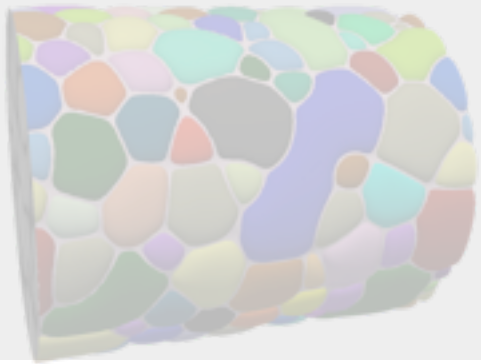
SAND2016-2815C

$$v_n = M\gamma H \qquad \gamma = \Delta F - \Gamma \frac{\partial f_{mix}}{\partial c}\Big|_{eq}$$

$$\frac{\partial \mathbf{c}}{\partial \mathbf{t}} = \nabla \cdot \left[\mathbf{M_c} \nabla \left(\frac{\delta \mathcal{F}_{\mathbf{tot}}}{\delta \mathbf{c}} \right) \right]$$



Experimental Investigation and Mesoscale Modeling of Irradiation-induced Grain Growth

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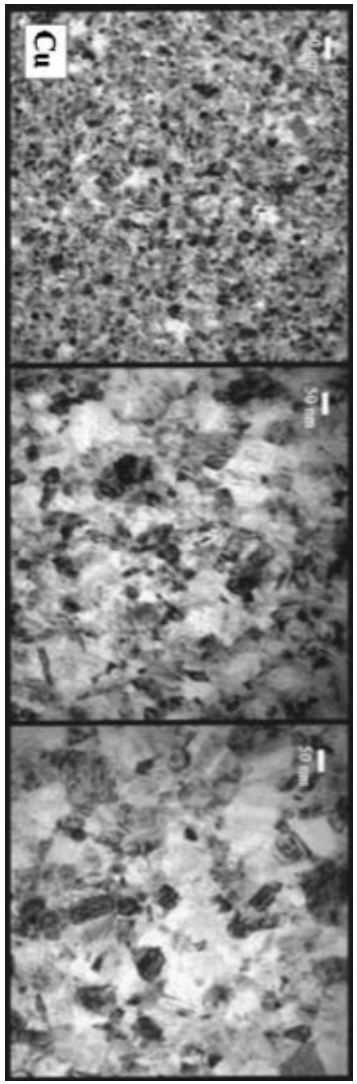
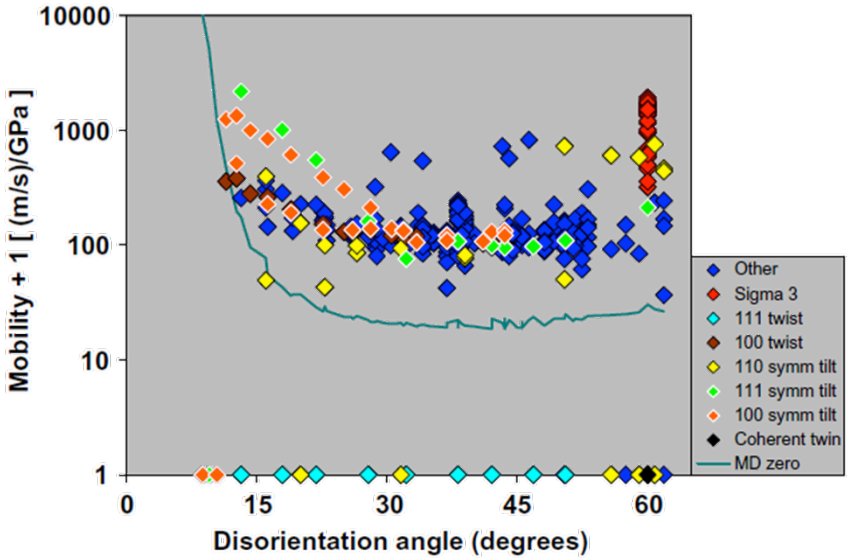
Motivation



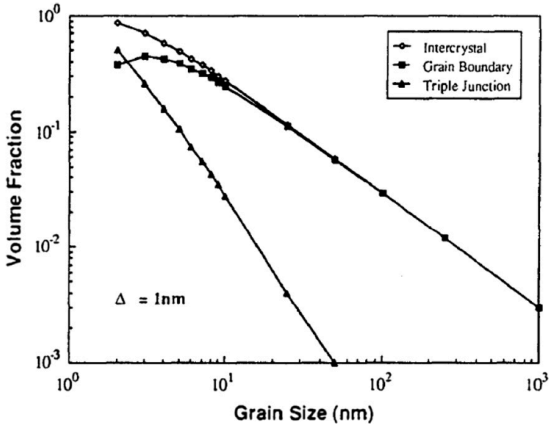
Kaoumi, *et al.*, J. ASTM Intl, (2006)

Nanocrystalline metals (NCs):

- Exemplary mechanical properties
- Abundant sinks for structural and chemical defects
- Ideal candidates for radiation-tolerant materials?

