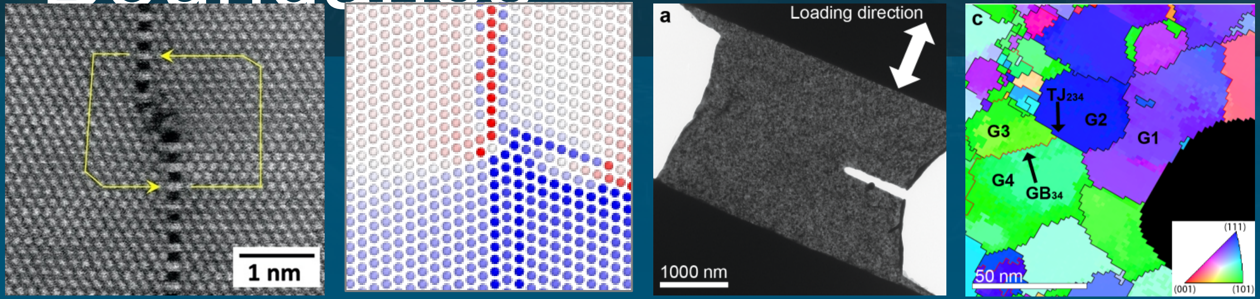
SAND2022-15573C

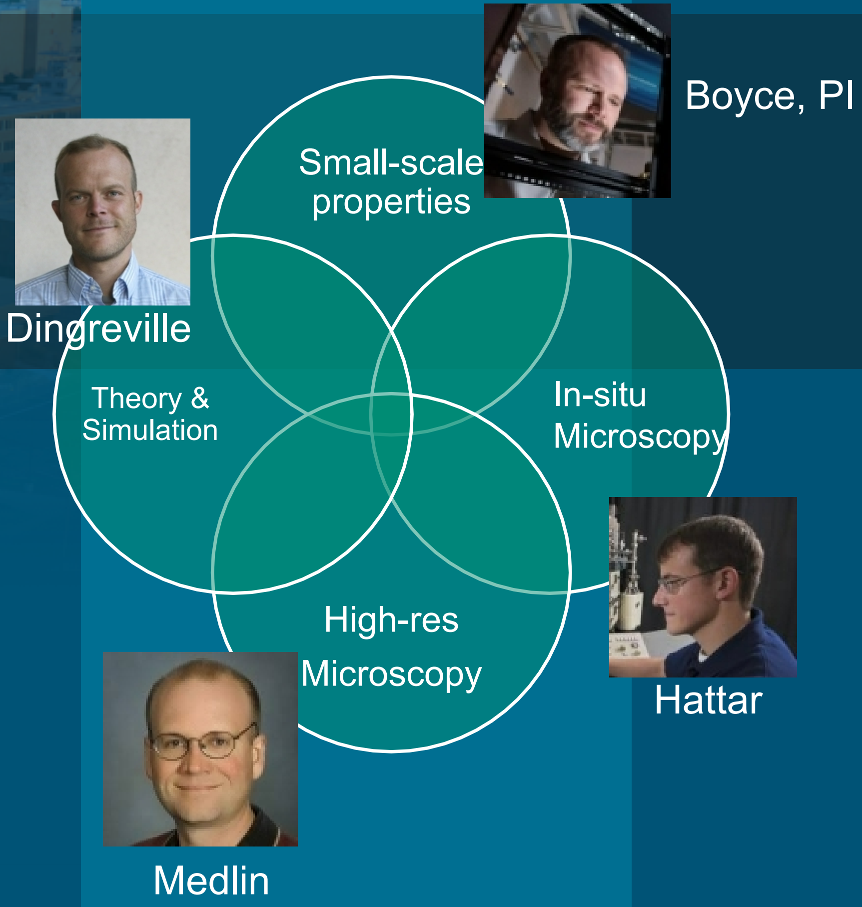
Sandia National Laboratories

Nanomechanics and Nanometallurgy of Boundaries



Brad L. Boyce, Khalid Hattar, Doug Medlin, Remi Dingreville

Sandia National Laboratories



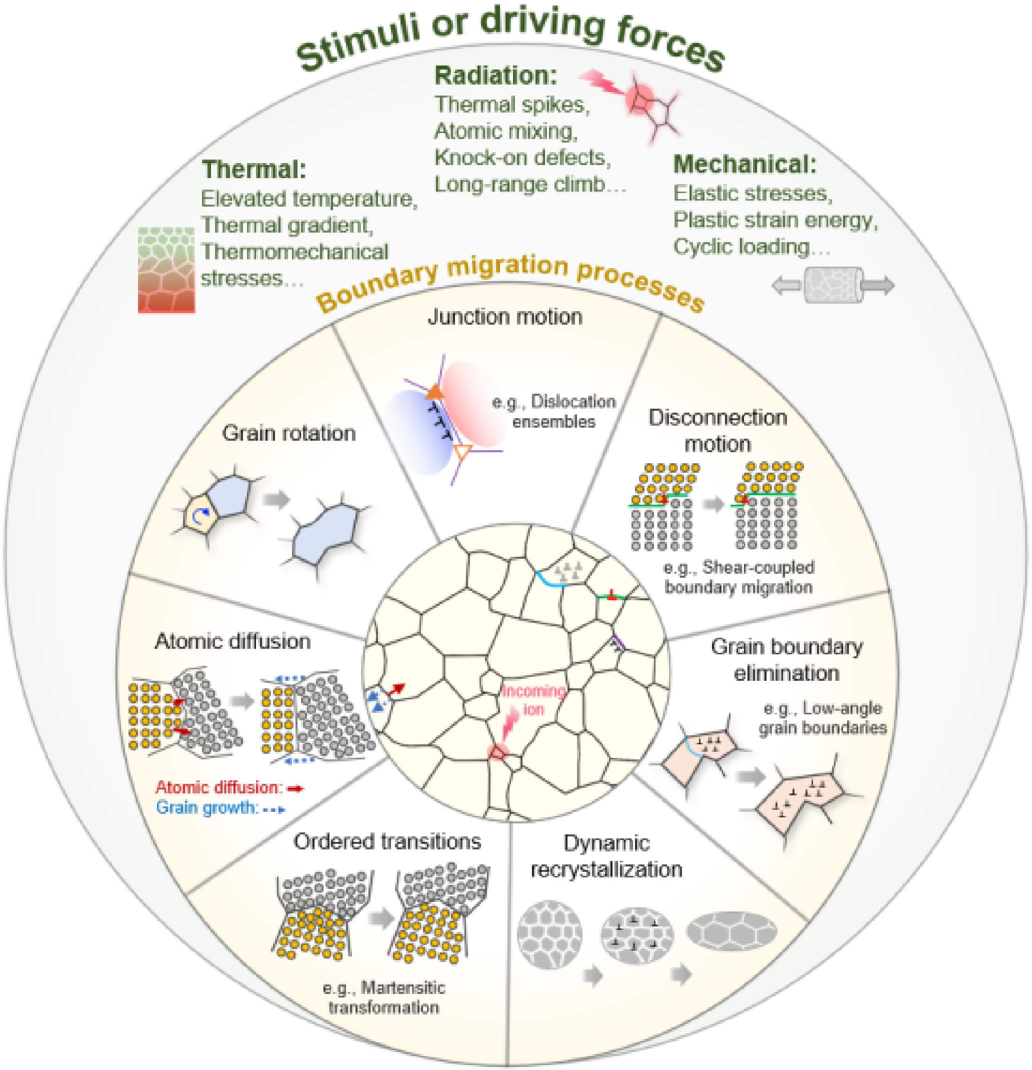
U.S. DEPARTMENT OF ENERGY NNSA

Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

Project Overview:

Guiding principle: By understanding the mediating role of grain boundaries and their networks, we can harness them to control monotonic and cyclic damage processes.

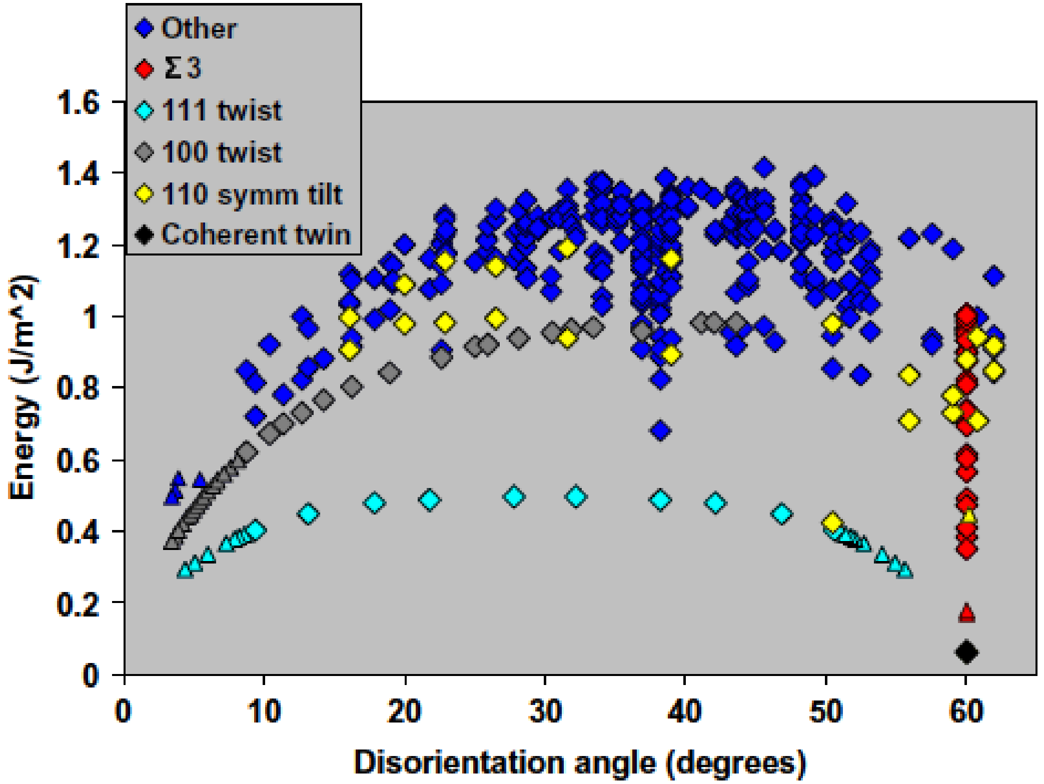


Nanocrystalline metals provides a unique **'microstructural grain boundary laboratory'** through which we can suppress better-understood mechanisms (e.g. dislocation plasticity) and amplify the unusual contributions of grain boundaries.

Current core hypothesis: the presence and evolution of defects within grain boundaries alter the GB behavior in response to thermal, irradiation, and/or mechanical driving forces

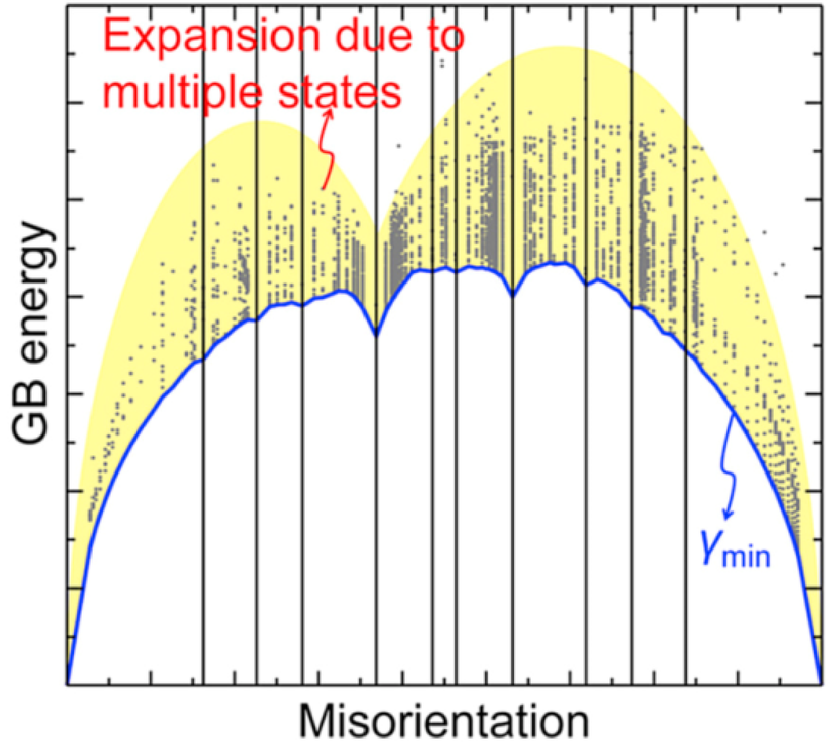
"Way back" in 2009…

Grain boundary properties depend strongly on character



Olmsted, Foiles, Holm, *Acta Mater*, 2009

Grain boundaries can occupy a multiplicity of states

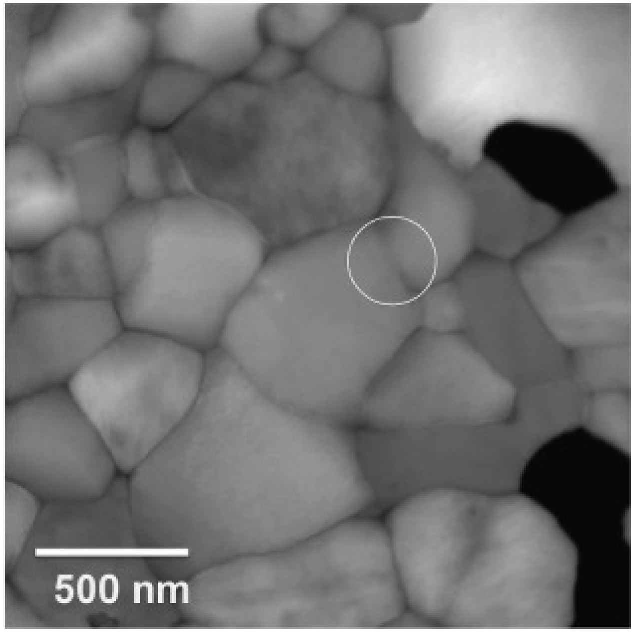


Han, Vitek, Srolovitz, *Acta Mater*, 2016

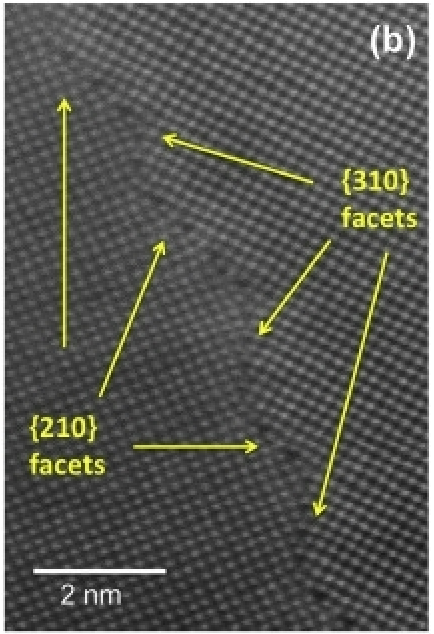
Theme of this presentation: **Defected defects…**

