Exploring the Role of Texture, Grain Boundary Character, and Grooving on the Grain Growth in Metallic Thin Films

SAND2017-2725C

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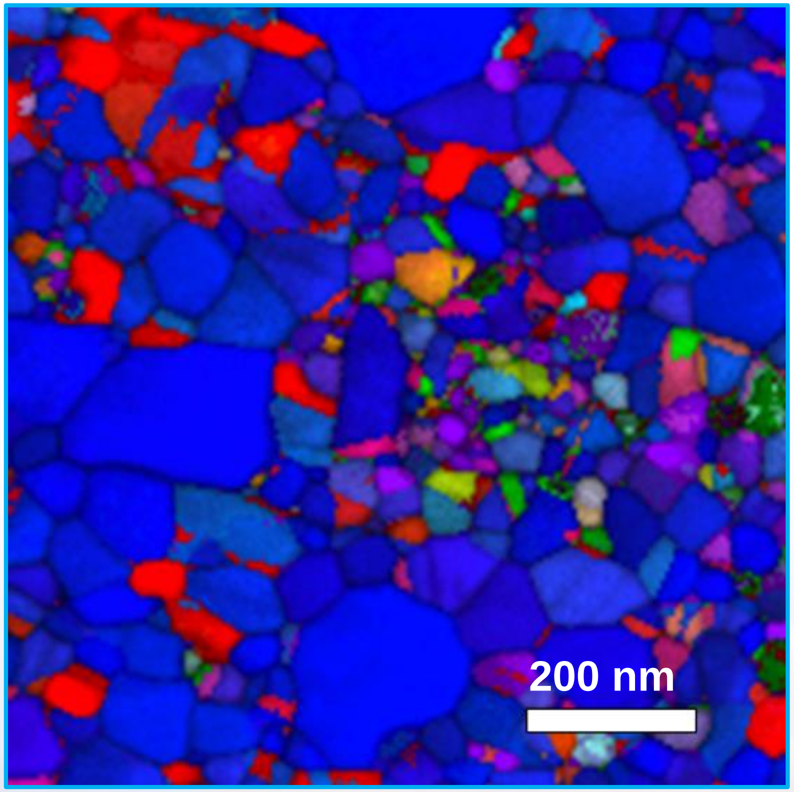
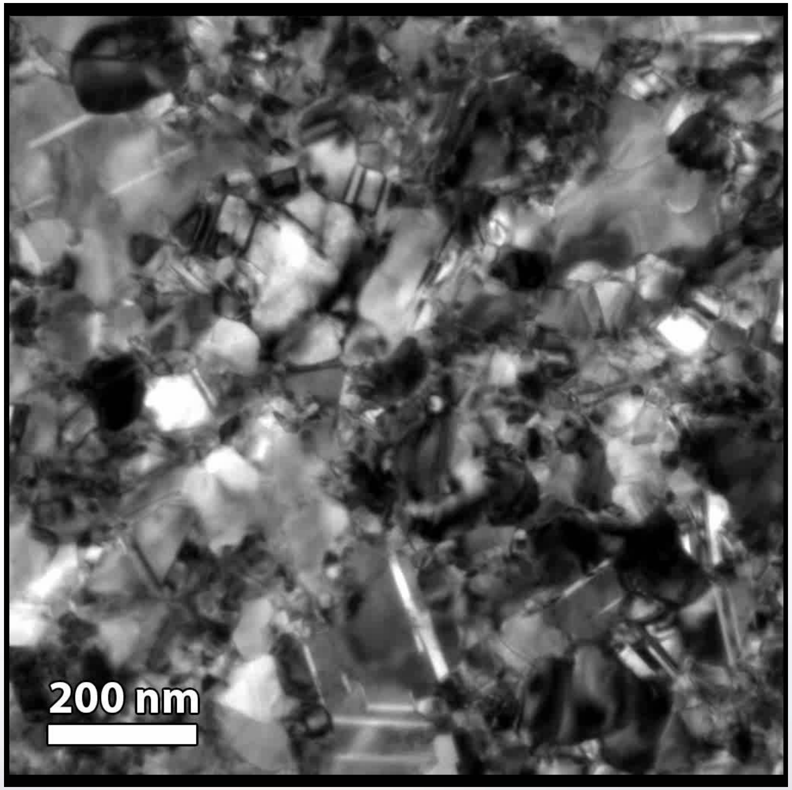
3/2/2017





Preliminary work to experimentally correlate the grain boundary stability with local grain orientation or grain boundary character during thermal or radiation driven grain growth

This work was supported by the US Department of Energy, Office of Basic Energy Sciences. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

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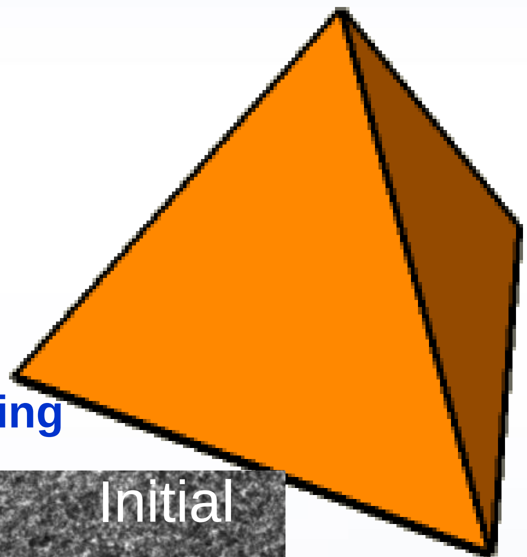
Mechanical Properties are Very Dependent on Grain Size in Nanocrystalline Metals

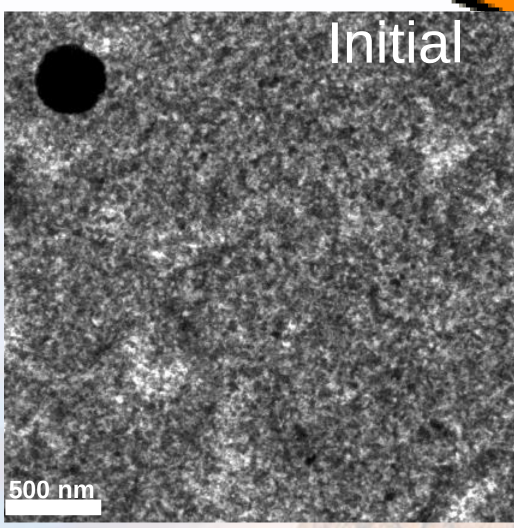
Performance

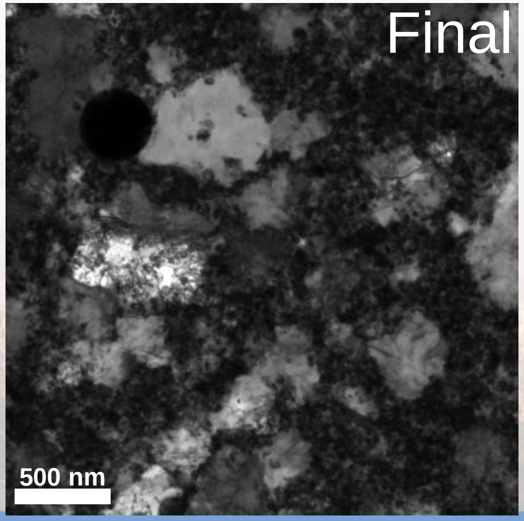
Properties

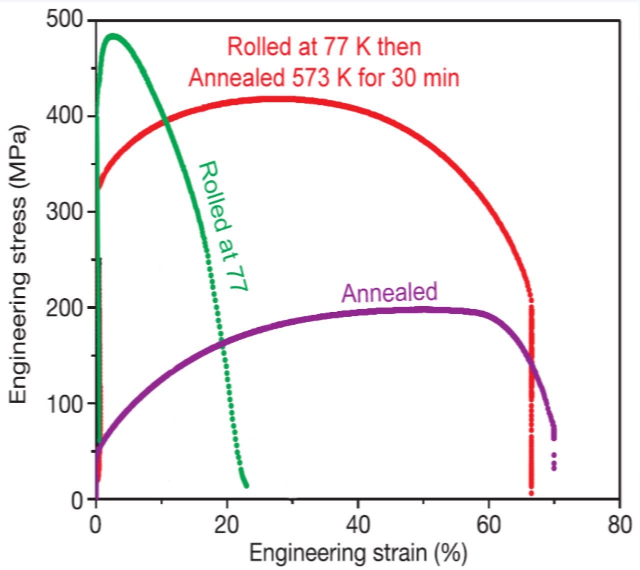
Processing



Microstructure







Wang et al. Nature 419 2002

Key questions:

- Identification of the governing deformation mechanism in each microstructure
- Optimization of the thermal processing to control the microstructure