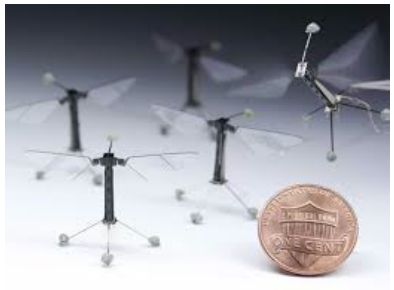


Olmsted *et al.*, Acta Mater. **57** (2009)



Palumbo *et al.*, Scr. Metall. Mater. **24** (1990)

RoboBee



Ma *et al.*, Science. **340** (2013)

What are the relationships among ion damage, grain boundary character, and grain growth?

Synergistic In Situ Capabilities

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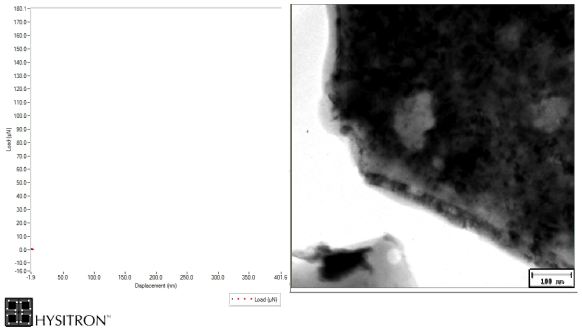
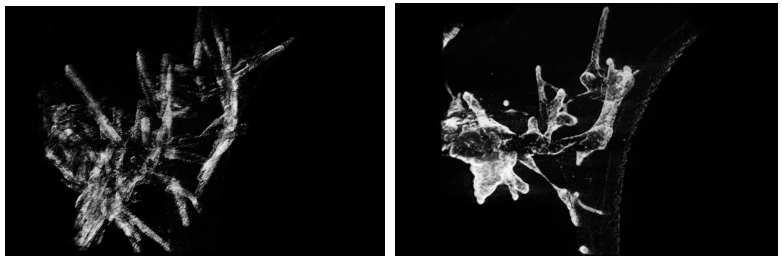
Mechanical



Direct correlation of dose and defect density with resulting changes in strength, ductility, and defect mobility

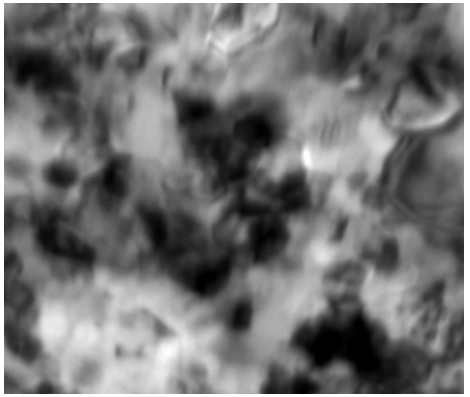
Structural

Morphology changes as a result of radiation damage



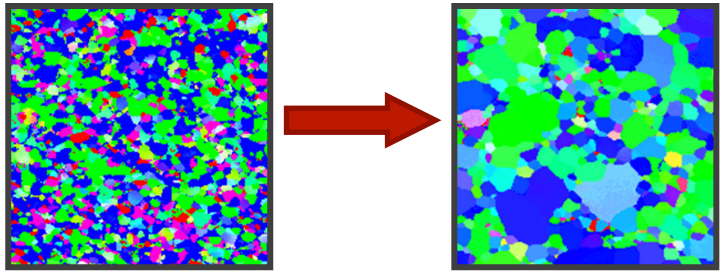
Thermal

Coupling effects of temperature and irradiation on microstructural evolution up to 800 °C



Texture

Quantifying orientation changes as a result of radiation, implantation, and heat.