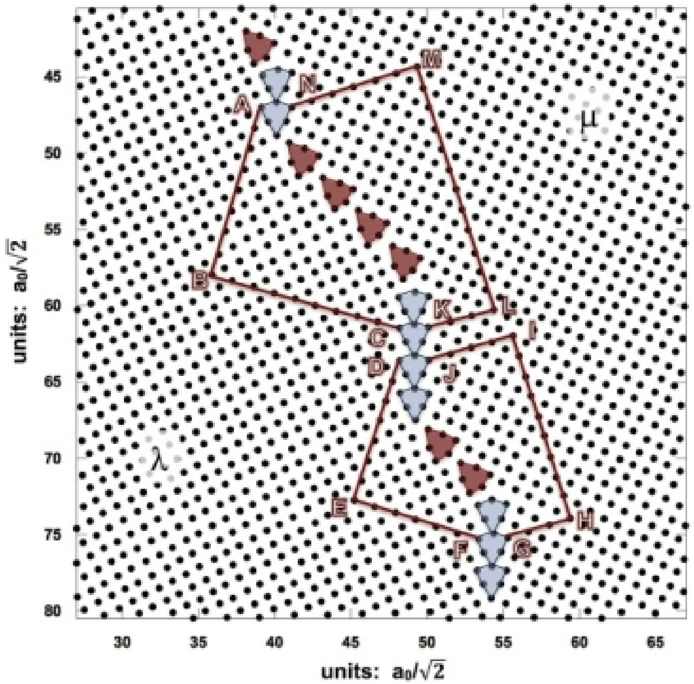
Grain boundaries are 2D defects that move through the evolution of 0D and 1D defects within them

Defected Defects

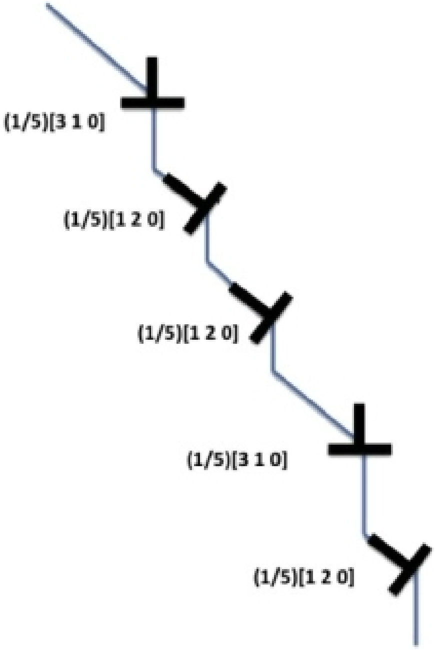


An “ordinary”
Σ=5 grain boundary





{310} and {210}
facets

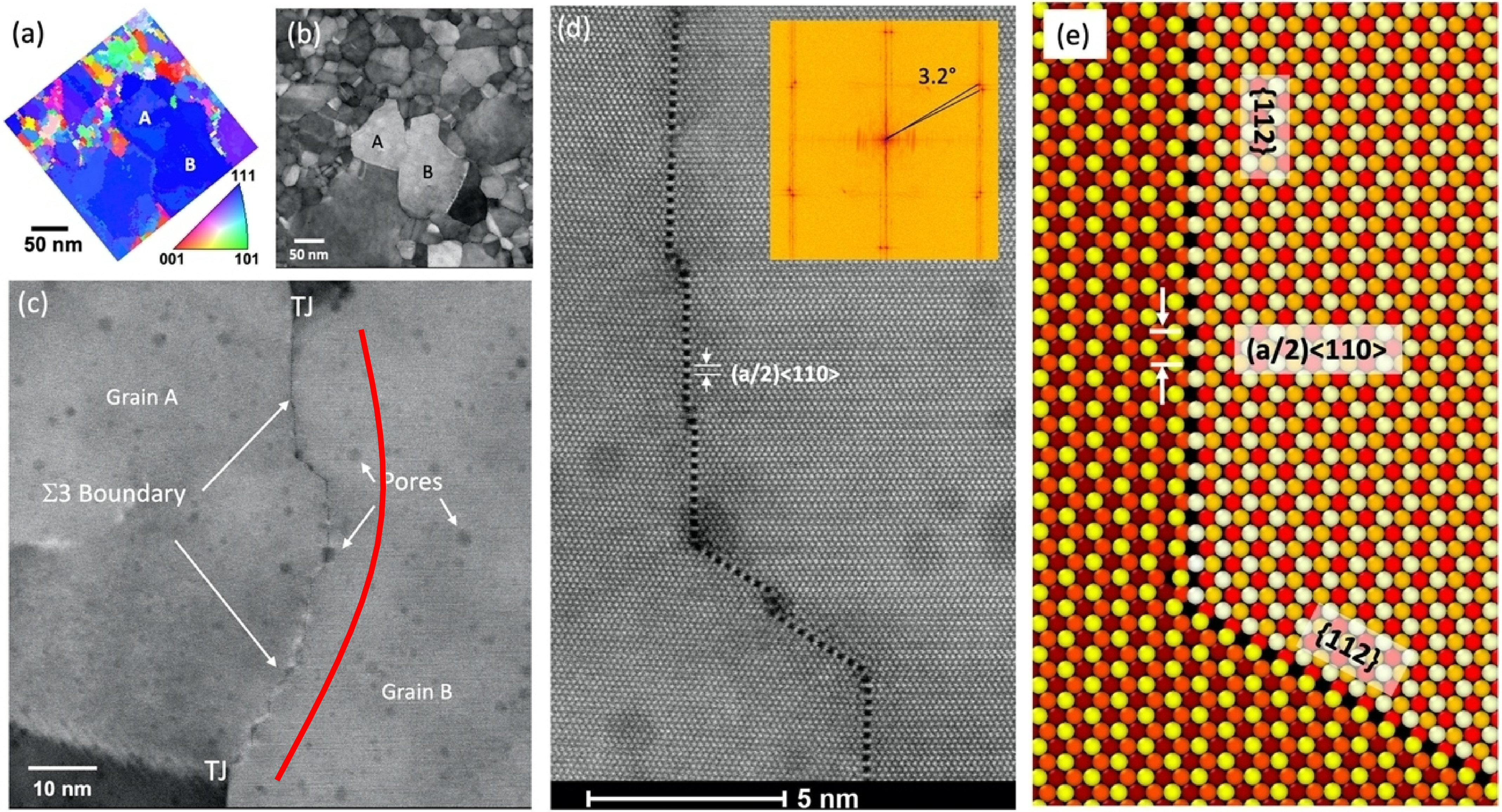


secondary grain
boundary dislocations

Facets are a common GB feature found in many vicinal low-CSL boundaries.
They are also found within many random HAGBs as the boundary locally tries to adopt a low energy structure

Medlin, Hattar, Zimmerman, Abdeljawad, Foiles, *Acta Materialia*, 2017

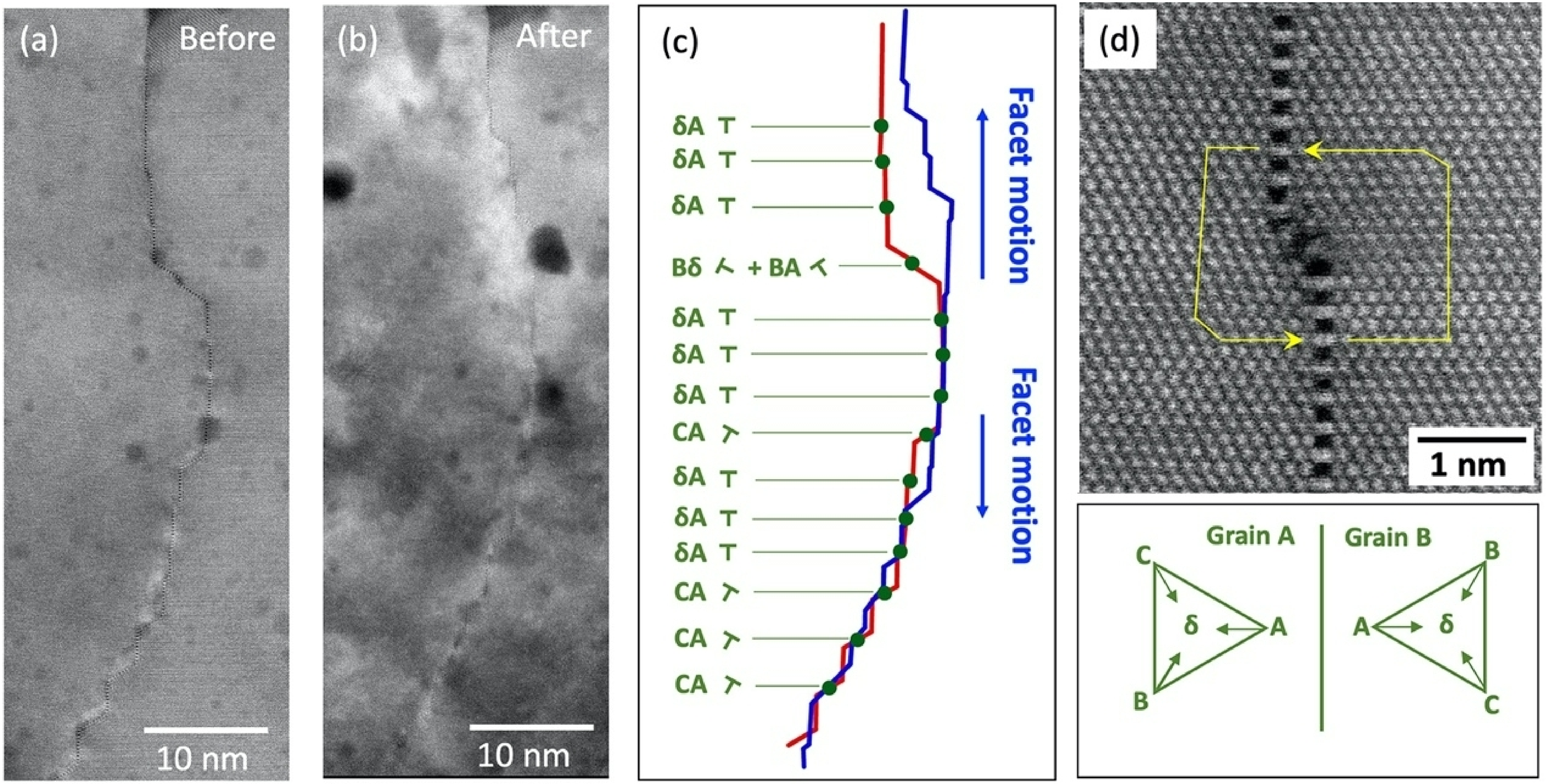
Defected Defects: Irradiation-induced migration of a ∑3 grain boundary



C.M. Barr, et al., *Science Advances*, 2022

Facet migration of a ∑3 grain boundary

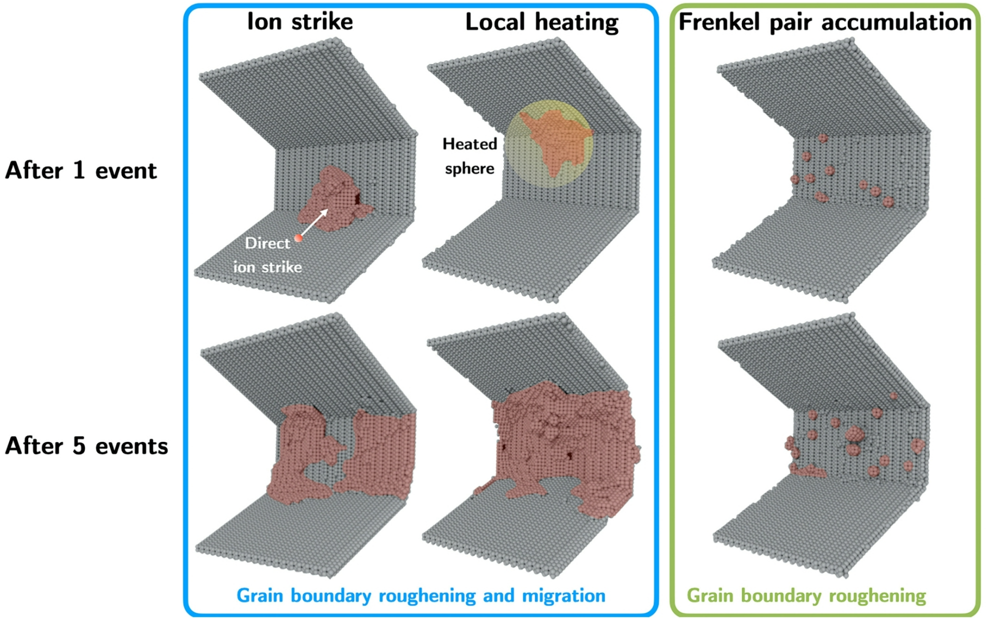
Irradiated with non-depositing 2.8 MeV Au^{4+}; Total dose during exposure: 1 dpa