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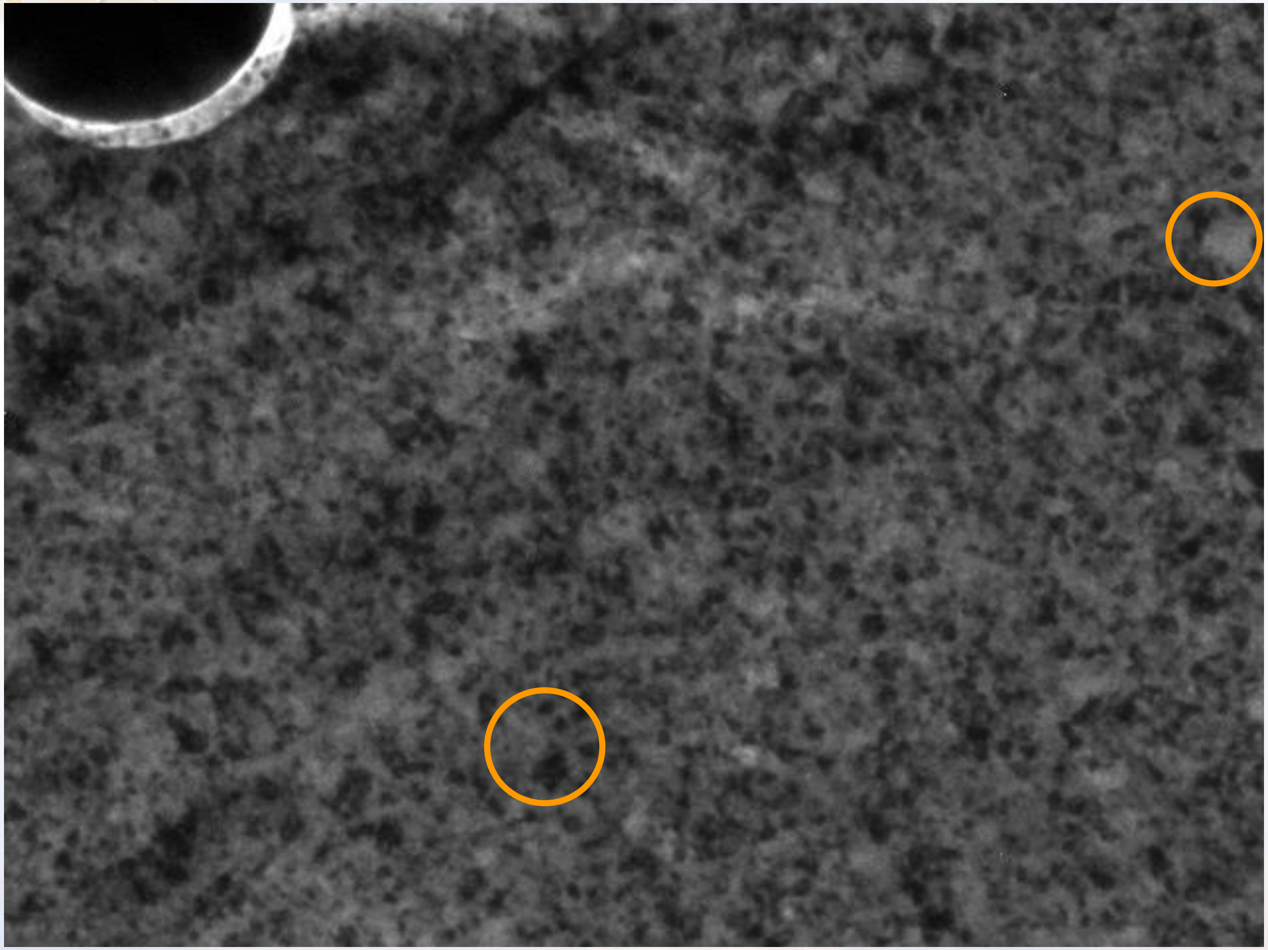
Dynamics of Abnormal Grain growth in PLD Ni



90 nm-thick PLD Ni during annealing at 350 ° C

400 nm

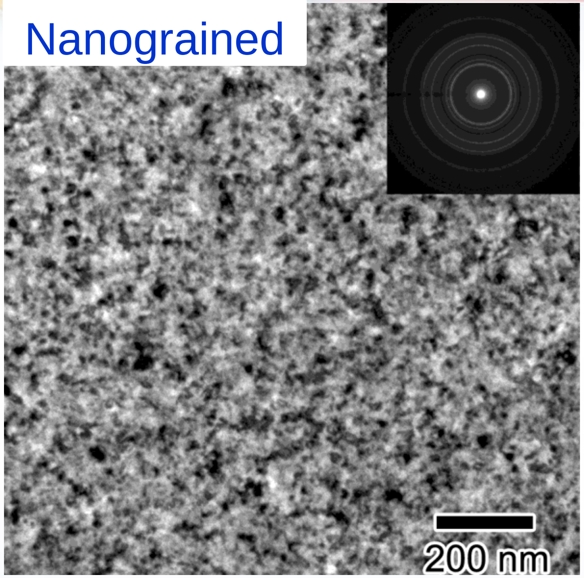
A few select grains grow at the expense of the remaining matrix

Abnormal Grain Growth is a function of:

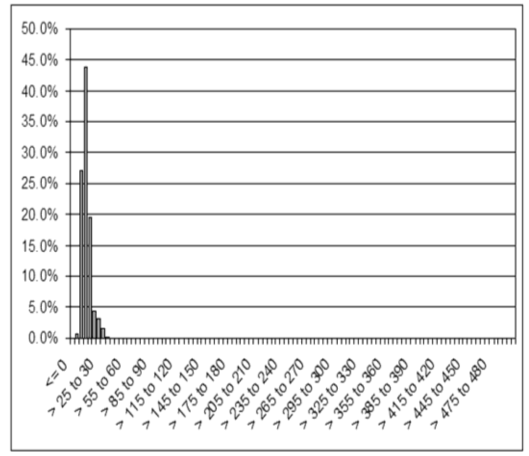
- Time
- Temperature
  - e^- beam illumination
- Film thickness
- 4 years of Aging
- Surface Abnormalities
  - Ledges
  - Splats – No effect
- Myriad of defects form in the abnormal grains