The application of advanced microscopy techniques to characterize synergistic effects in a variety of extreme environments

In Situ Irradiation

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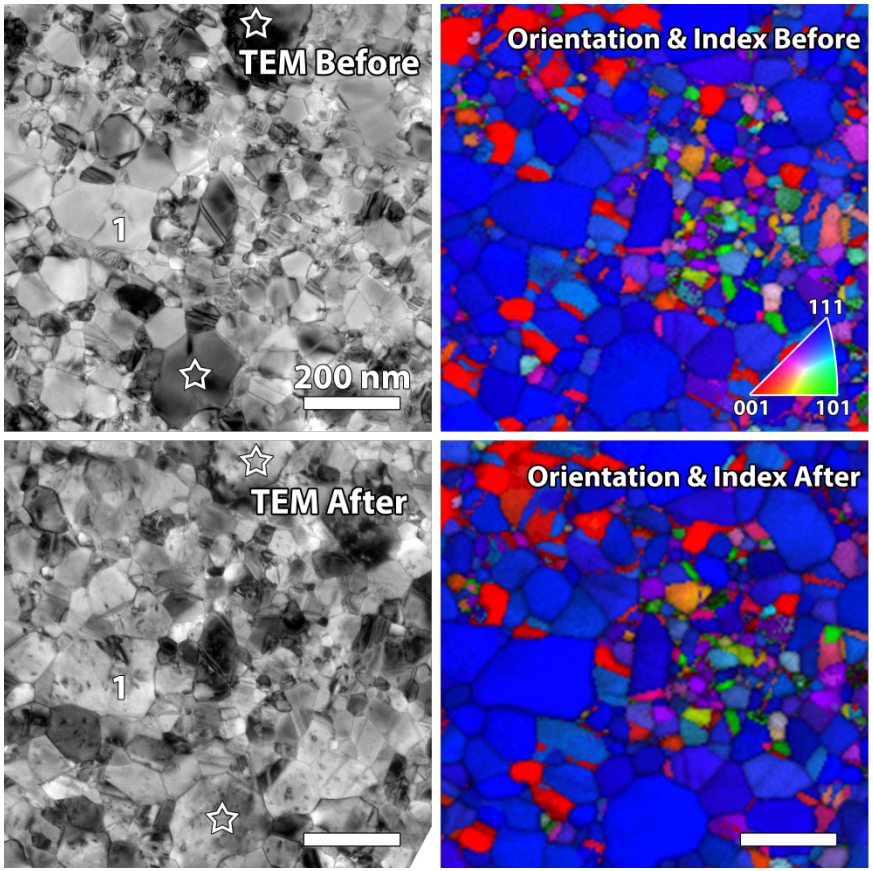
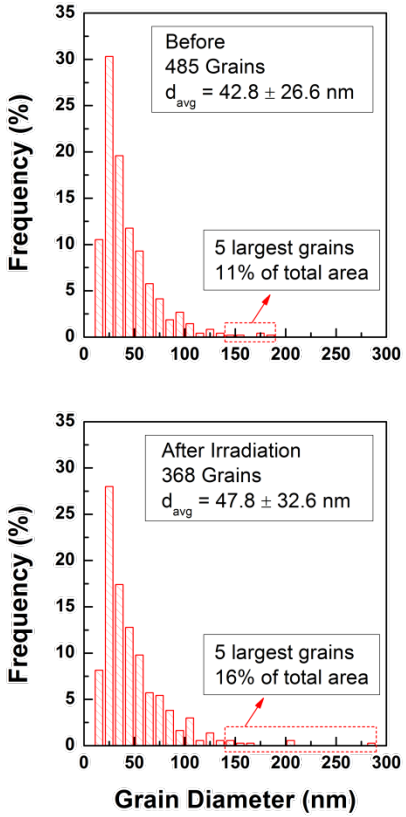
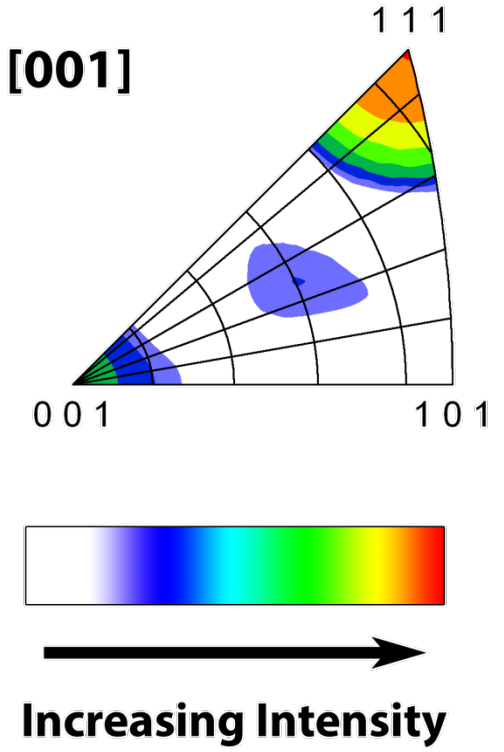
- Au foil during bombardment with 10 MeV Si3+
- ~22 s of 4000s total experiment time

Locations of single ion strikes and resulting microstructural change captured.