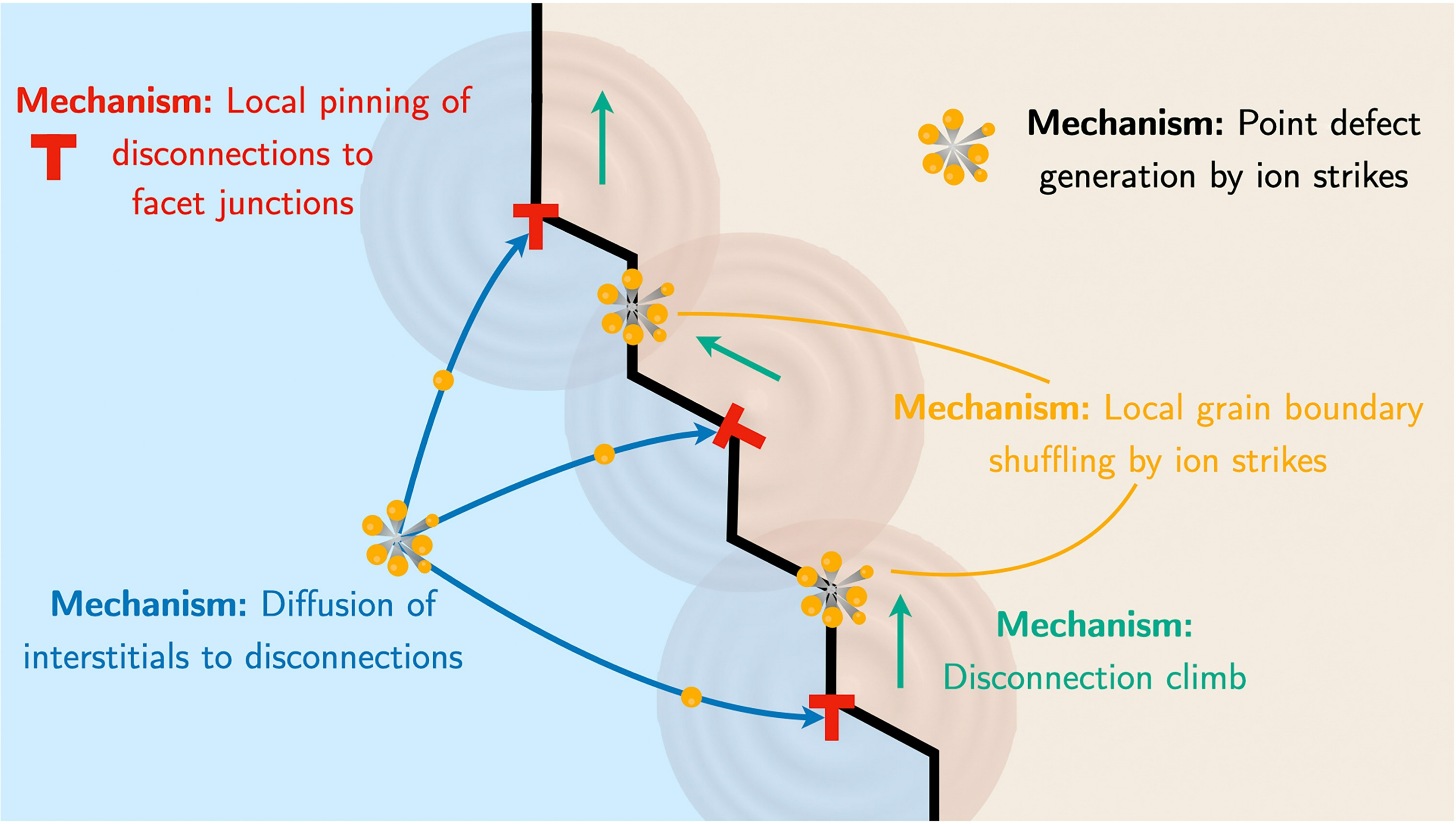
What atomic process(es) drive this migration of the facet junctions?

C.M. Barr, et al., *Science Advances*, 2022

Irradiation induces a suite of processes that facilitate boundary migration

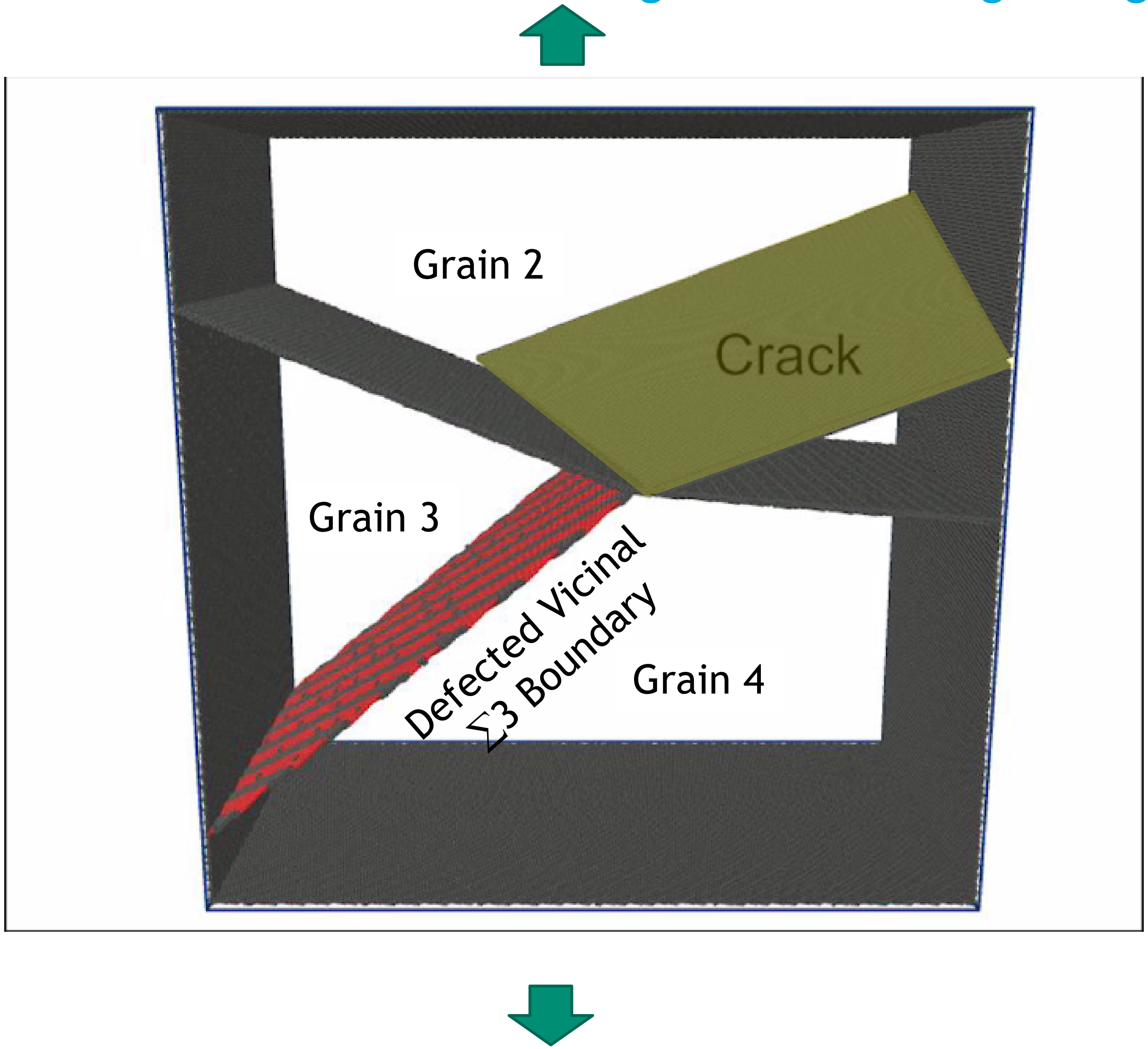


Three simulation techniques:
Localized heating
Ion strike (PKA)
Frenkel pair accumulation (NRT-dpa)



C.M. Barr, et al., *Science Advances*, 2022

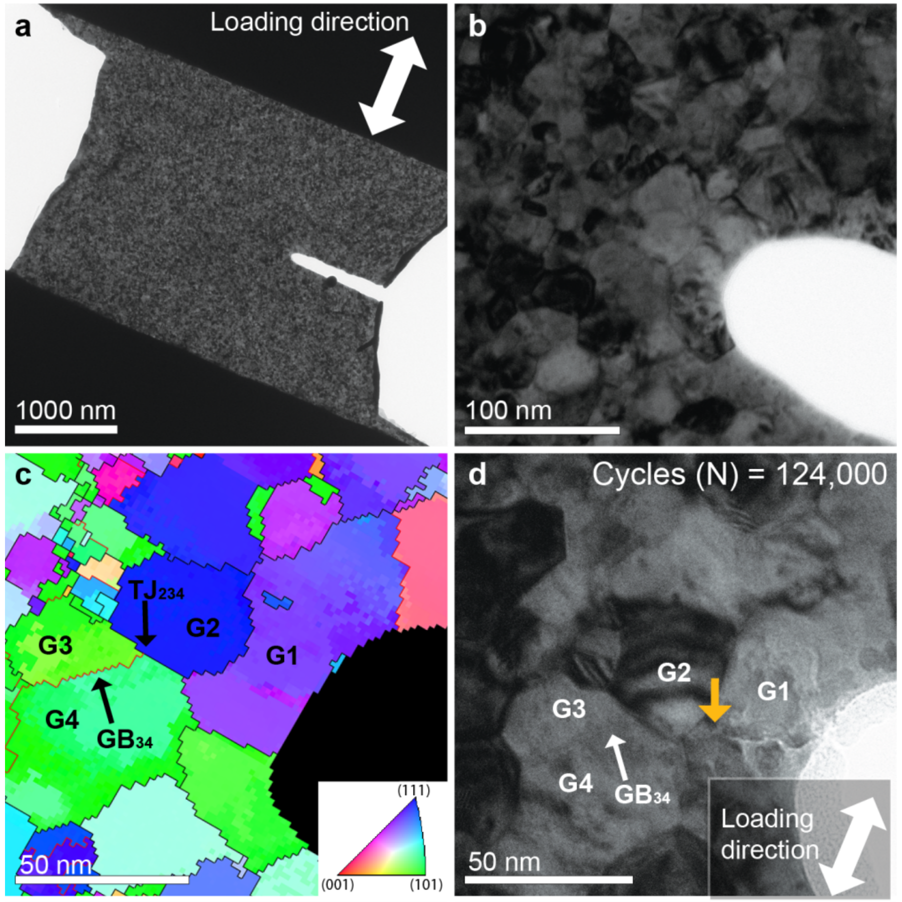
Defected Defects: Simulation of fatigue-induced gb migration



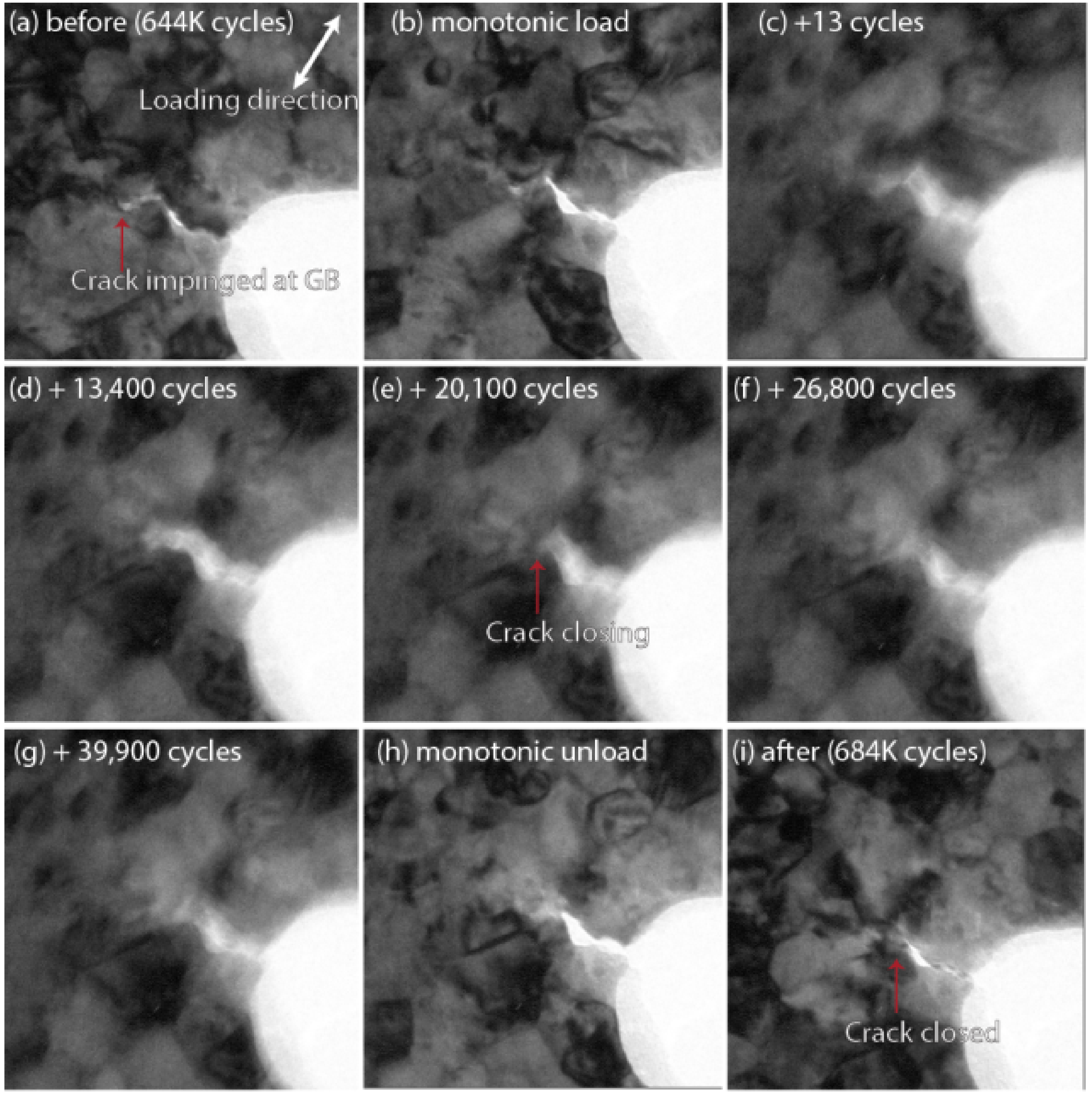
C.M. Barr *et al.*, in review
(a collaboration with M. Demkowicz)

High-cycle fatigue-induced vicinal boundary migration

Polycrystalline Pt



200 times every second,
we apply 17 μN, a force equivalent
to merely 10,000 C-C bonds.