Microstructural Control through Annealing in PLD Ni

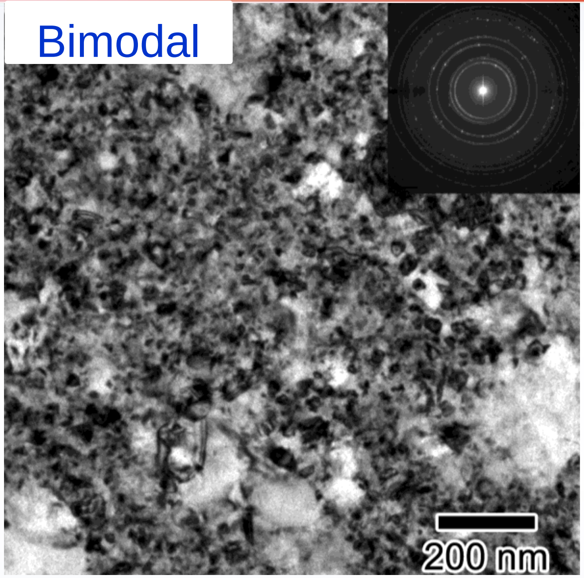
Nanograined



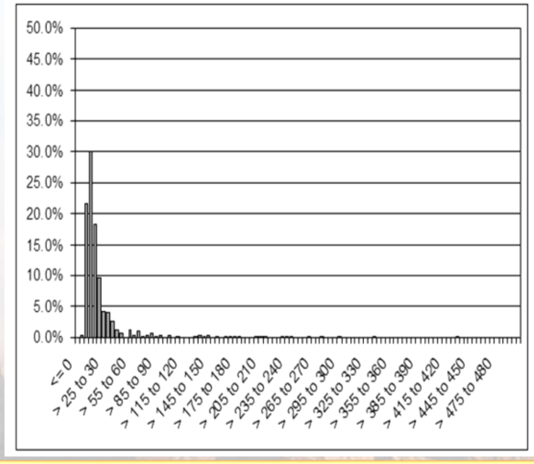
80 nm-thick As-deposited on Si



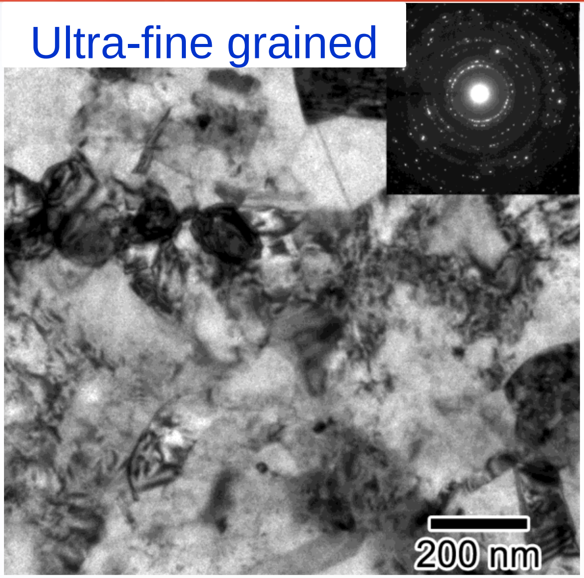
Bimodal



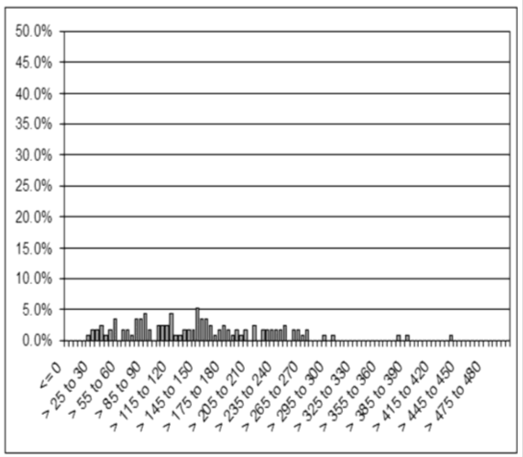
1 hr at 275 ° C



Ultra-fine grained



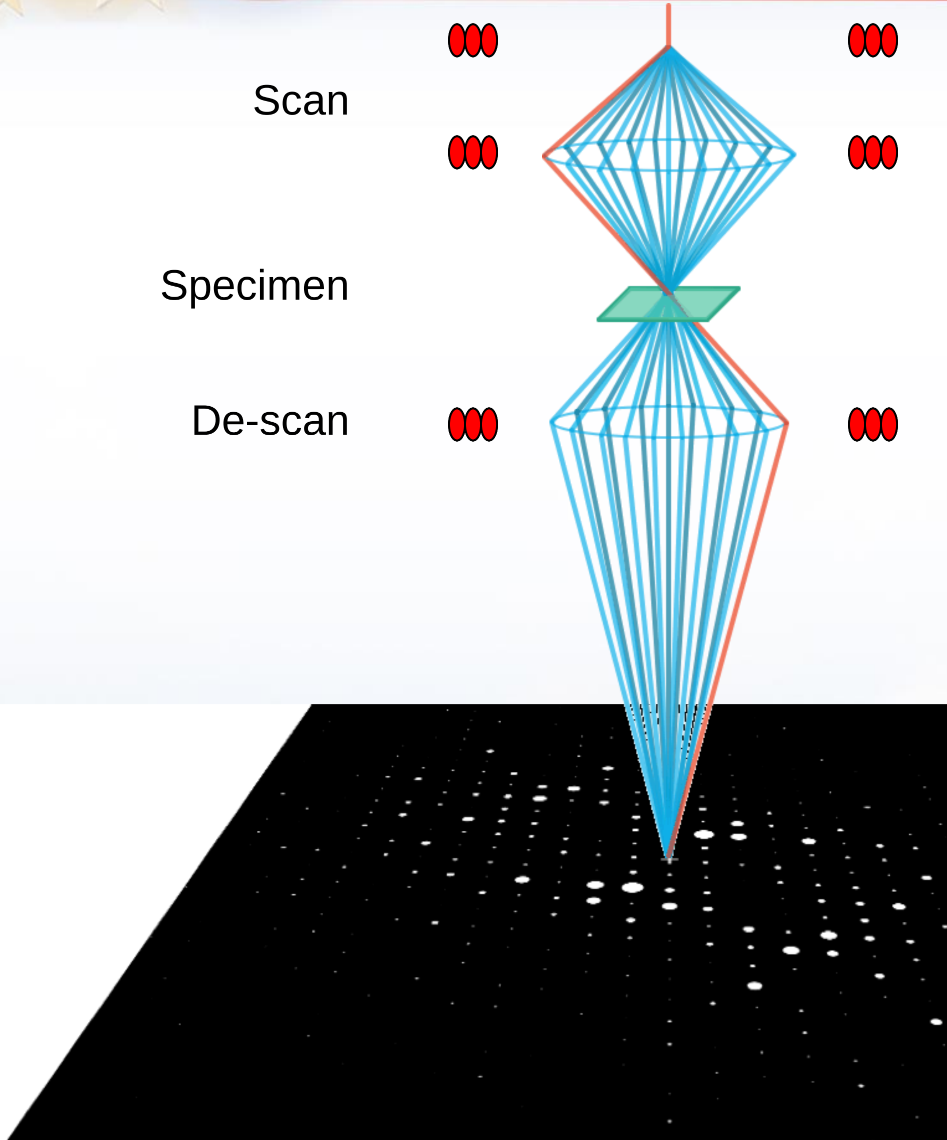
1 hr at 375 ° C

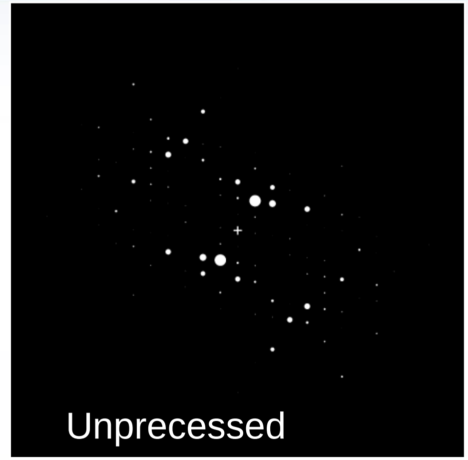


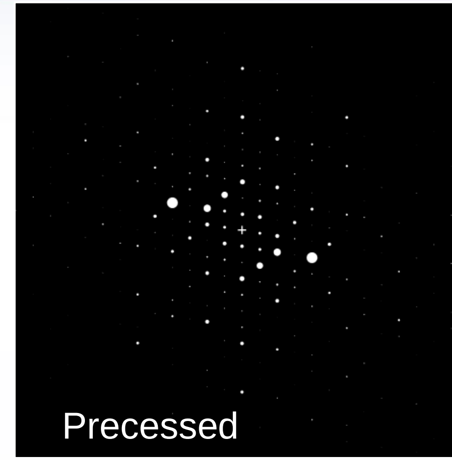
Grain size can be quantified from BF images, but not much else.

Precession Electron Diffraction (PED) Microscopy

Collaborators: K.J. Ganesh, S. Rajasekhara, & P.J. Ferreira







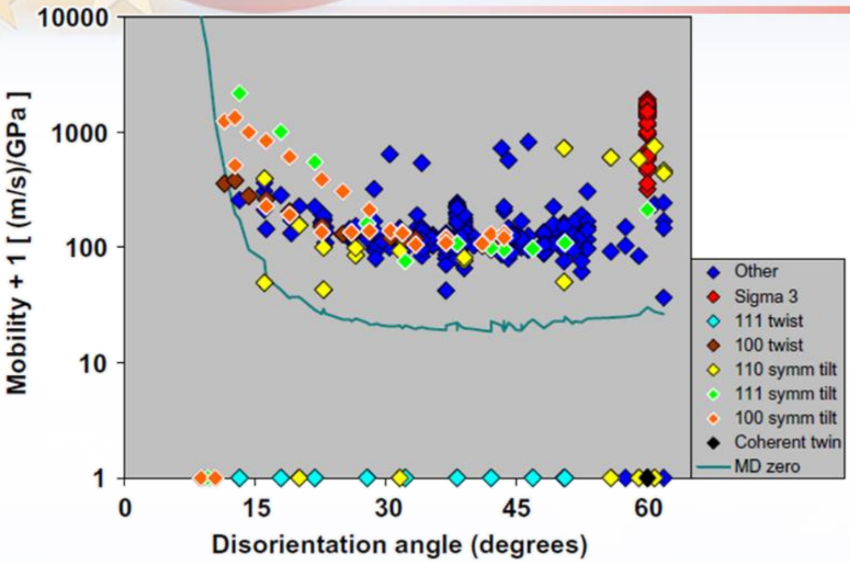
Advantages

- **< 10 nm spatial resolution**
- **Near kinematical electron diffraction**
- **Symmetry ambiguities are resolved**
- **Fast and automated acquisition**
  - **~200 grains in 15 min.**

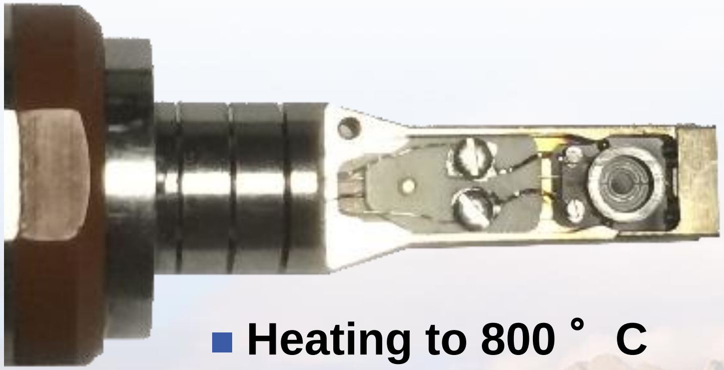
Chris Own, PhD Dissertation, Northwestern University, 2004

Slide courtesy: K. J. Ganesh

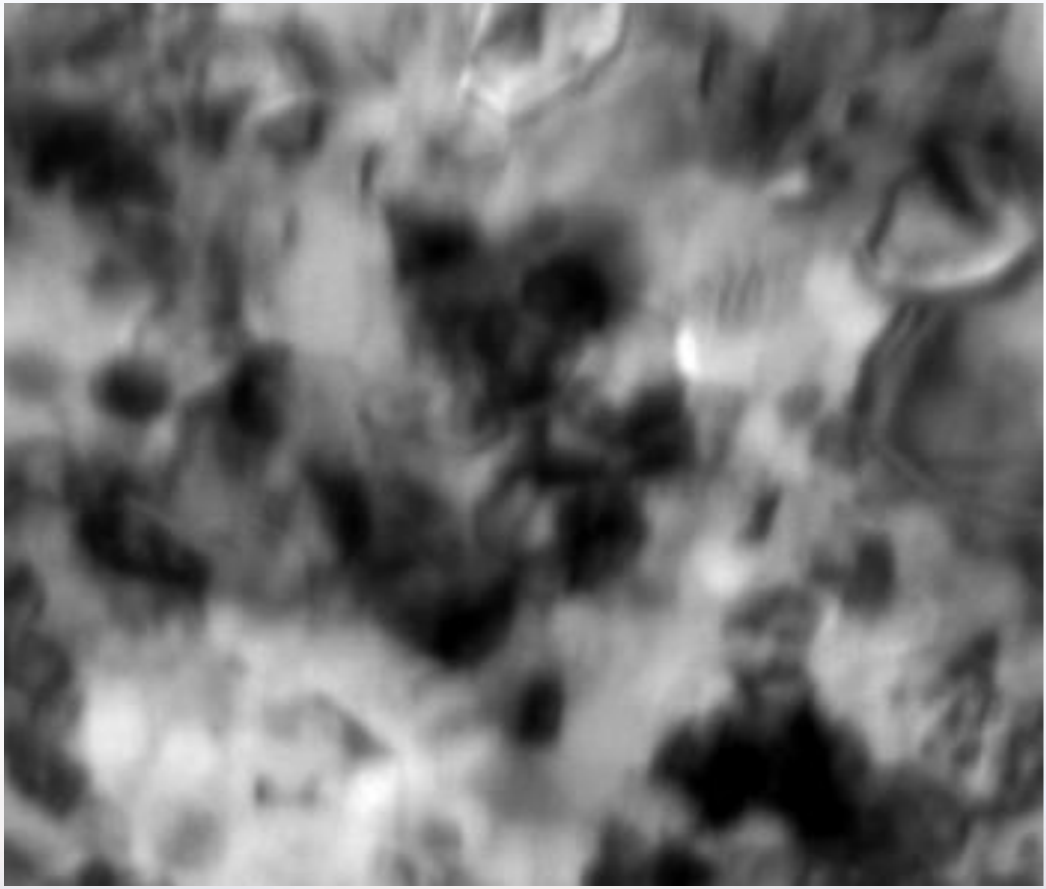
Can Grain Boundary Role be Determined from In situ Annealing?