Quantification: Overall







- Same area characterized before and after irradiation.
  - Local grain size, orientation, boundary character
  - Hundreds of grains counted in minutes

Bufford, *et al.*, Appl. Phys. Lett., **107** (2015)

Rapid quantification of statistically relevant numbers of grains and boundaries.

Quantification: Local

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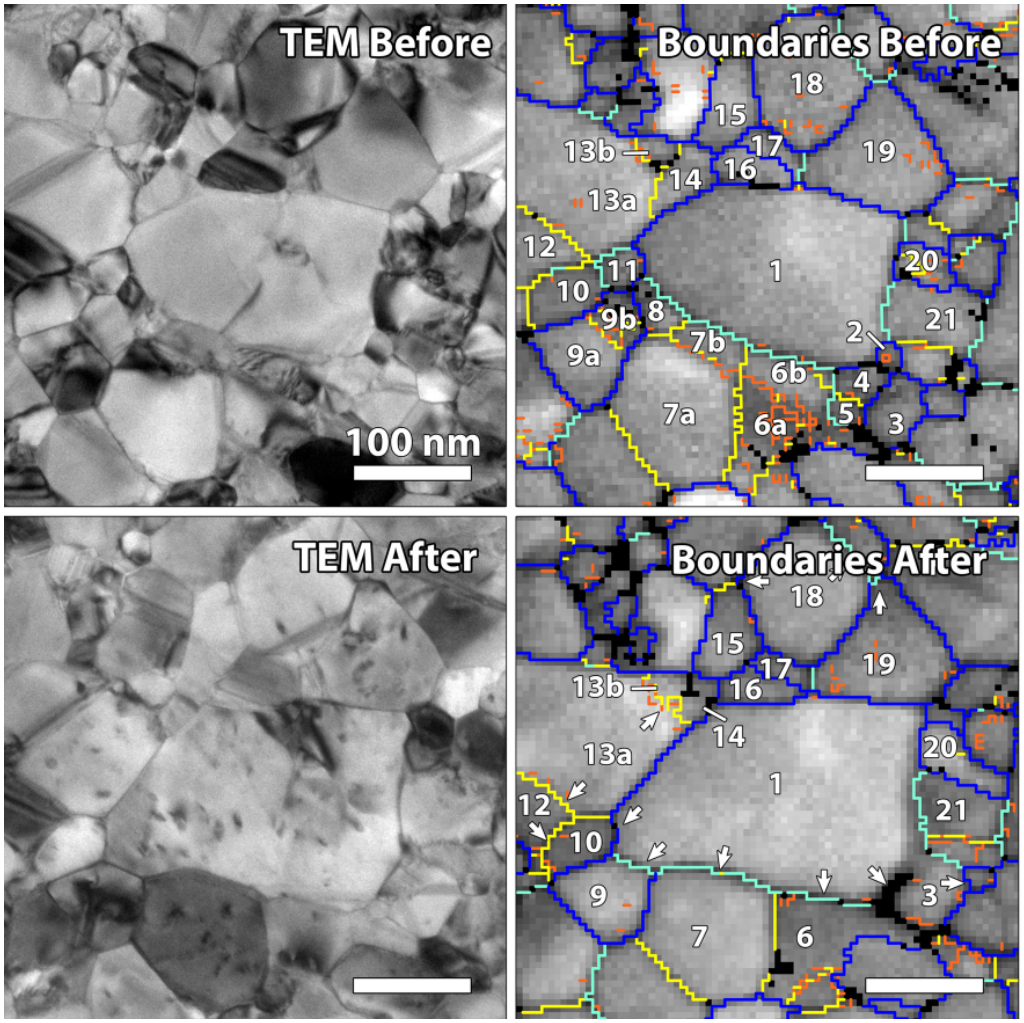
- The same grains identified before and after irradiation
- Individual grain boundary misorientation angles and axes quantified
- Correlation of GB properties and radiation-induced changes



θ < 3°

3° ≤ θ < 15°

15° ≤ θ < 30°

30° ≤ θ

Bufford, *et al.*, Appl. Phys. Lett., **107** (2015)