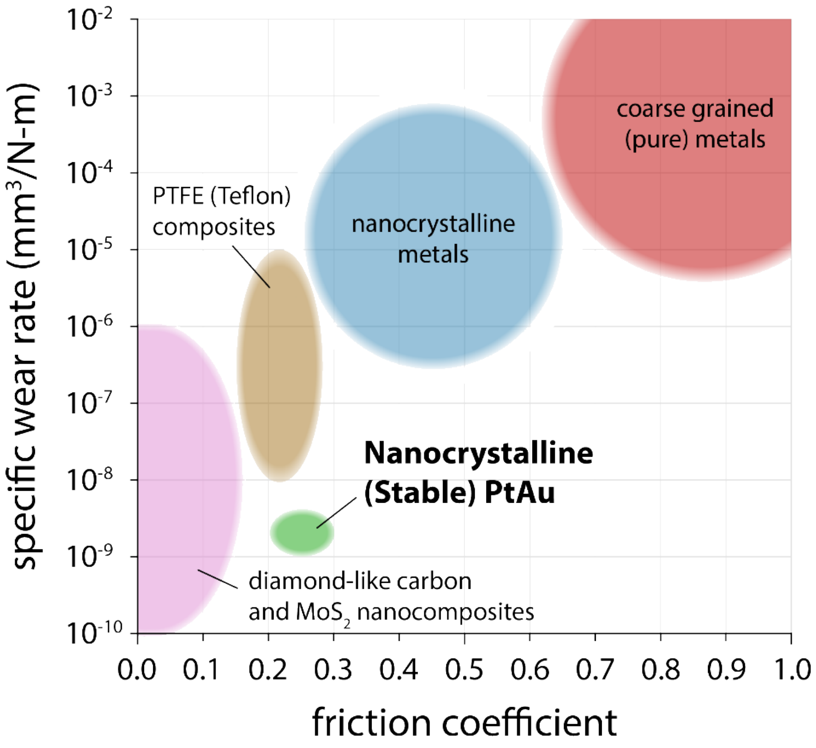


Similar observations of crack healing have been made multiple times in Pt, and also in Cu

Defected Defects:
Added complexity with alloying

How does chemistry (solute content) affect these processes?

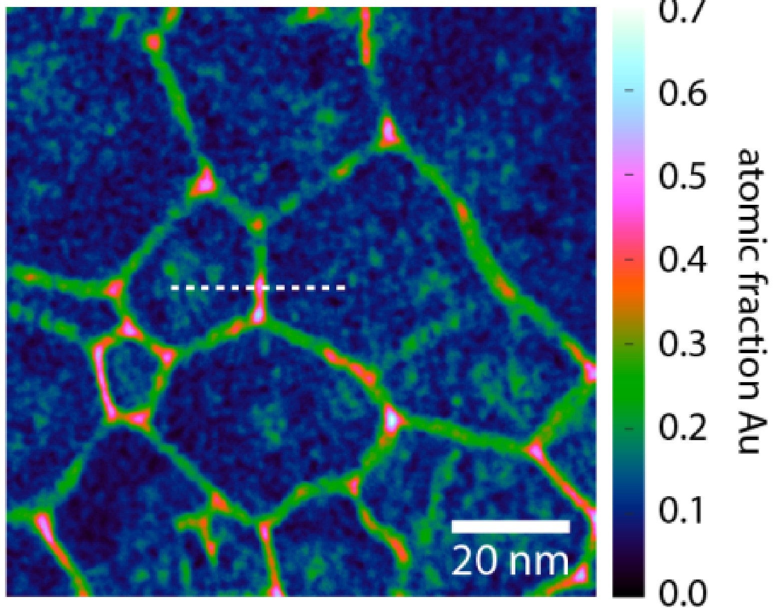
Cover art:
Barr, et al., *Nanoscale*, 2021
(simulations from Fadi Abdeljawad)

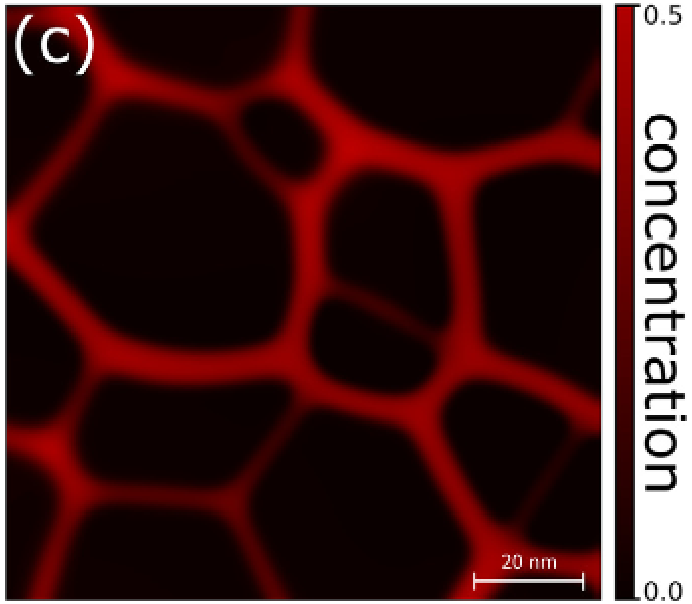


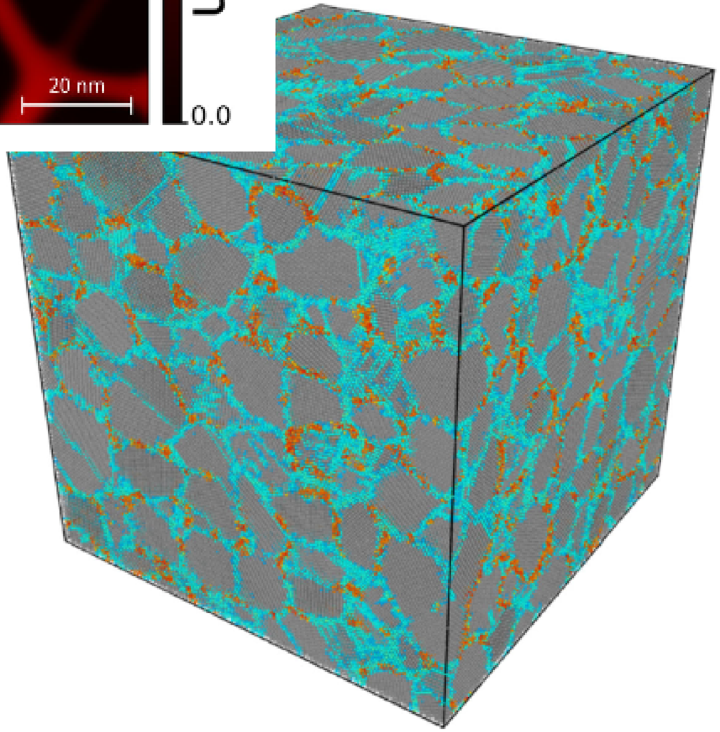
Wear Properties: Curry, et al., *Advanced Materials*, 2018
Tribocatalytic DLC formation: Argibay, et al., *Carbon*, 201

Pt-Au: the most noble binary nanocrystalline alloy

STEM-EDS



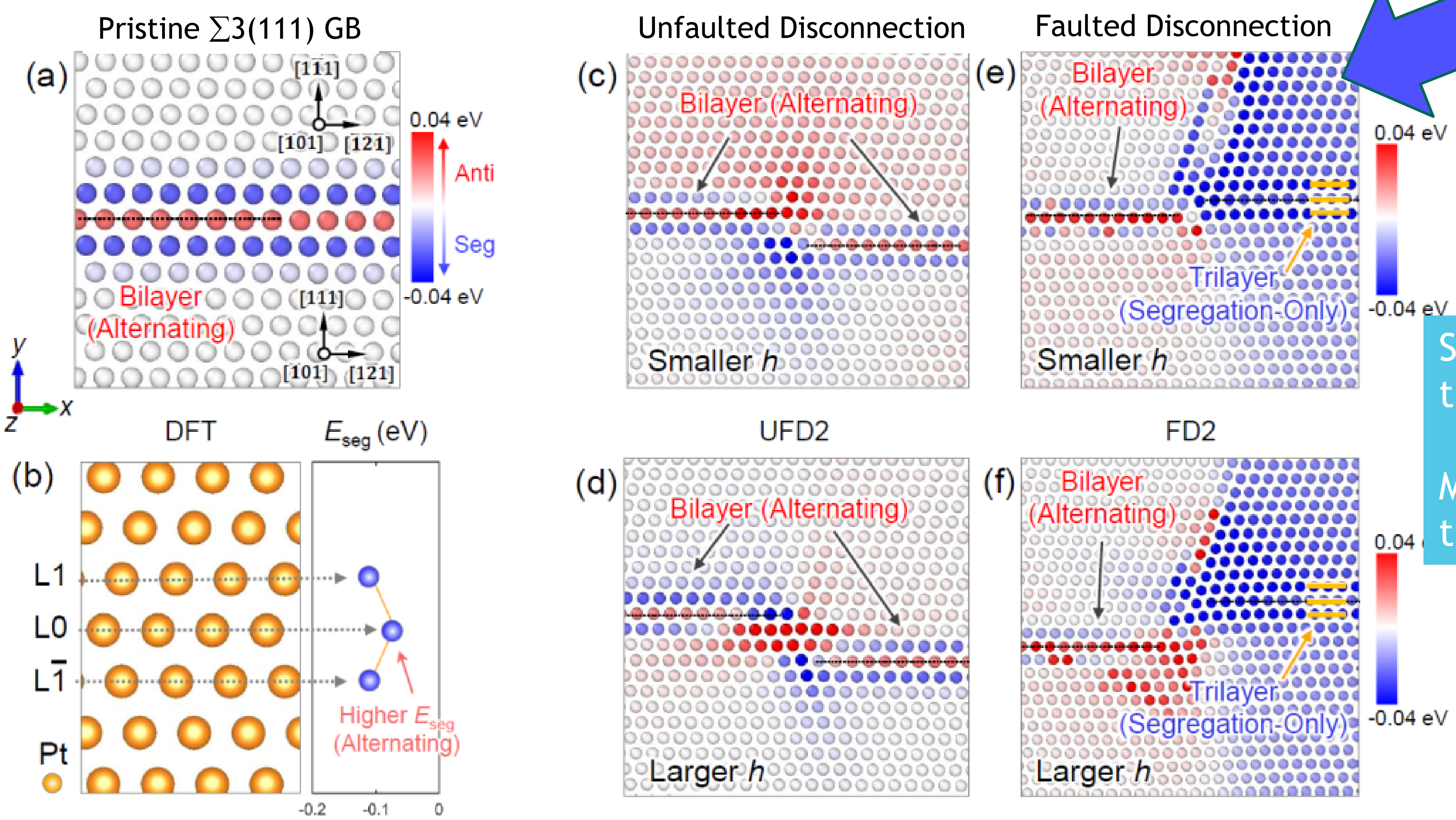




Phase Field with Heterogeneous Segregation: J. Monti et al., *Acta Mater*, 2022
GB character: C.M. Barr, et al., *Nanoscale*, 2021
GB Spinodal decomposition: X. Zhou et al., *Acta Mater.*, 2021 (collab with G. Thompson, D. Raabe)
GB phase transformations: C.J. O'Brien et al., *J. Mater. Sci.*, 2018
Tensile behavior: N.M. Heckman et al., *Nanoscale*, 2018

Defected defects distort compositional effects

The local segregation potential depends on the nature of the defect structure.



Extensive changes in segregation potential as a result of defect type.

Some defects may trigger phase separation,

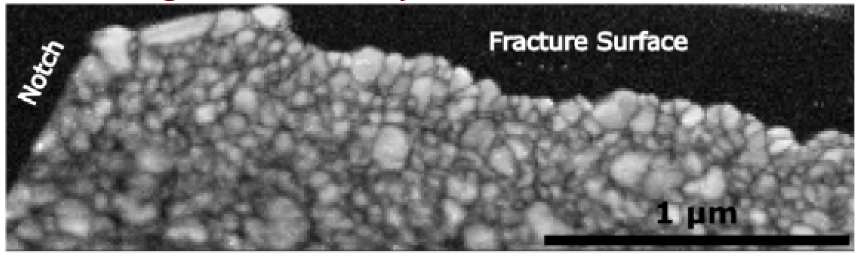
Moreover, defects may become trapped by the excess solute

In Pt-Au alloy: Hu, Medlin, Dingreville, *J. Phys. Chem. Lett.*, 2021
In 12 additional binary alloys: Hu, Berbenni, Medlin, Dingreville, in review

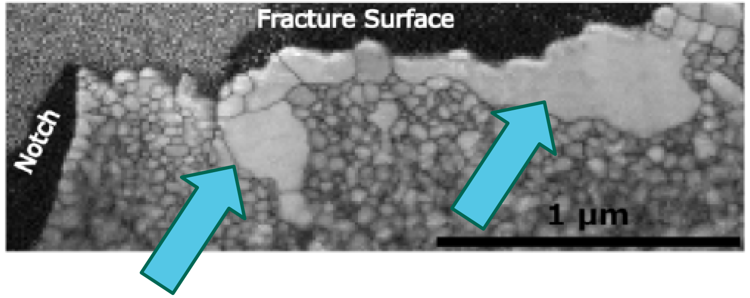
Ok, how do these chemically-stabilized GB defects alter macroscale polycrystalline behavior?