Olmstead, *et al*, Acta Mater, 2009.

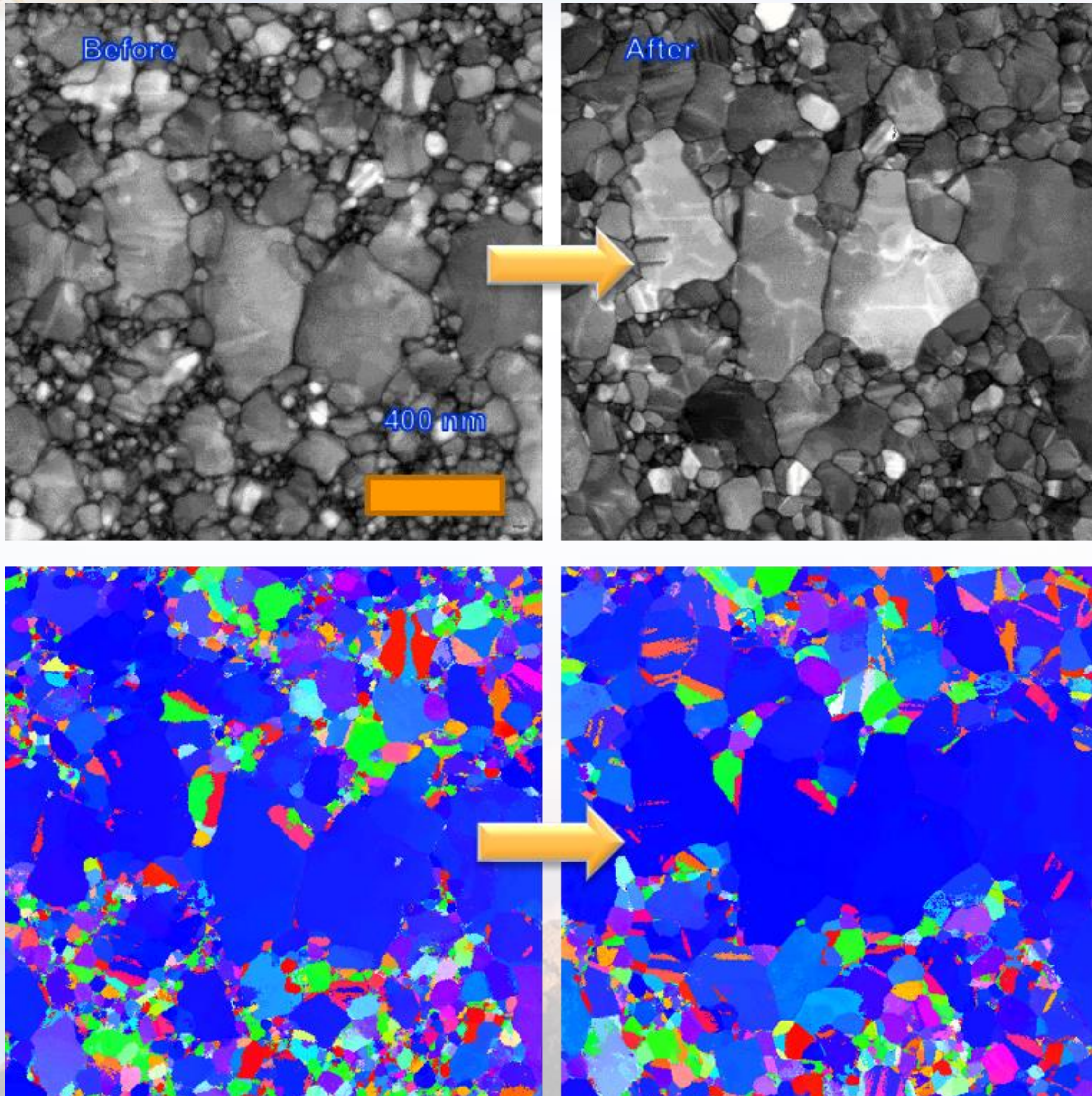


- **Heating to 800 ° C**

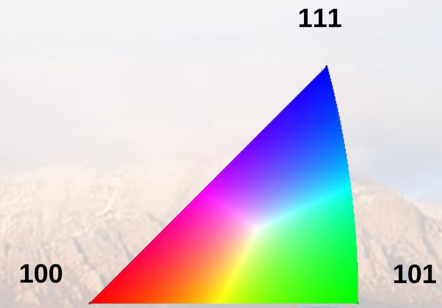


In-situ annealing of PVD Au

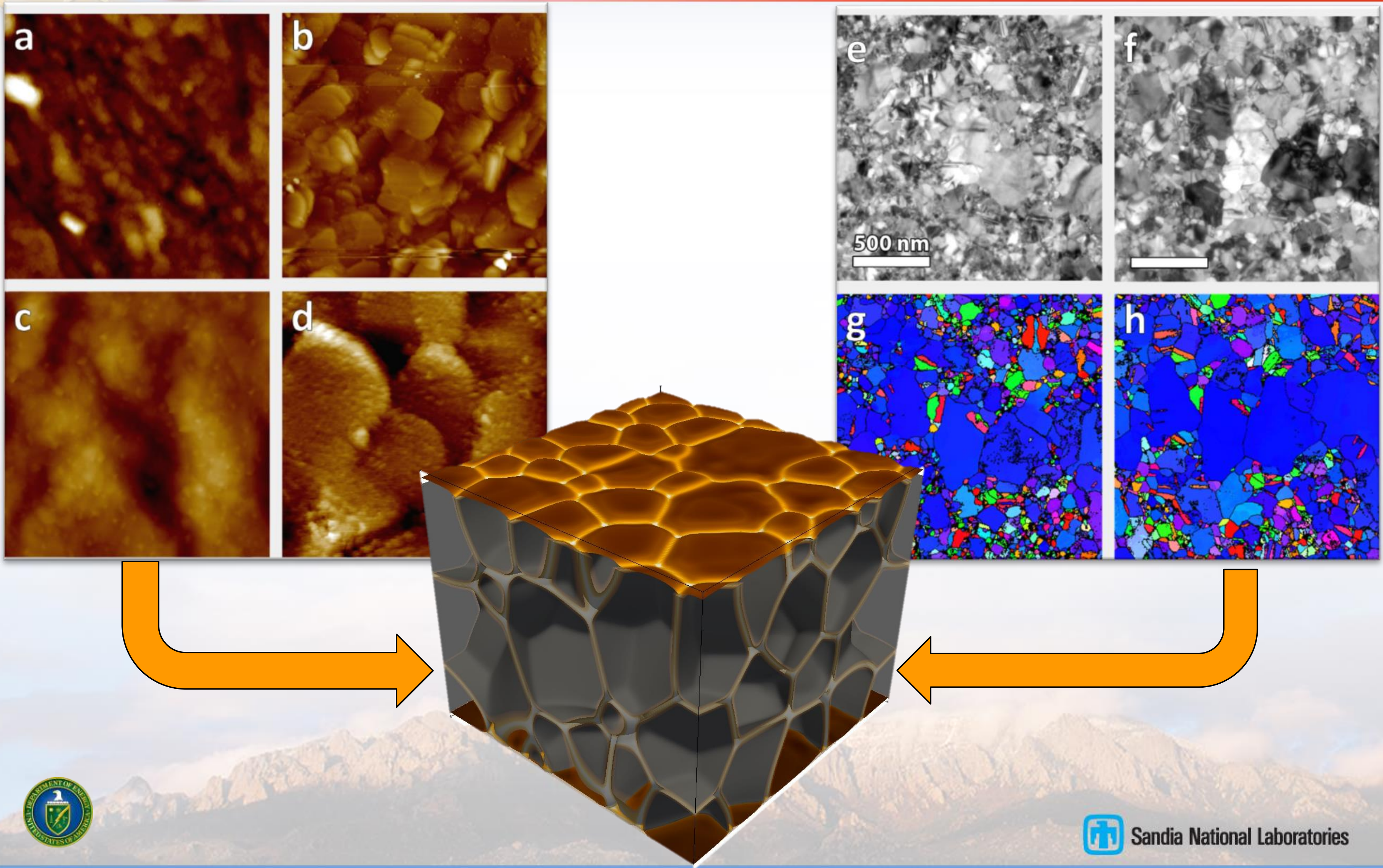
PED Provides Insight into the Role of Texture and Grain Boundary Character