Grain boundary misorientation angle and axes quantified

Modeling Approach: Phase Field

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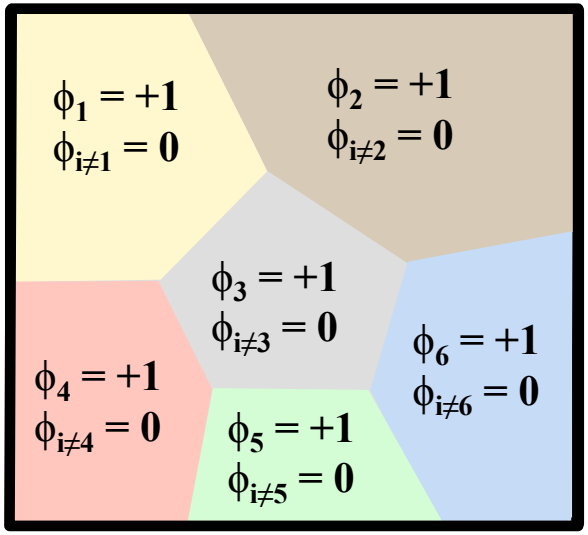
- Total free energy

$$\mathcal{F}_{tot} = \int d\mathbf{r} \left[W_\phi f_{grain}(\phi_i) + \sum_i^{n_\phi} \frac{\epsilon_i^2}{2} |\nabla \phi_i|^2 \right]$$

Bulk GB energy



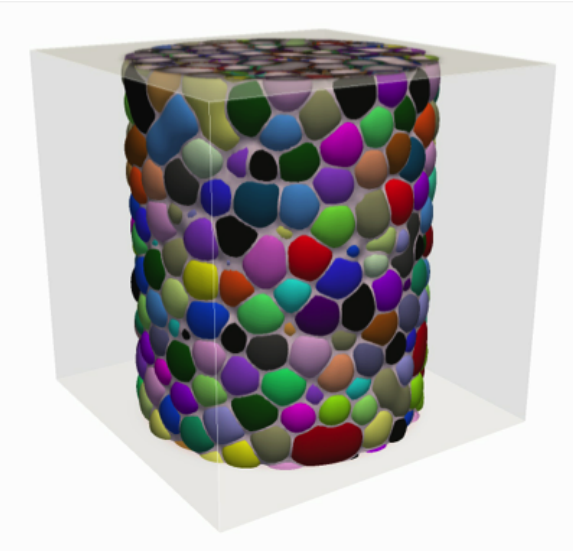
- Dynamics

$$\frac{\partial \phi_i}{\partial t} = -L_i \left(\frac{\delta \mathcal{F}_{tot}}{\delta \phi_i} \right)$$

Allen-Cahn Eq.

L_i: GB kinetic parameter

- GB properties
  - Energy: $\gamma_{gb} = \frac{2\sqrt{2}}{3} \epsilon_i \sqrt{W_\phi}$
  - Mobility: $M_{gb}\gamma_{gb} = L_i \epsilon_i^2$



Abdeljawad and Foiles, Acta Mater. **101** (2015)
Bufford, *et al.*, Appl. Phys. Lett., **107** (2015)