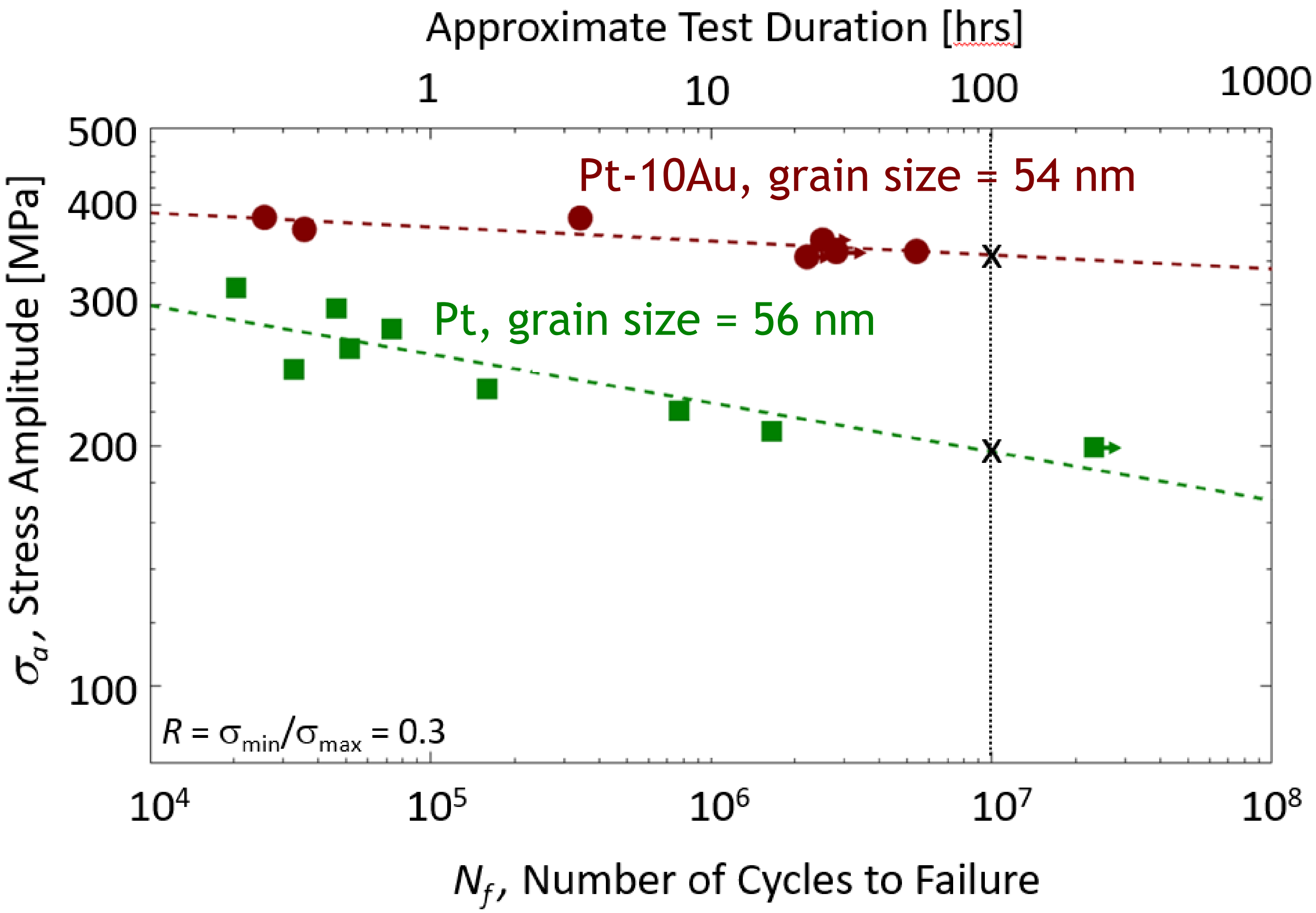
Net effects: Au in Pt stabilizes grain structure and enhances fatigue resistance

Pt-10Au, (initial grain size = 54 nm)
Fatigued ~1M cycles to failure



Pt, (initial grain size = 56 nm)
Fatigued ~1M cycles to failure

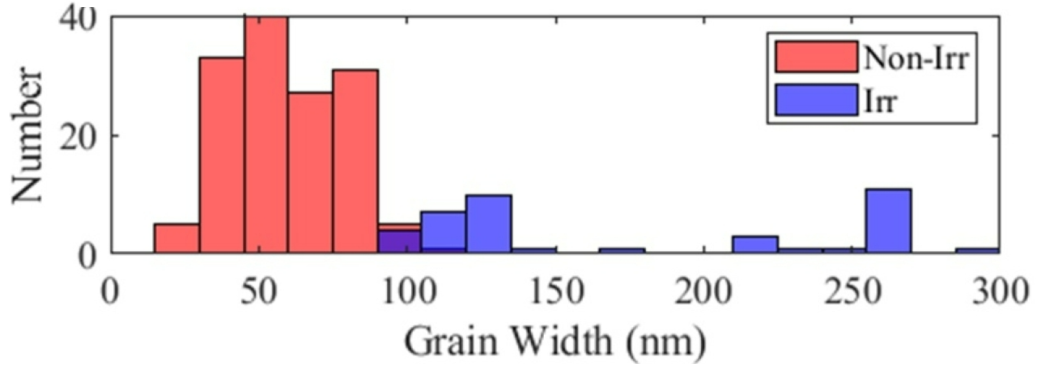




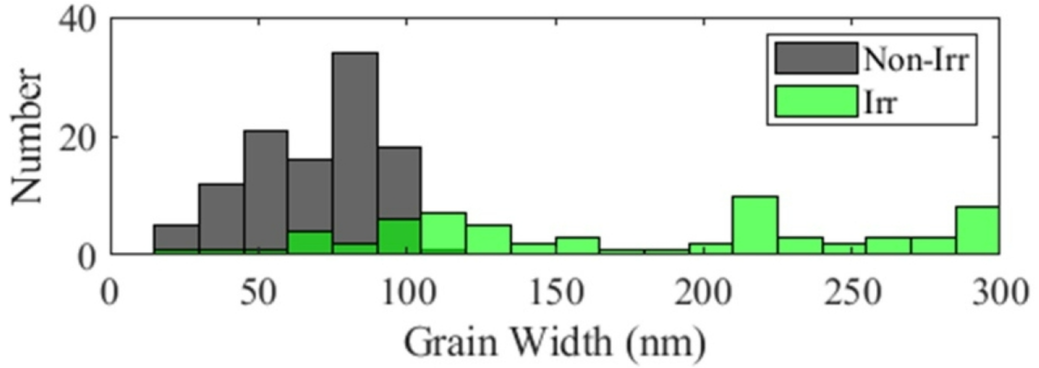
N.M. Heckman, et al., *Acta Materialia*, 2022

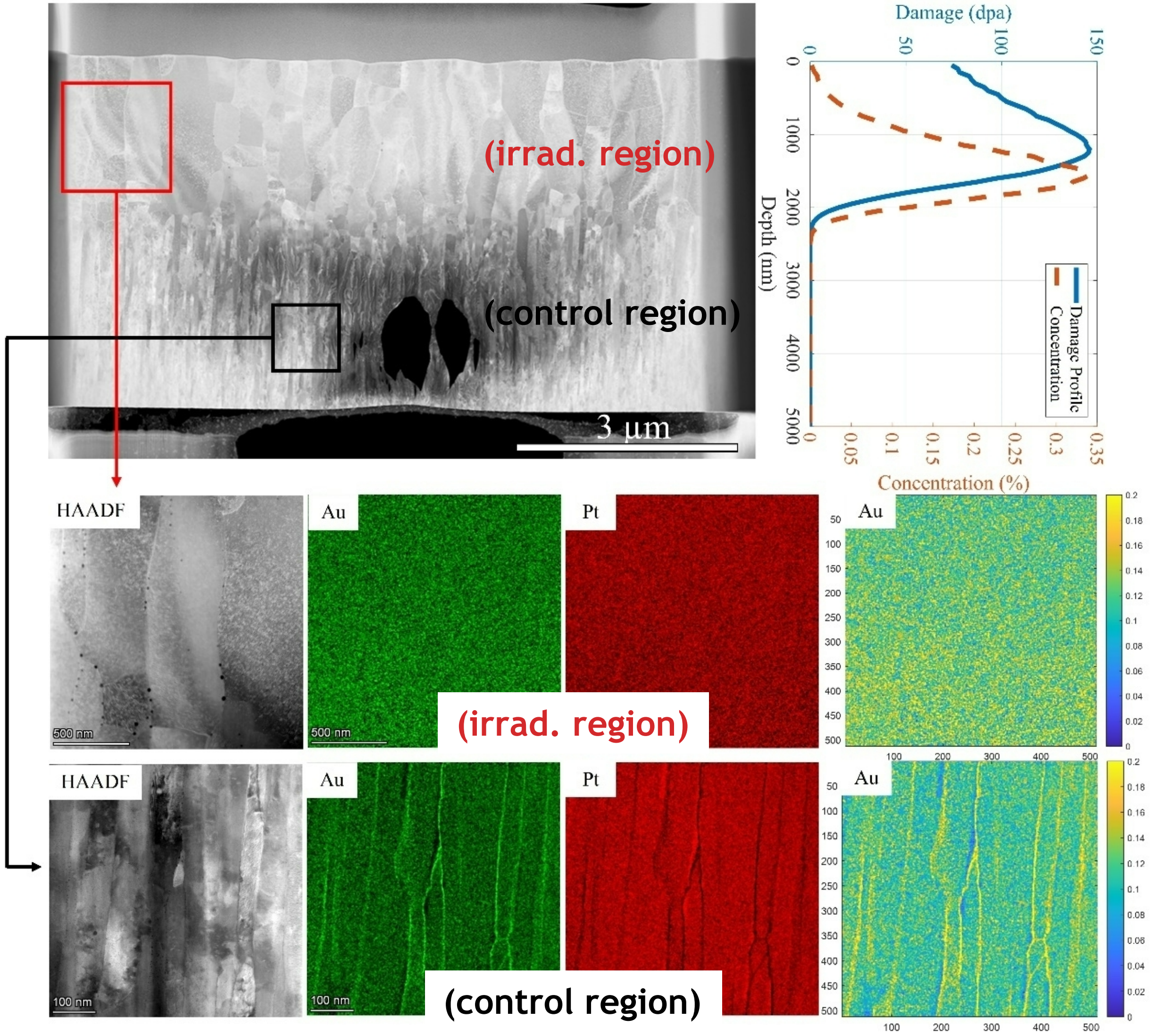
But the presence of Au at the GB does not resist irradiation-induced growth

Pt irradiation-indued grain growth



Pt-10Au irradiation-indued grain growth

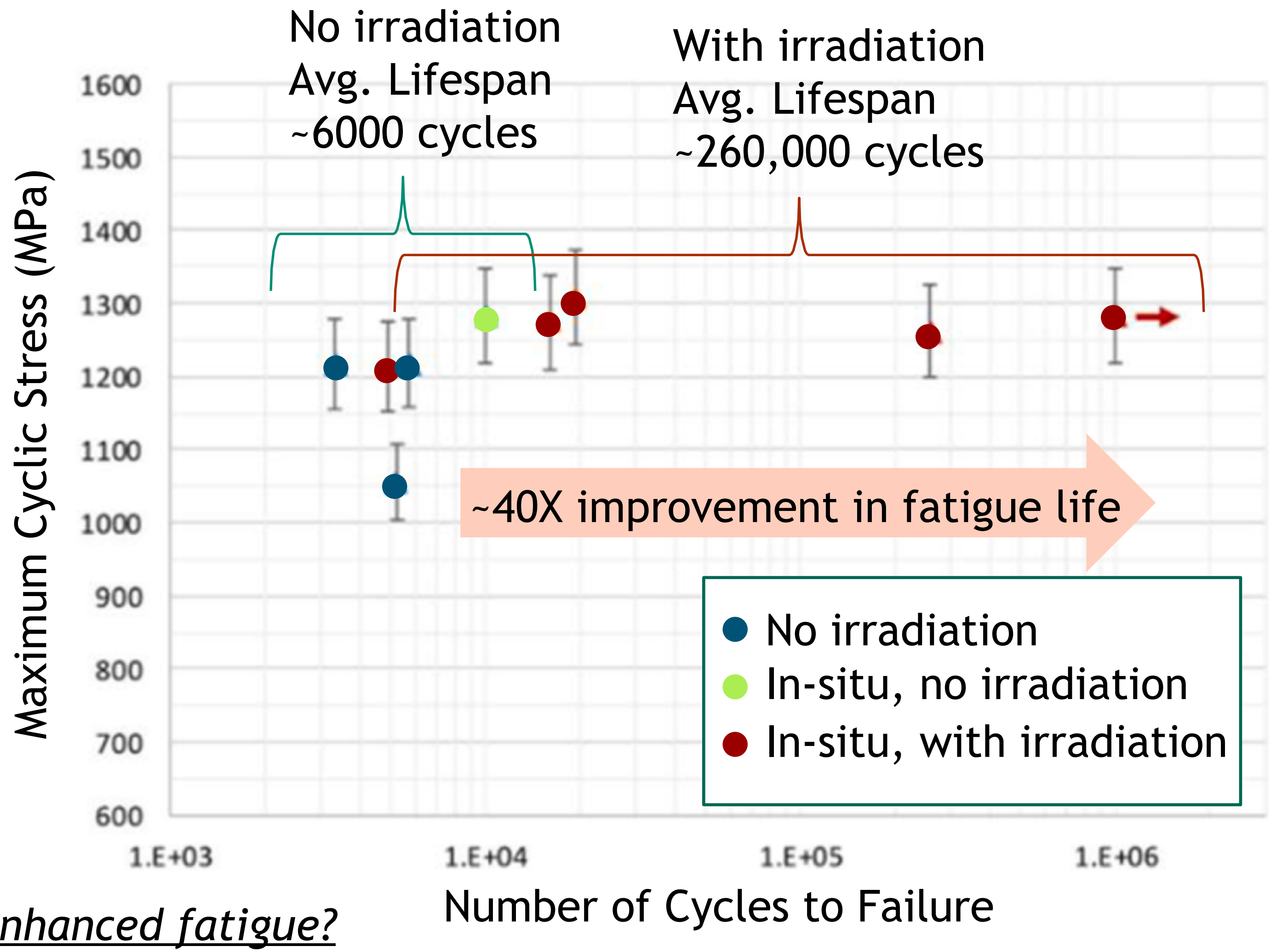




20 MeV Au^{4+} ion irradiation room temperature to a fluence of 2×10^{16} ions/cm^2

Schoell et al., *unpublished*

Simultaneous Irradiation + High-cycle Fatigue



What causes radiation-enhanced fatigue?