- **Freestanding Au foil**
  - 40 nm thickness
  - Annealed to 300 °C
- **PED orientation mapping to digitize the microstructure**
  - <10 nm resolution
- **Captures changes in structure**
  - Orientation
  - Grain size
- **Direct input for use in computational models**



Combining PED with AFM Creates at Tool to Examine Grain Boundary Grooving Role on Abnormal Grain growth



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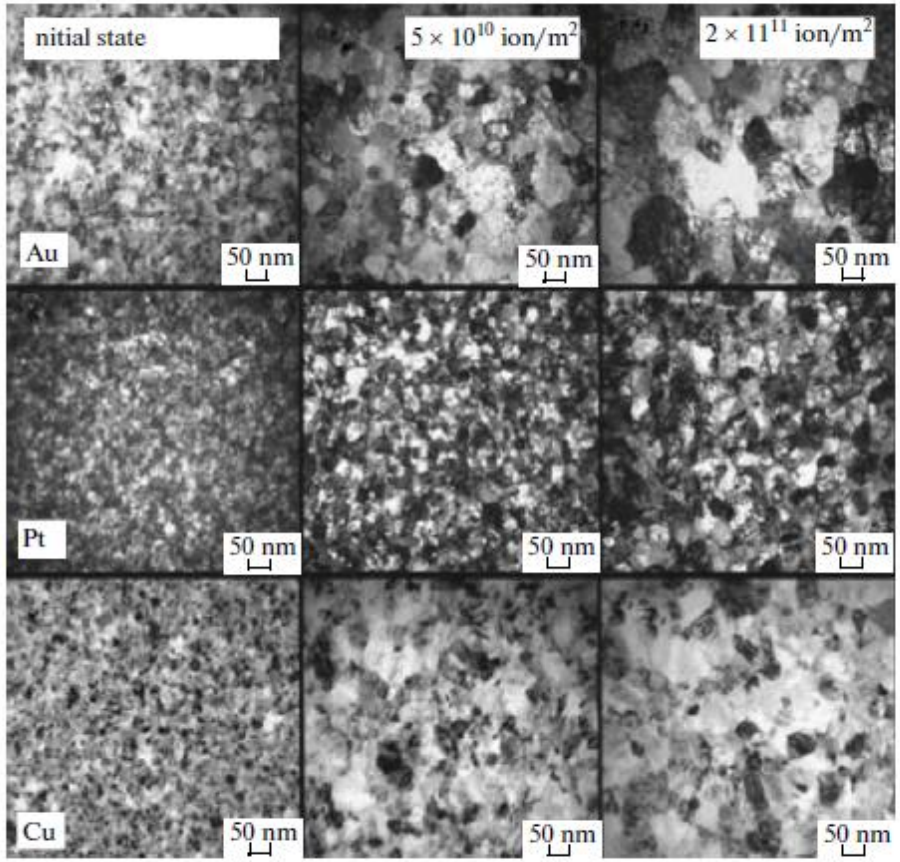
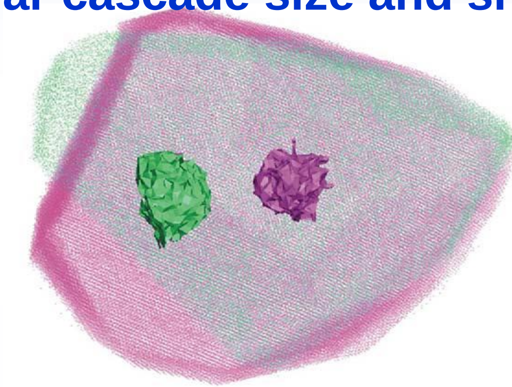
Radiation Tolerance from Nanocrystalline Metals

Variation in radiation tolerances



Kaomi et al., JAP: 2008. 104 073525

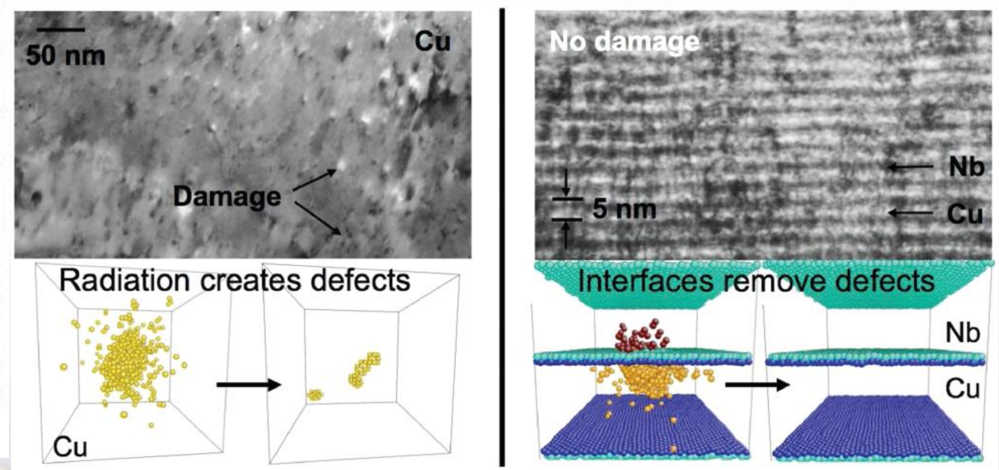
Similar cascade size and shape predicted



BCC Fe
FCC Ni

Samaras et al., J. Nuc. Mat.: 2006. 351

Nanolamellars are radiation tolerant



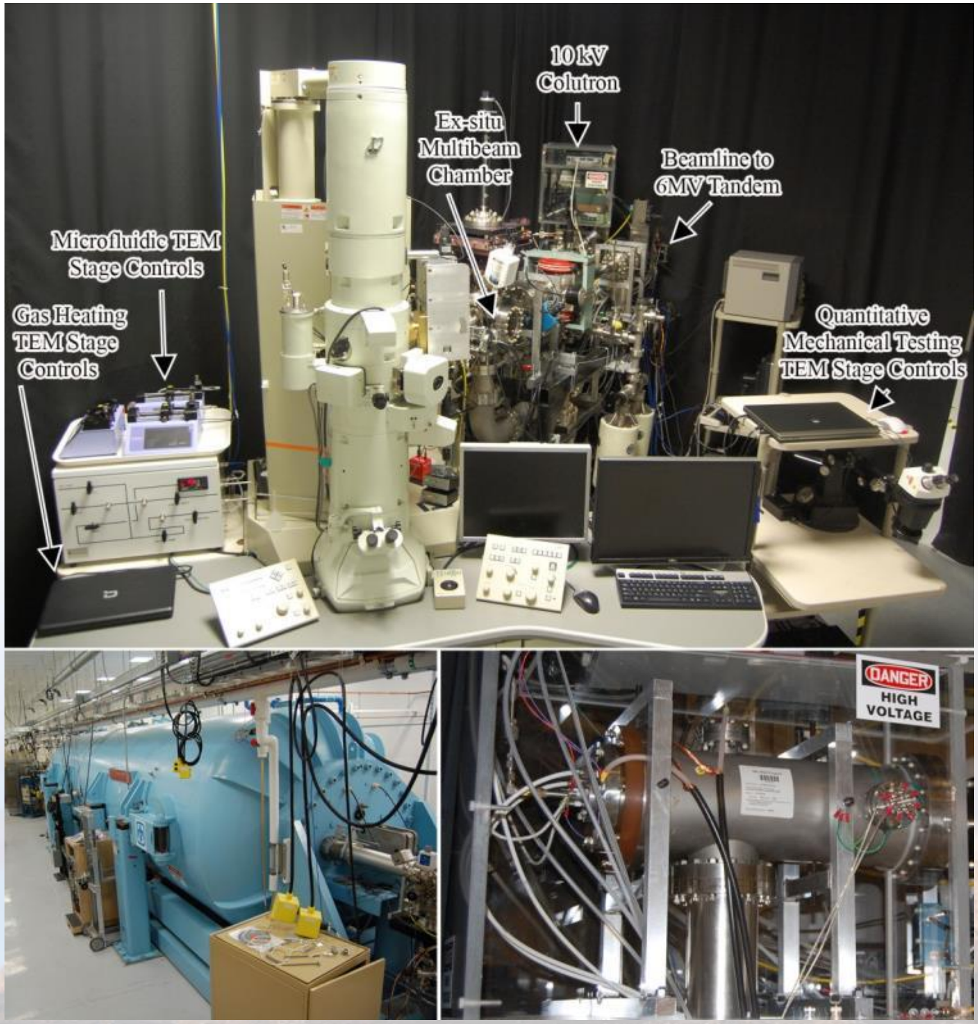
Demkowicz et al., MRS Bulletin: 2010. 35

To a first order mean grain size comparison, these reports appear conflicting.
Not necessarily the case if initial microstructural details and associated properties are considered