Trends in GB Mobility

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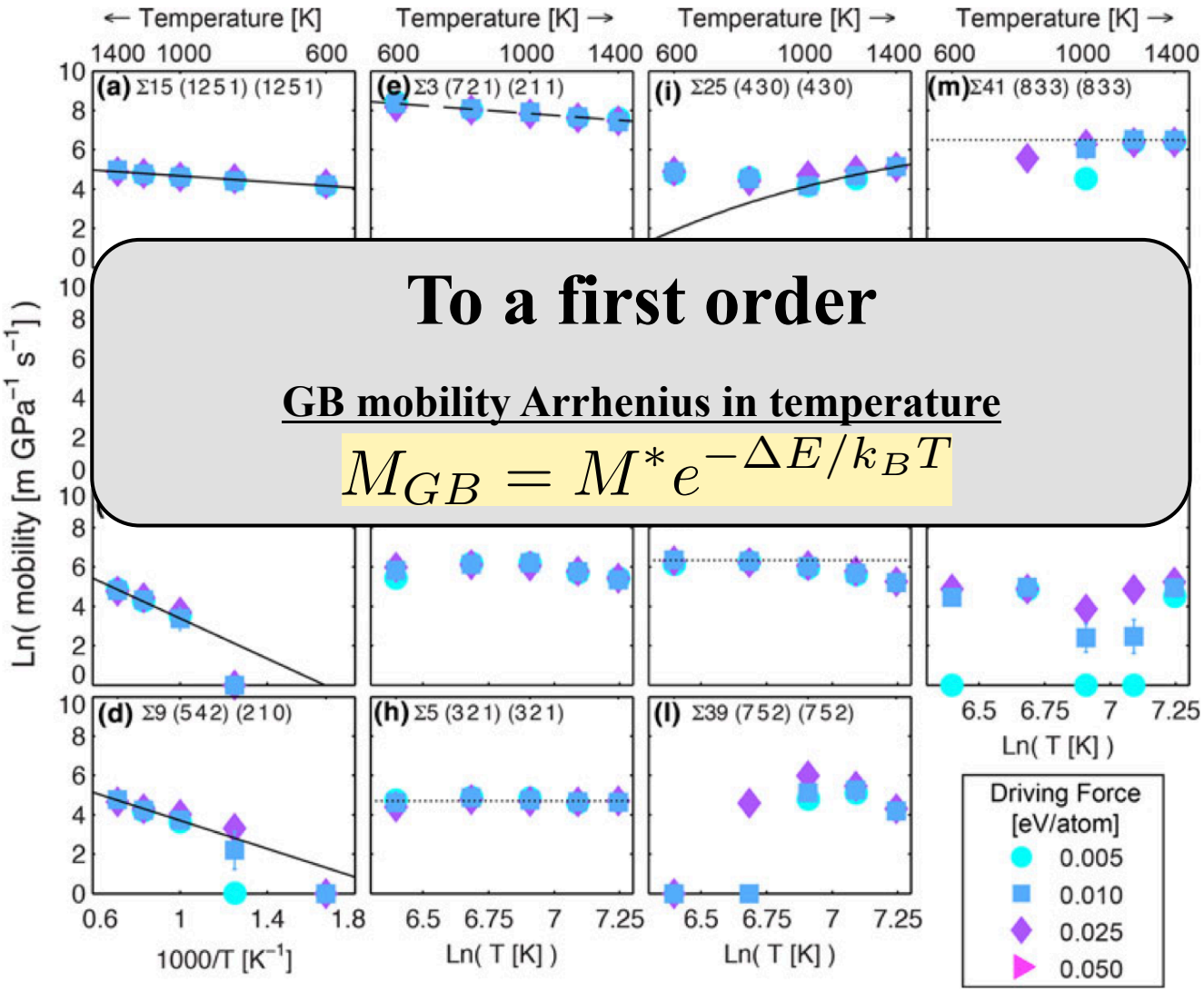

To a first order

GB mobility Arrhenius in temperature

$$M_{GB} = M^* e^{-\Delta E / k_B T}$$

Homer, *et al.*, JOM, **66** (2014)

Modeling Approach

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- **GB Mobility**
  - T_{ref}: Reference far-field temperature
  - T_o: Temperature at center of thermal event
  - N_{spike}: # of thermal events (ion flux)

Mobility parameter:
(In terms of the far field reference temperature)

$$L(T) = L(T = T_{ref}) \exp\left[-\frac{\Delta E}{k_B T_{ref}}\left(\frac{1}{T/T_{ref}} - 1\right)\right]$$

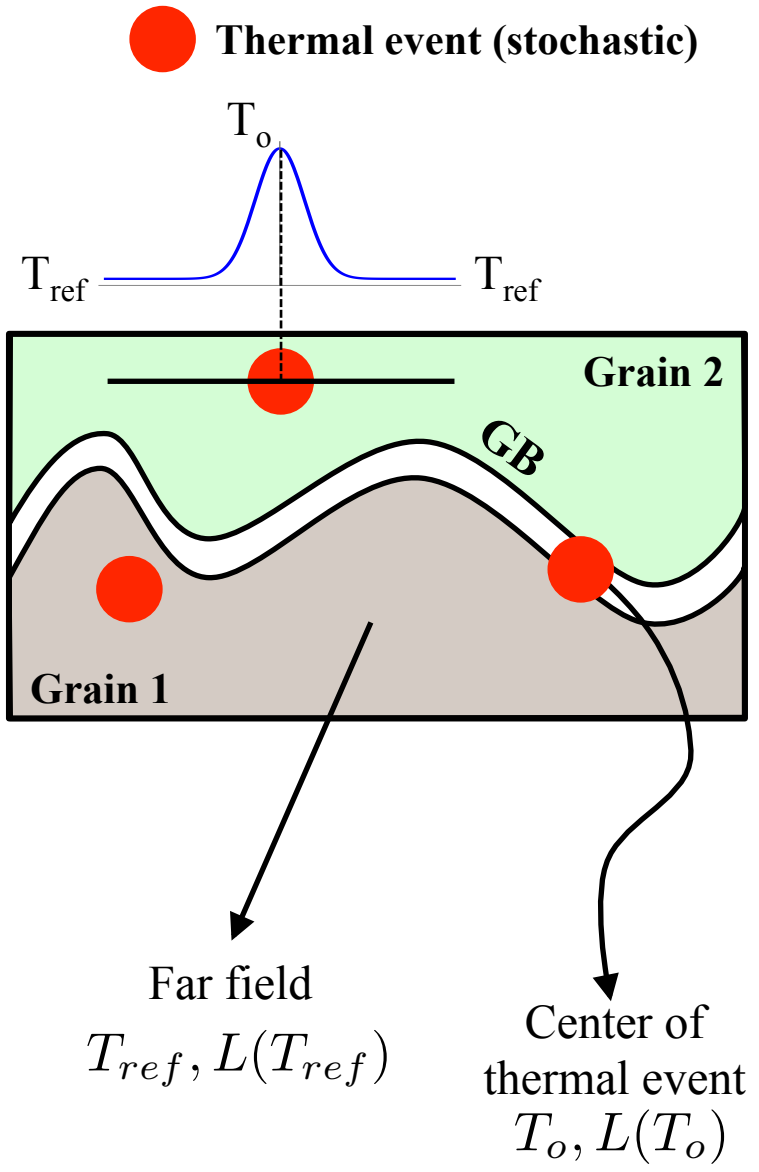
Temperature field:
(Gaussian shapes for thermal events)