COLLECTIVE DEFECTS:

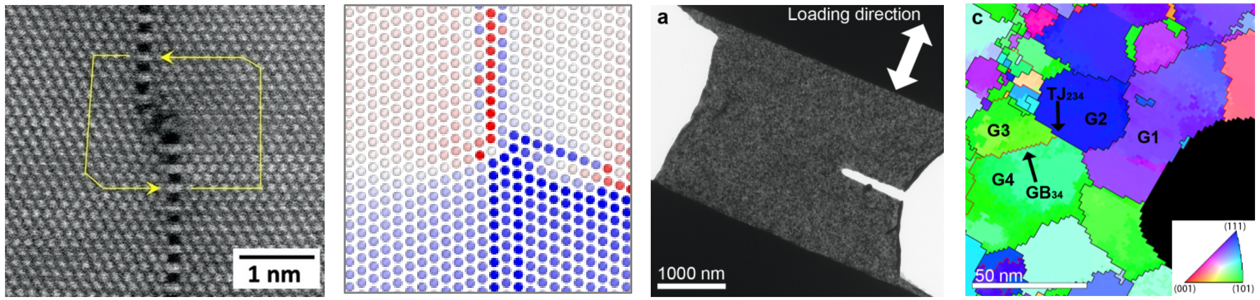
Compressive residual stress?

Radiation-induced hardening?

Complex superimposed defect-interactions?

Briggs et al., *Nucl Inst. Meth. Phys. Res.*, 2021

Summary



While there are many distinct unit processes for grain boundary migration in response to thermal, radiation, and mechanical stimuli, a unifying theme is the critical role of defects within the grain boundary.

Questions?

BIG SCIENCE AT THE NANOSCALE

U.S. DEPARTMENT OF ENERGY | Office of Science

- Comprehensive nanoscience capabilities
- Free access with a successful 2-page user proposal

CINT is a user facility providing cutting-edge nanoscience and nanotechnology capabilities to the research community.

Access to our facilities and scientific expertise is **FREE** for non-proprietary research.

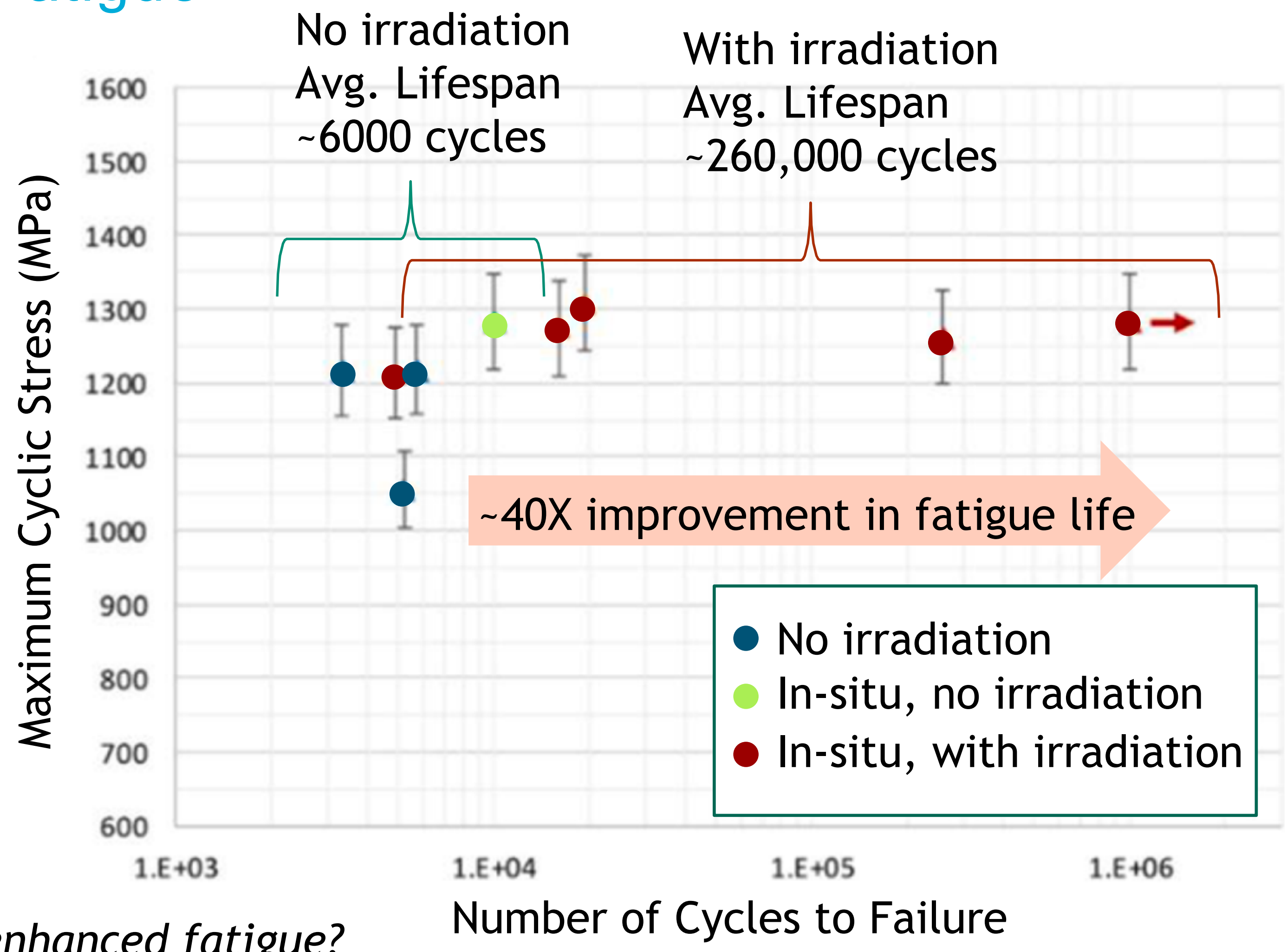
Research areas:

- Quantum Materials Systems
- Nanophotonics and Optical Nanomaterials
- ***In-Situ Characterization and Nanomechanics***
- Soft, Biological, and Composite Nanomaterials

To learn more and apply to use the facilities, visit: https://cint.lanl.gov

Backu
p

Irradiation + Fatigue



What causes radiation-enhanced fatigue?

Compressive residual stress?

Radiation-induced strengthening?

Complex superimposed defect-interactions?

What else?

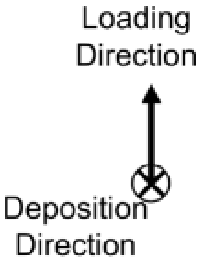
Briggs et al., *Nucl Inst. Meth. Phys. Res.*, 2021

Did the Pt-Au actually resist fatigue-induced grain growth?