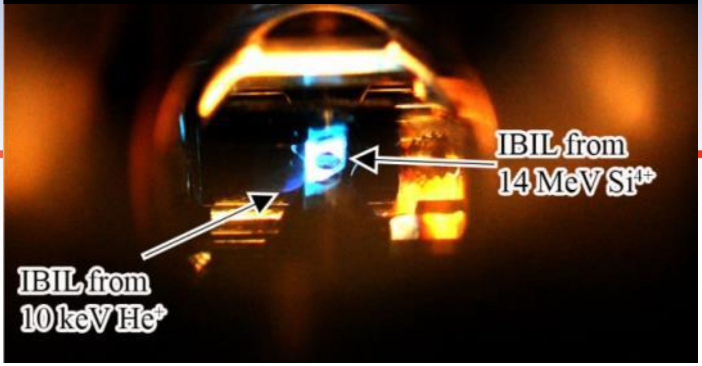
Sandia's Concurrent *In situ* Ion Irradiation TEM Facility

Collaborator: D.L. Buller

10 kV Colutron - 200 kV TEM - 6 MV Tandem

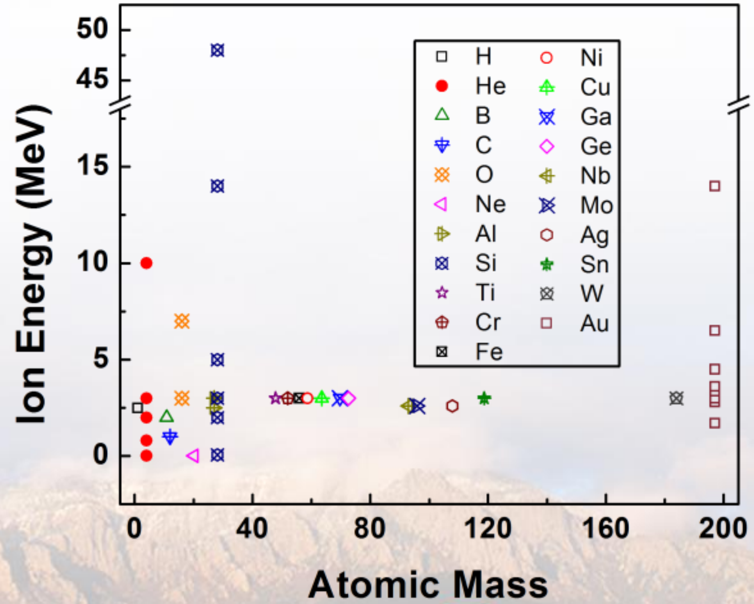


IBIL from a quartz stage inside the TEM



Direct real time observation of ion irradiation, ion implantation, or both with nanometer resolution

Ion species & energy introduced into the TEM



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Grain Growth from *In Situ* Irradiation

- **Au foil during bombardment with 10 MeV Si^{3+}**
- **~22 s of 4000s total experiment time**

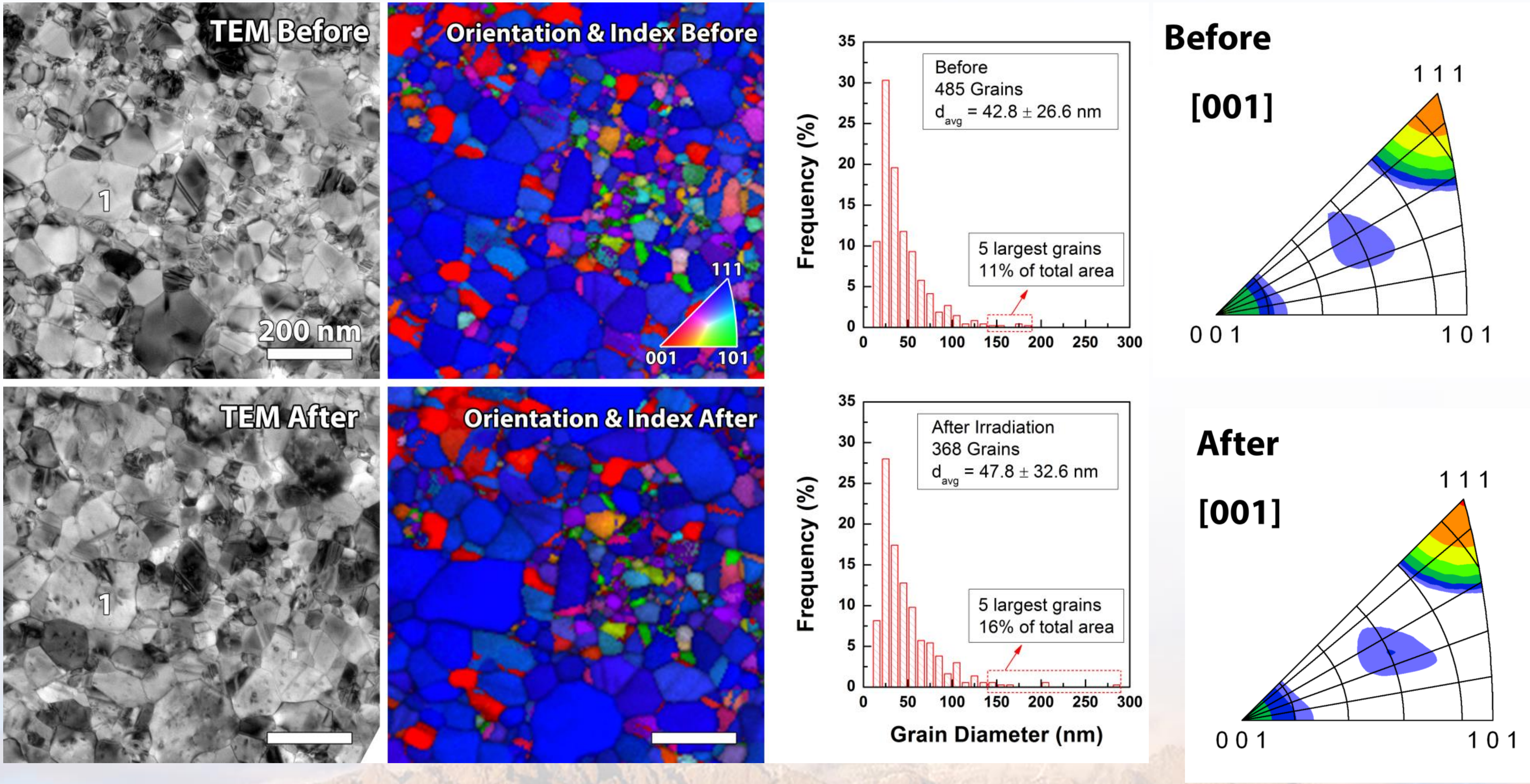
In situ ion irradiation TEM: 10 MeV Si into nanocrystalline Au.

Playback at 2 × real time.

2 × real time

Locations of single ion strikes and resulting microstructural change captured.

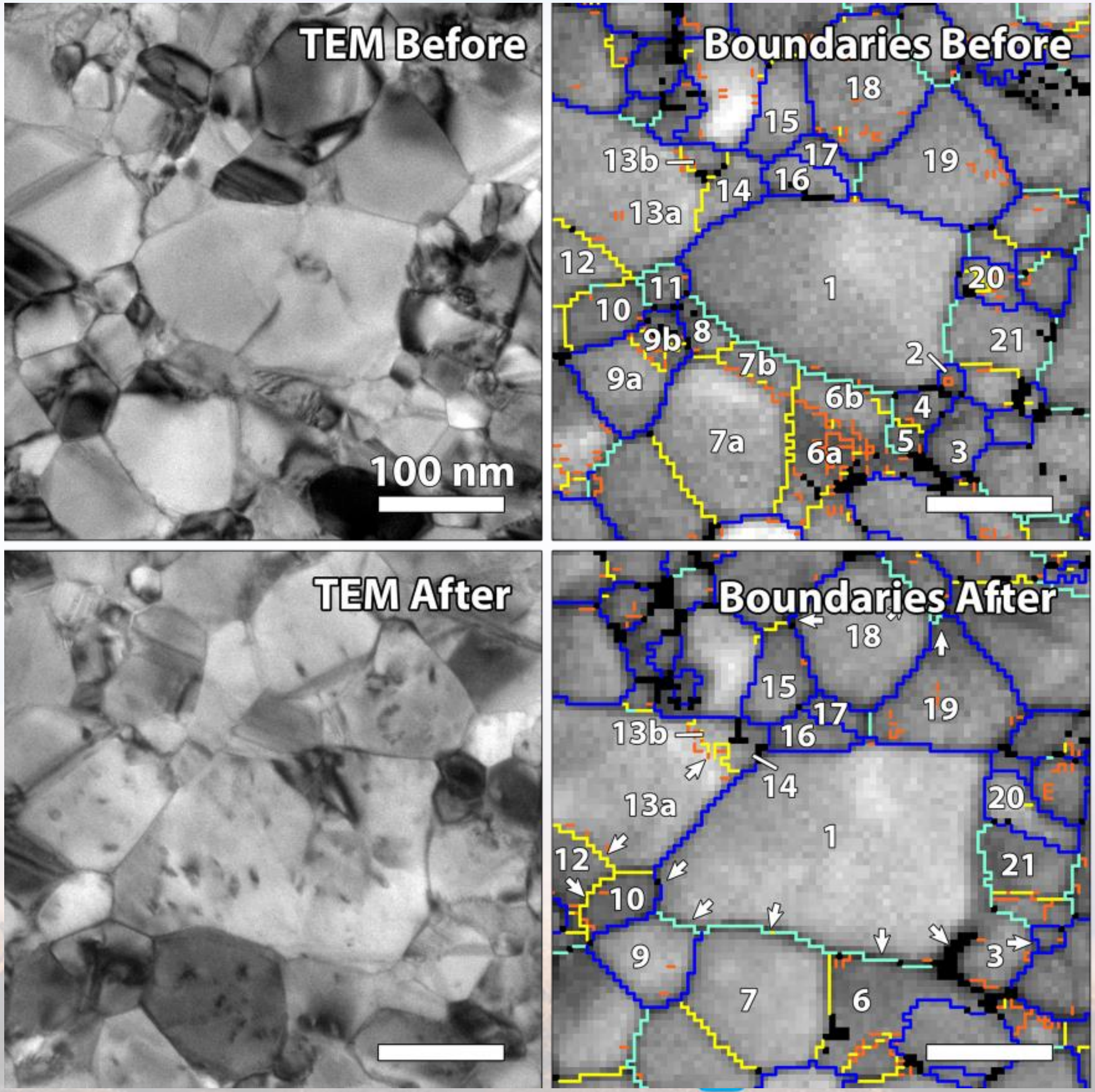
Global Quantification of Nanocrystalline Au Stability During 10 MeV Self-Ion Irradiation