$$T(\mathbf{r})/T_{ref} = 1.0 + \sum_{i=1}^{N_{spike}} \left[(T_o/T_{ref}) - 1.0\right] e^{-(\mathbf{r}-\mathbf{r}_i)^2/2\sigma^2}$$

In this study

$$T_o/T_{ref} = 10$$

$$L(T_o)/L(T_{ref}) = 100 \ (\Delta E/k_B T_{ref} = 5.12)$$



Results

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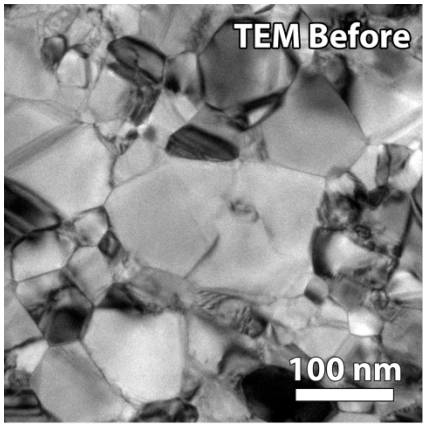
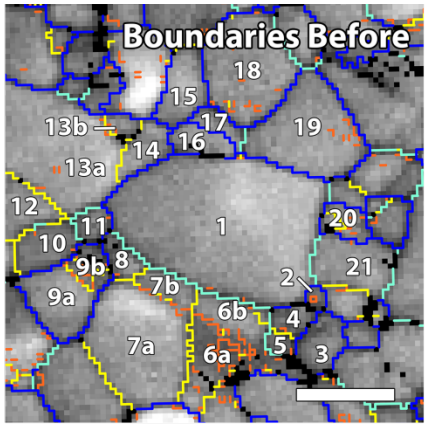
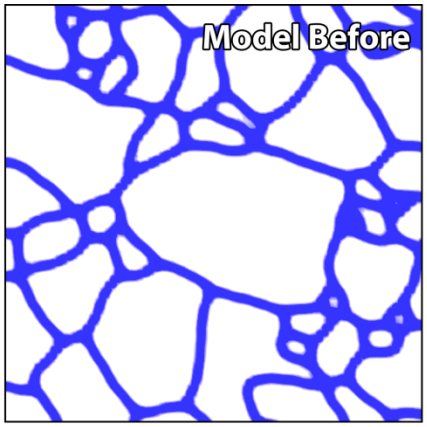
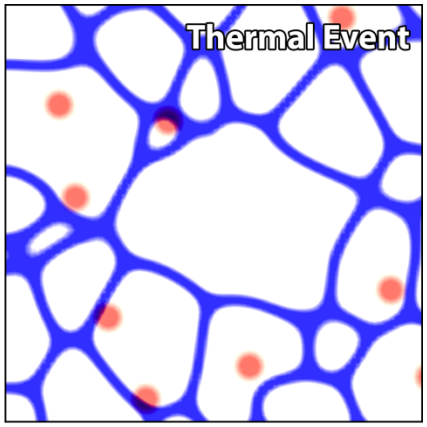
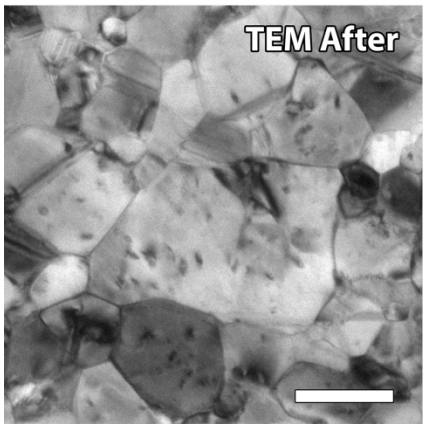
Results