Pt

$N_f = 8.5\times10^5$ cycles

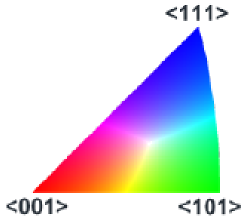
$\sigma_a = 104$ MPa

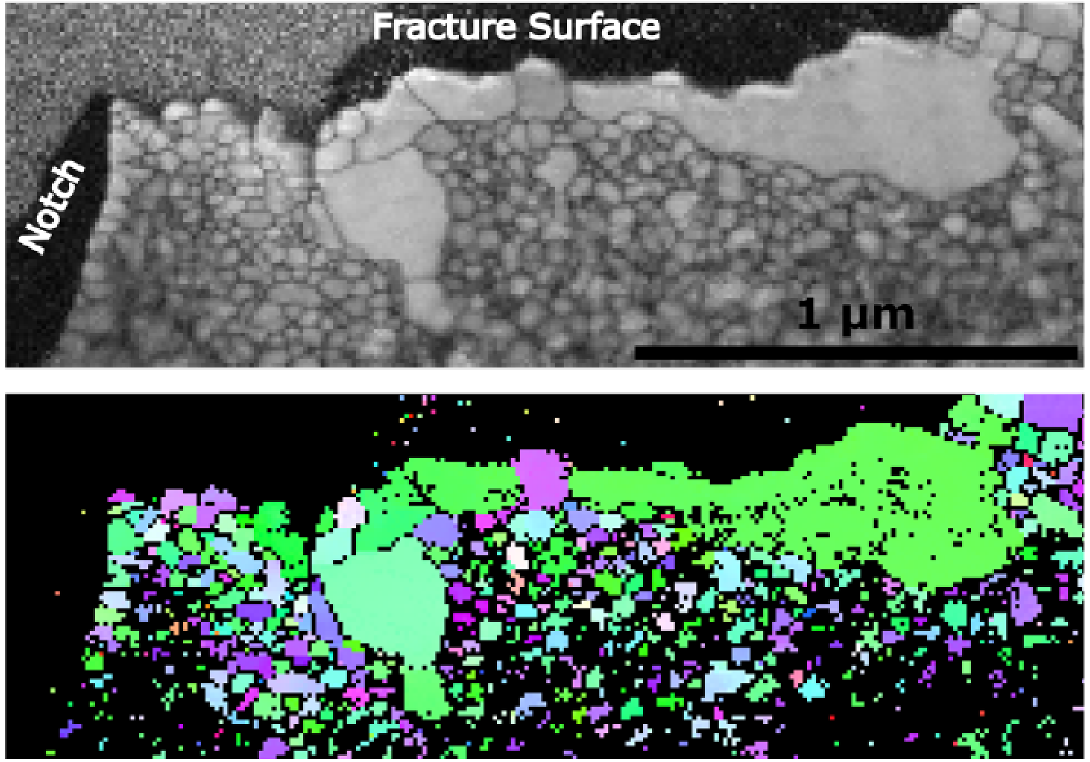


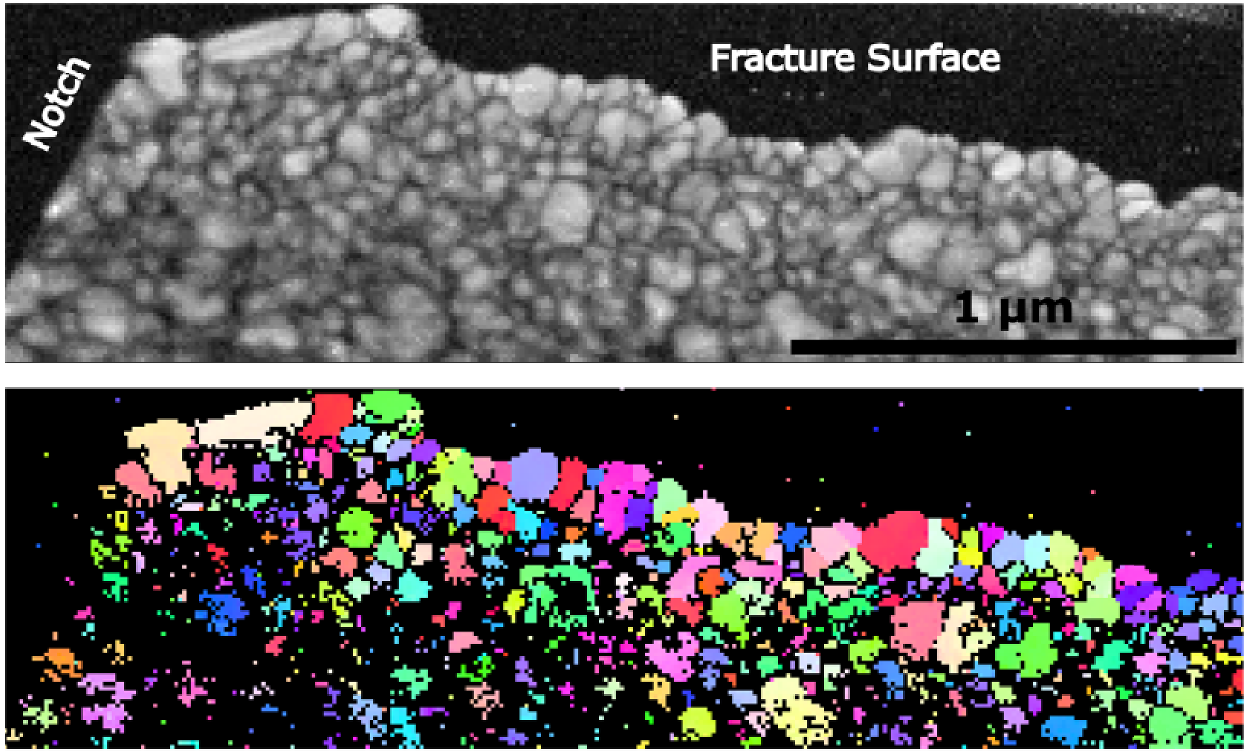
Pt-10Au

$N_f = 7.1\times10^5$ cycles

$\sigma_a = 126$ MPa

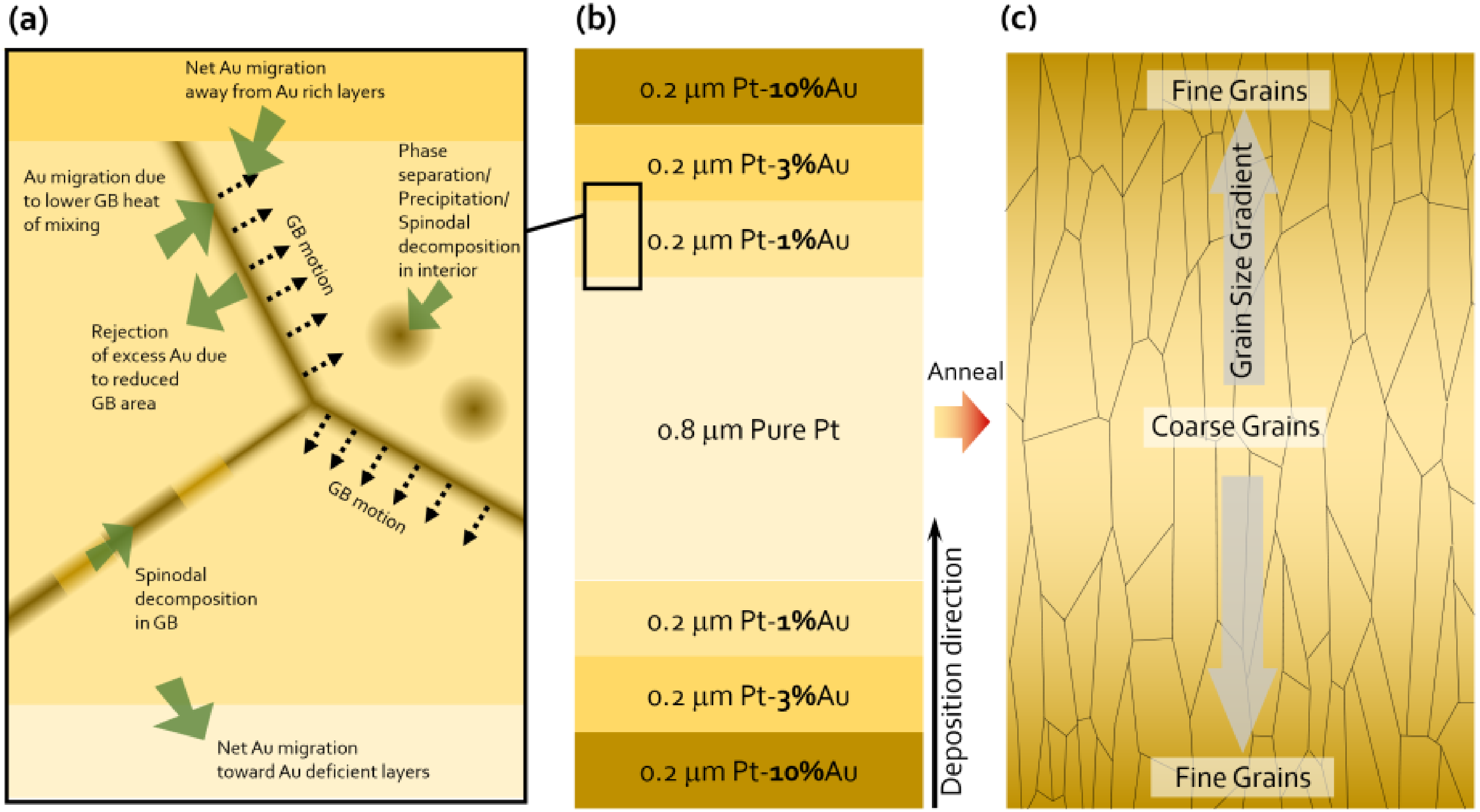




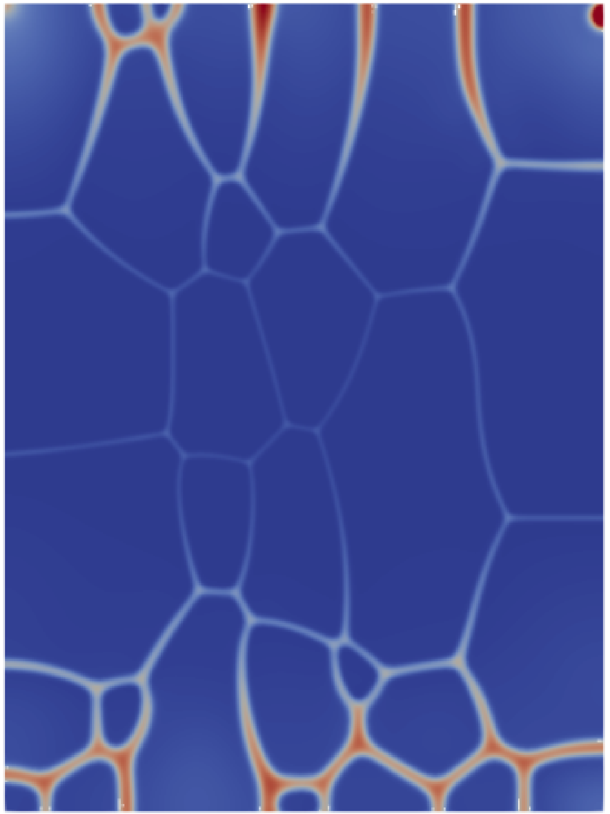


N.M. Heckman, et al., *Acta Materialia*, 2022

Gradient Pt-Au by composition not severe plastic deformation

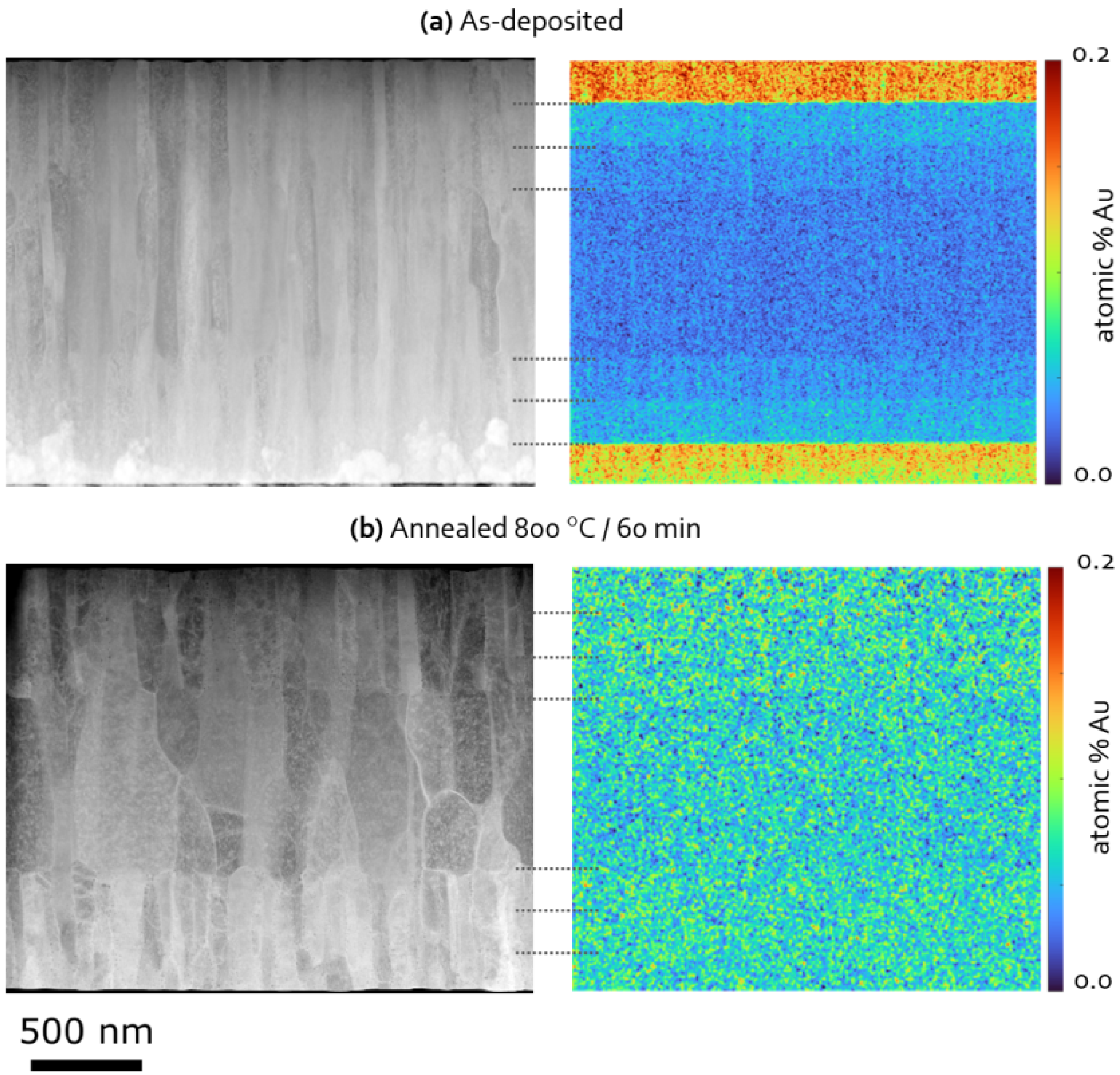


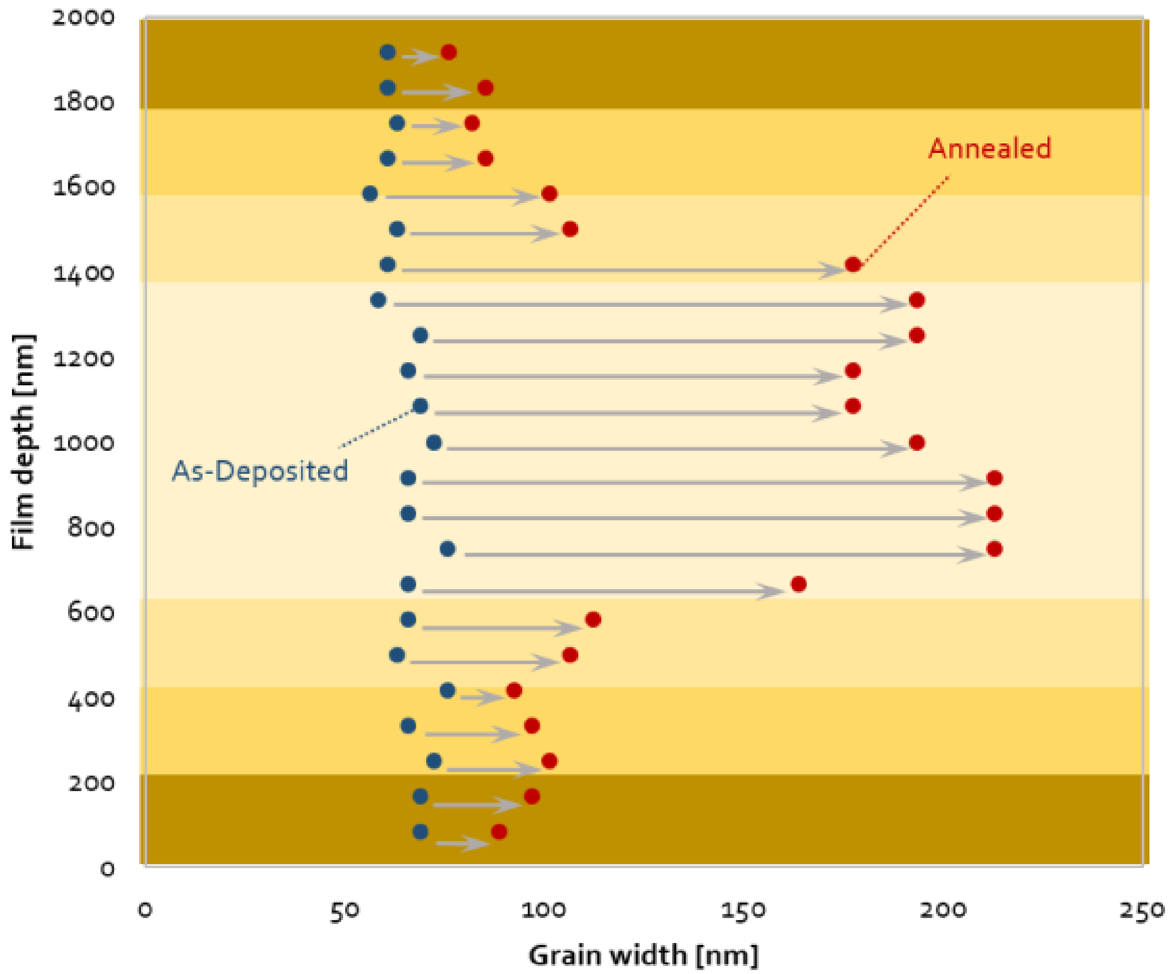
Phase field prediction of Gradient Grain size