The initial and post grain diameter, diameter distribution, and texture evolution can be compared to the *in situ* video

Local Quantification of Nanocrystalline Au Stability During 10 MeV Self-Ion Irradiation

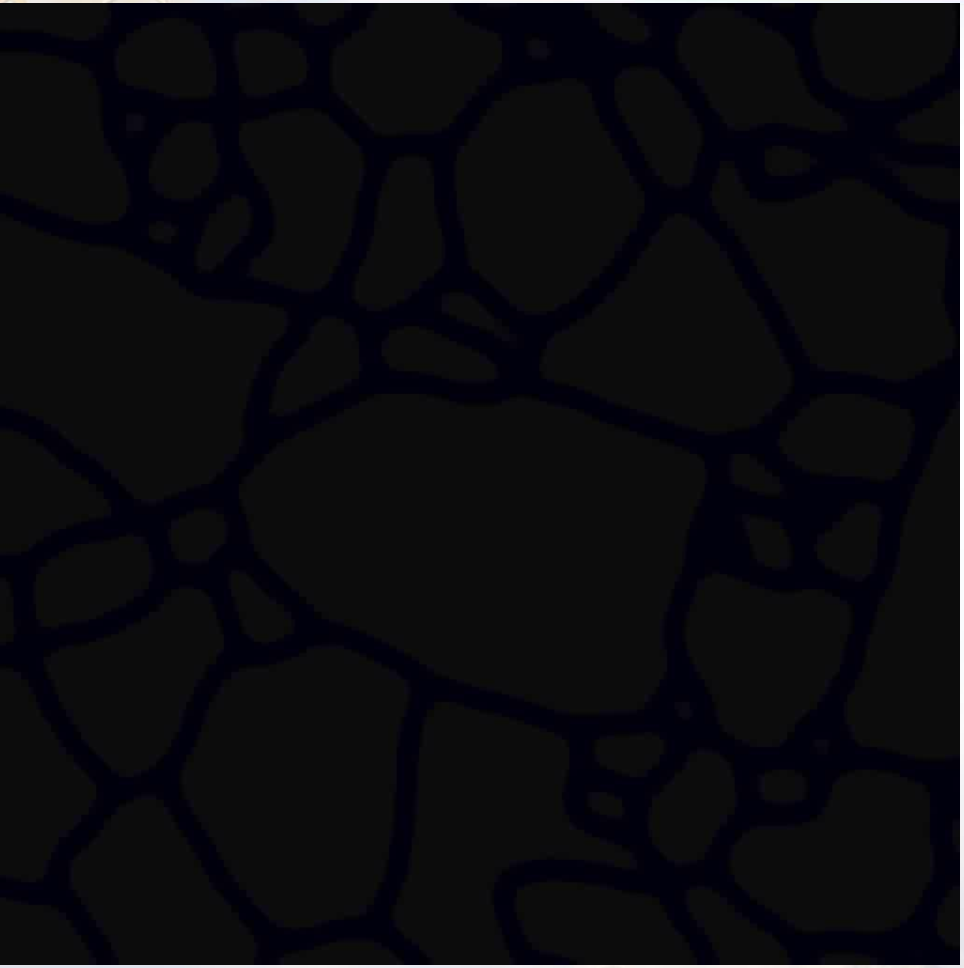
- The same grains identified before and after irradiation
- Individual grain boundary misorientation angles and axes quantified
- Correlation of GB properties and radiation-induced changes

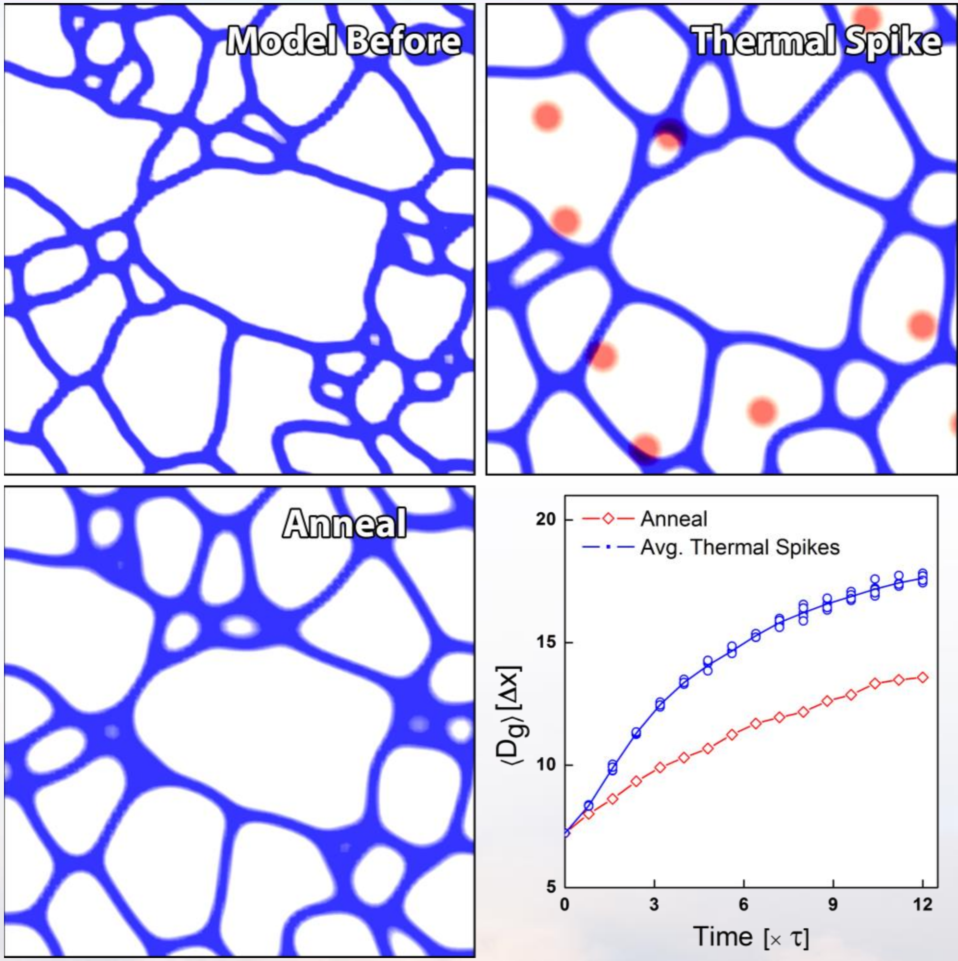


φ < 3°
3° ≤ φ < 15°
15° ≤ φ < 30°
30° ≤ φ

Grain boundary misorientation angle, boundary length, and axes of those migrating boundaries can be identified

