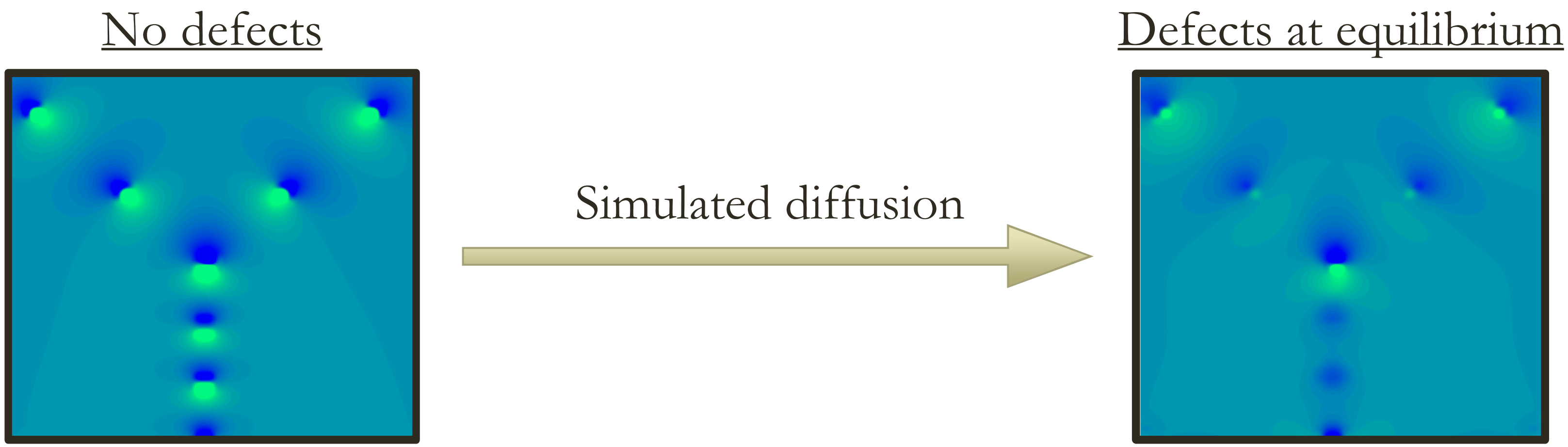
# Susceptibility to radiation-induced segregation

- **Metric:** Width of the vacancy depleted zone (VDZ).
  - In general, grain boundaries with very small misorientations (<10°) produce smaller VDZs.
  - GBs with larger misorientations tend to produce larger VDZ, implying that they better resist radiation damage.



# Conclusion

- This method can easily be extended to any domain where the elastic fields can be calculated.
- It is currently being used to investigate defect segregation around triple junctions, i.e. areas where three grain boundaries meet:




- The methodology and results shown in this presentation are being submitted to the *Journal of Nuclear Materials*

# Personal: Patrick Zarnas

- Previously worked as a manufacturing engineer at GE Aviation and project engineer at Aerotech.
- Currently a mechanical engineering PhD student at Northwestern University, focusing on solid mechanics and radiation damage.