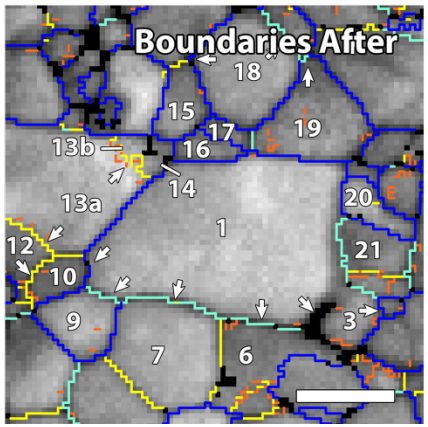


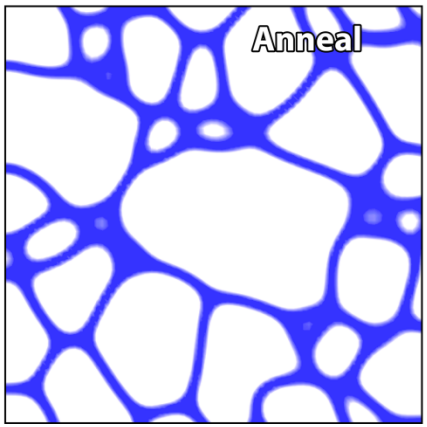


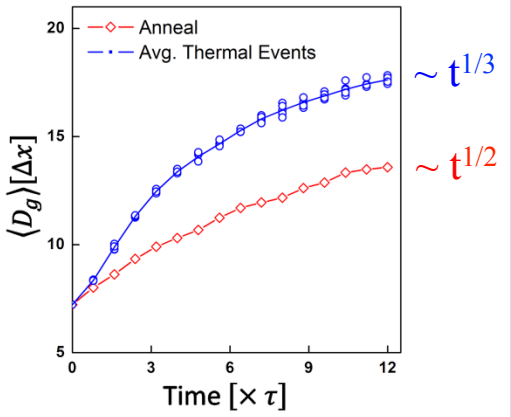










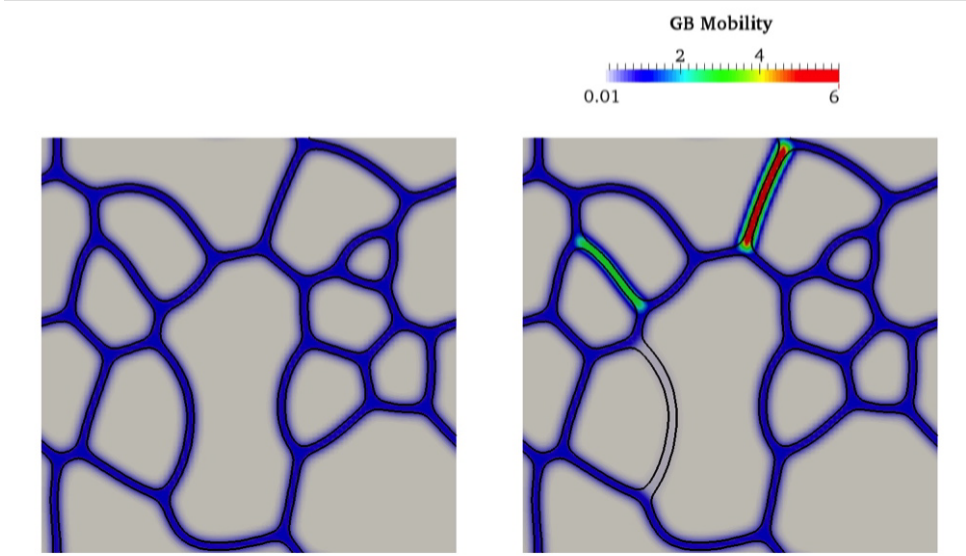


- Overall scaling laws appear consistent
- Subtle deviations from homogenous grain growth
- Avg. grain size vs. time deviates from traditional $t^{1/2}$ scaling
- Analytical treatments suggest scaling $t^{1/3}$ Kaoumi *et al.*, J. Appl. Phys., **104** (2008)

Bufford, *et al.*, Appl. Phys. Lett., **107** (2015)

Conclusion and Future Work

- TEM orientation mapping at various ion fluences
  - Analyzed and used as direct input for a phase field model
- Stable grains are characteristic of known low mobility grains
- Our first attempt to compare experimentally observed and modeled grain growth under irradiation.
  - Differences attributed to GB character



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Thank You

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In print: Bufford, *et al.*, Appl. Phys. Lett., **107** (2015)