Directly Inputted into and Comparison to Mesoscale Modeling



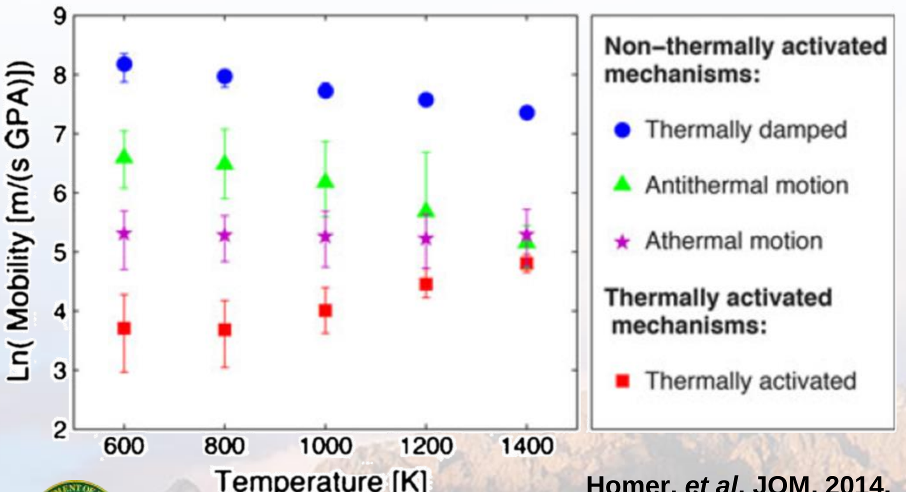


PED data can be directly inputted into Mesoscale and MD modeling

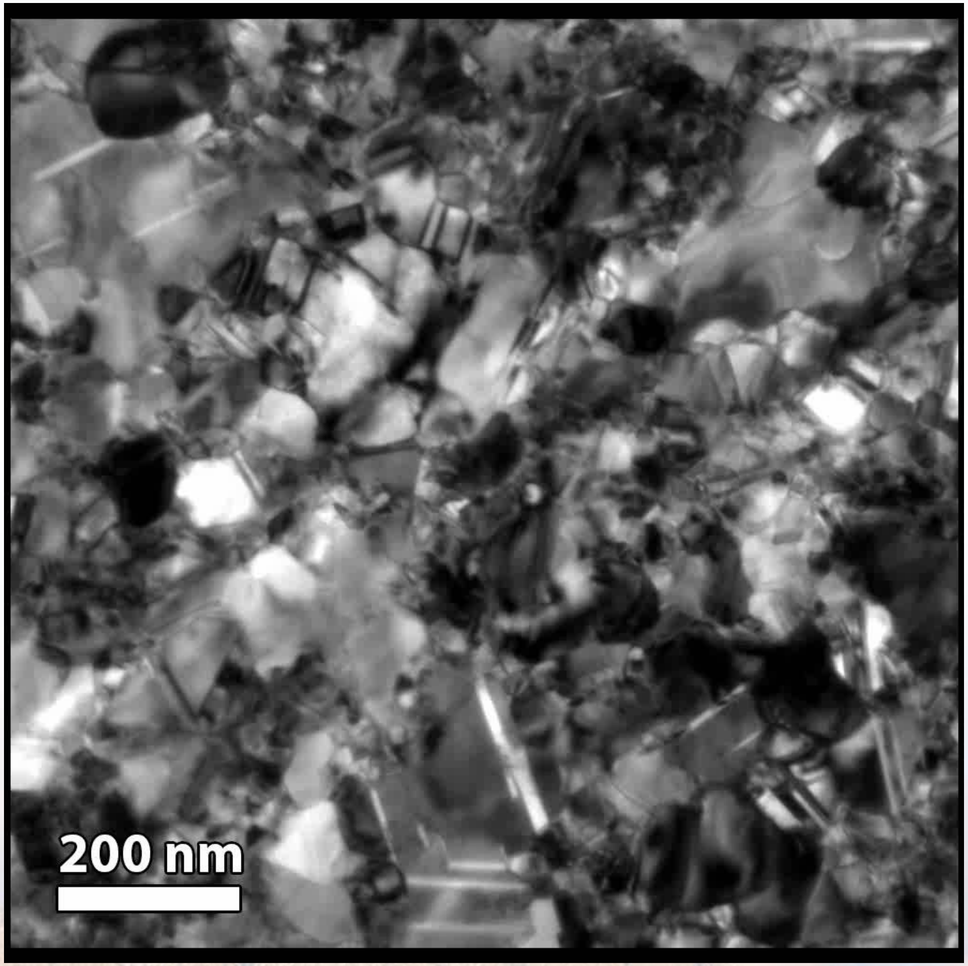
Mechanisms in modeling can be directly compared to in-situ observations

Future Directions

- **Nature of Ion Interactions**
  - Nuclear and electronic stopping
  - Point defects and defect clusters
  - Dose rate
- **Other materials and alloy systems**
- **Better informed GB mobility in model**

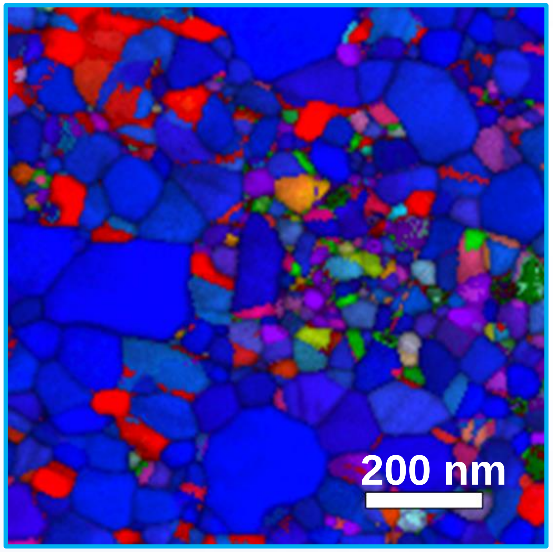


Homer, *et al*, JOM, 2014.



Implementation of heterogeneous boundary mobility

Summary



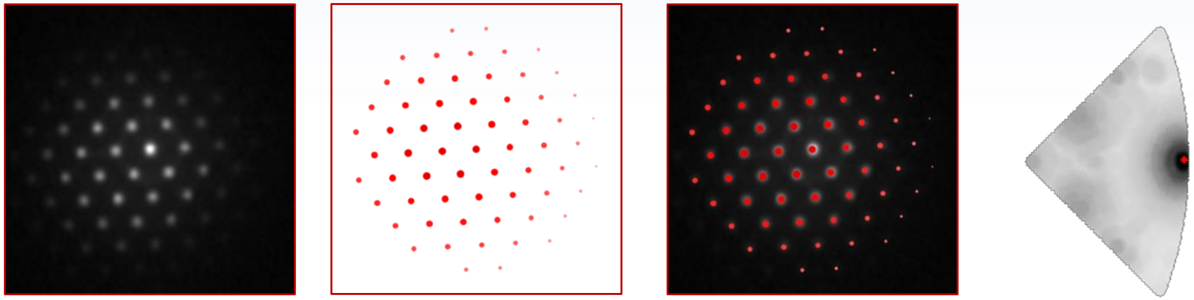
In situ ion irradiation
TEM: 10 MeV Si into
nanocrystalline Au.

Playback at 2 × real time.

Combining precession electron diffraction with in situ TEM grain growth provides new direct correlation to mesoscale modeling and further insight into nano- and micro structural stability.

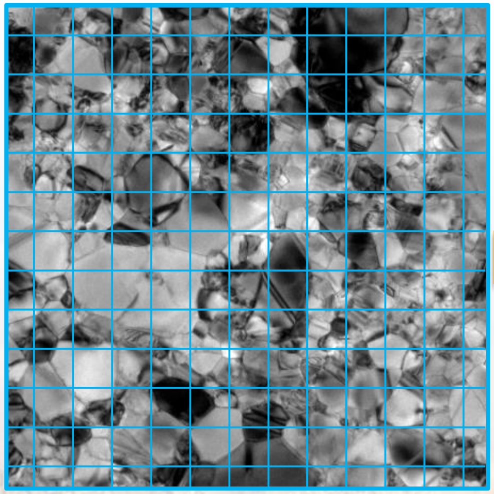
Fully supported by the Division of Materials Science and Engineering, Office of Basic Energy Sciences, U.S. Department of Energy. Sandia National Laboratories is a multiprogram laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

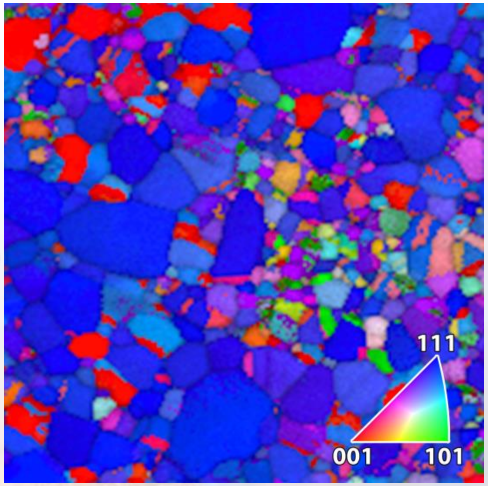
Approach: Experimental



Experimental Pattern | Theoretical Template | Template Matched | Point Mapped To IPF

- **Automated diffraction orientation mapping**
  - Point by point grid of orientations mapped
  - 5 nm resolution
- **Analogous to EBSD**

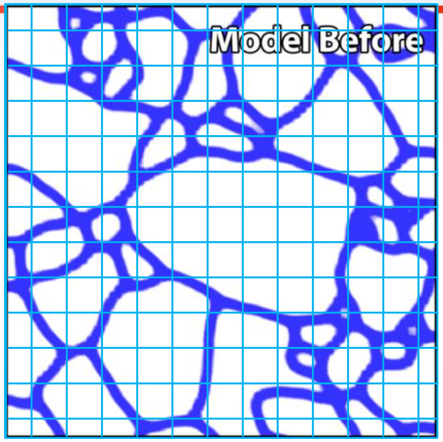


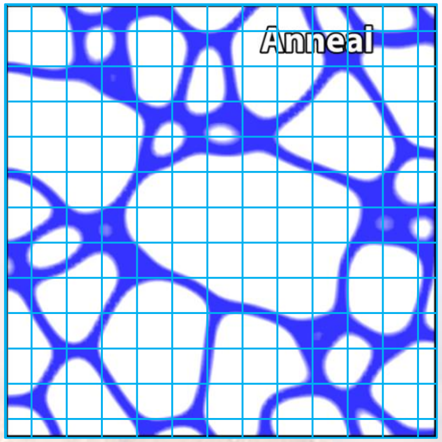


Point diffraction data

Approach: Modeling

- **What is phase field modeling?**
  - Mathematical model for solving interfacial problems, like solidification, growth, etc.
- **Example grain growth model**
  - Thermodynamic free energy function
    - $dF = d(\gamma A) = \gamma dA$ (γ: GB energy, A: GB area)
  - Model for kinetics
    - $V = M\gamma h$ (M: GB mobility, h: GB curvature)
  - Solve at each pixel for a predetermined timestep
- **See Abdeljawad and Foiles, Acta Mater, 2015 for more information**





Can directly use experimental maps as input structures, and then compare evolutions!

Model Data Analysis

- **During simulated annealing grain growth scales approximately with $T^{1/2}$**
  - Expected for homogenous grain growth
- **During simulated irradiation, grain growth scales with $T^{1/n}$, where n ≈ 3**
  - Initially faster, but stagnates sooner