Monti et al., *Acta Mater*, 2022

Experimental confirmation of gradient Pt-Au

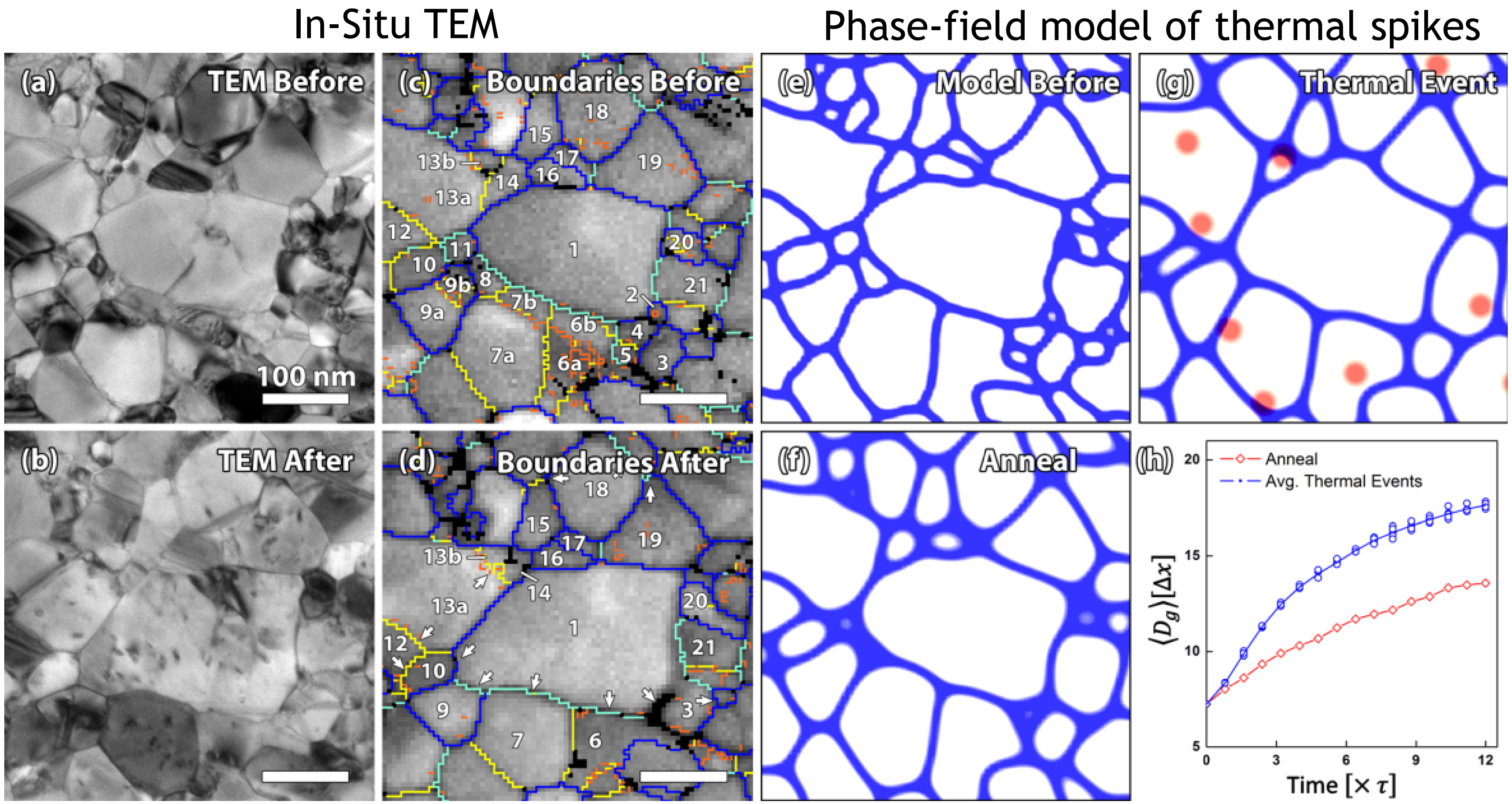




Barrios et al., *in review*

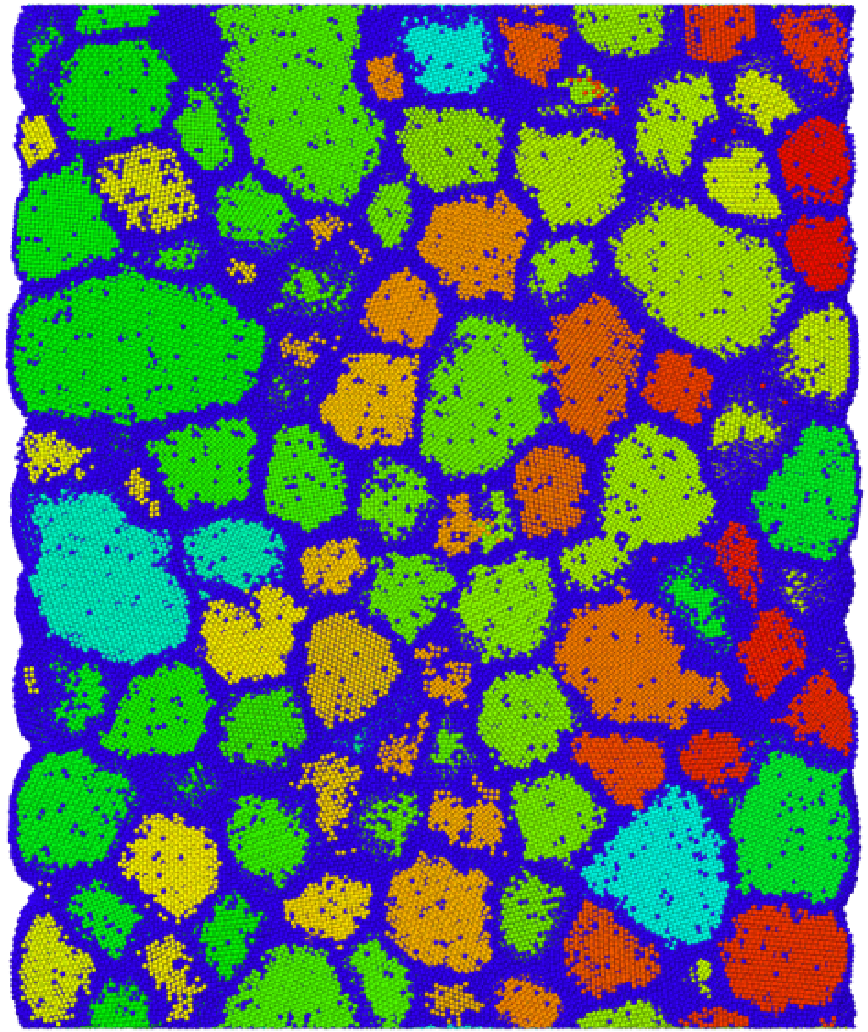
A macroscopic view of irradiation-induced evolution

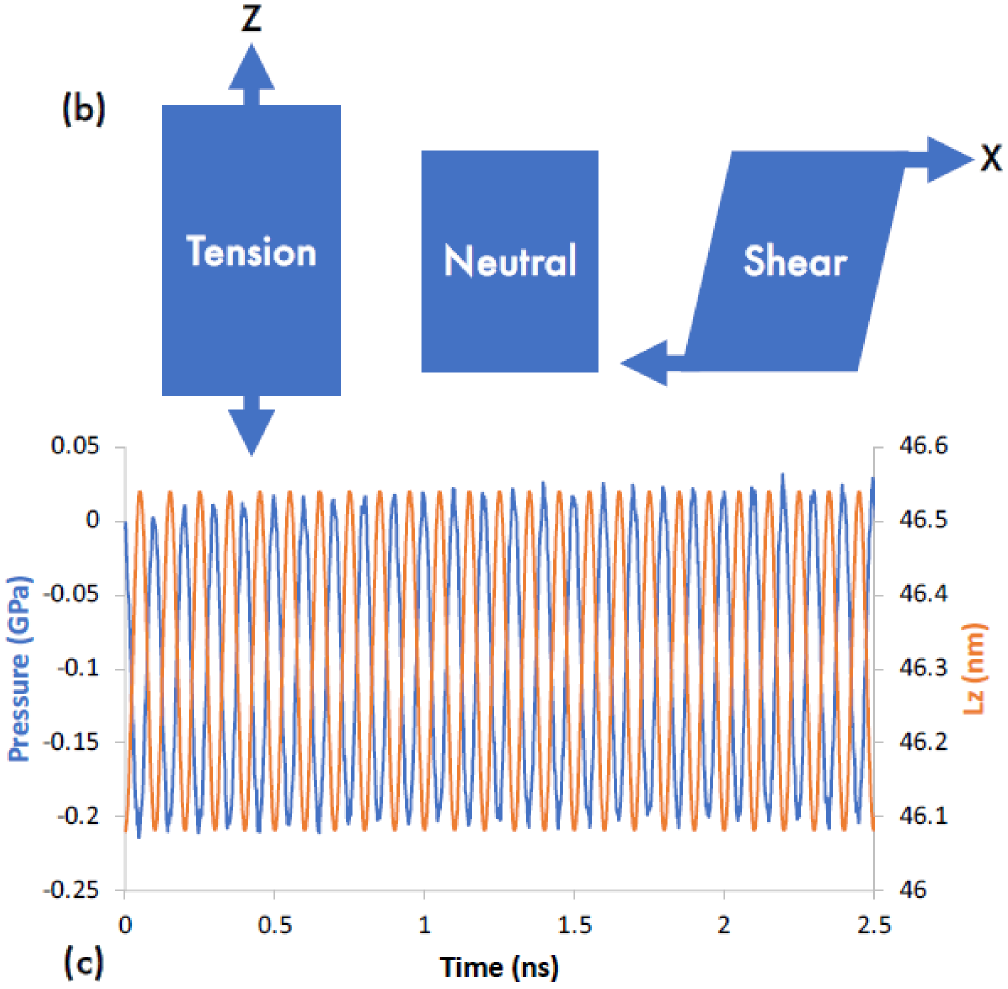
Au foil during bombardment with 10 MeV Si3+



Bufford, Abdeljawad, Foiles, and Hattar, *Appl. Phys. Lett.*, 2015

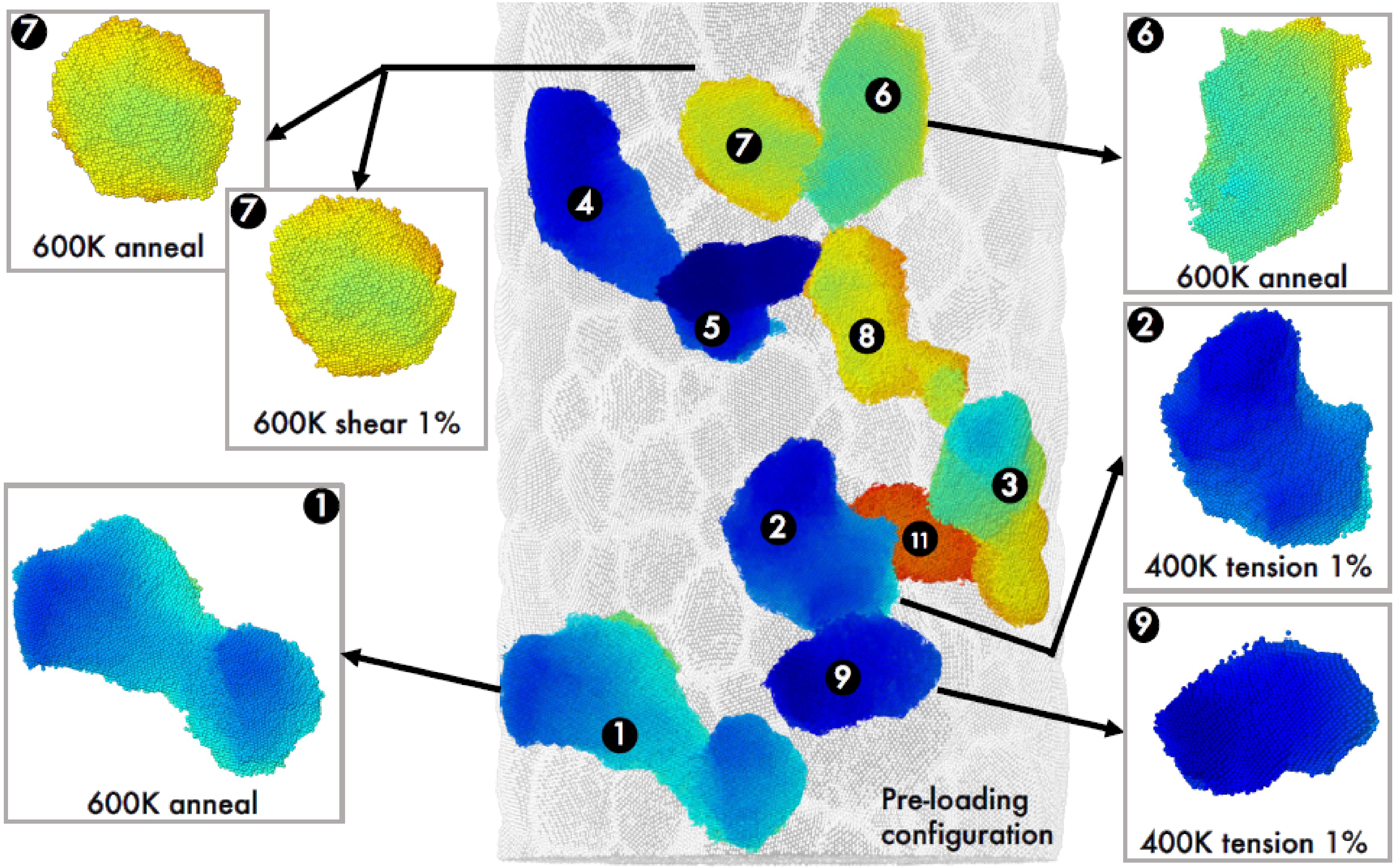
Collective activity of stimulated polycrsytals: a complex statistical picture





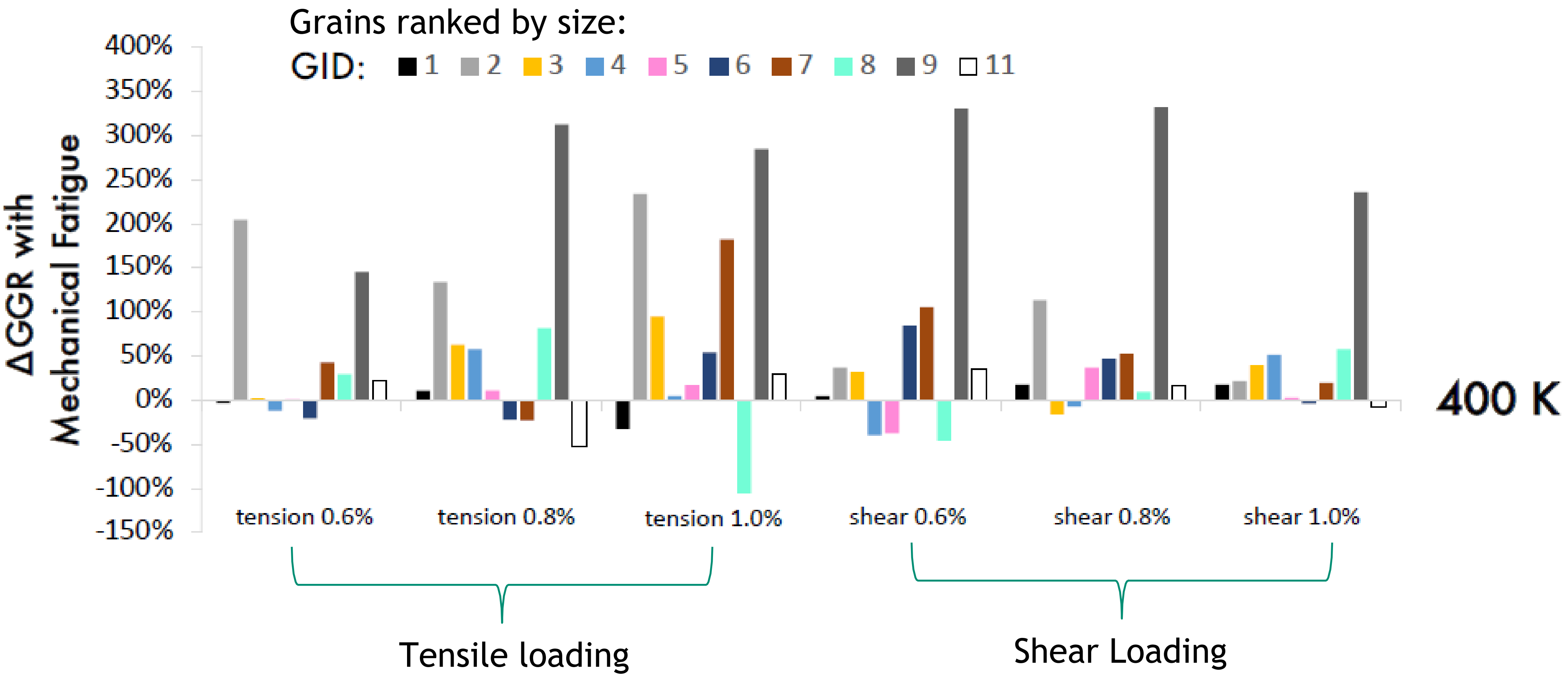
E.Y. Chen et al., submitted

Parsing the response of the 10 biggest grains under 6 different stimuli



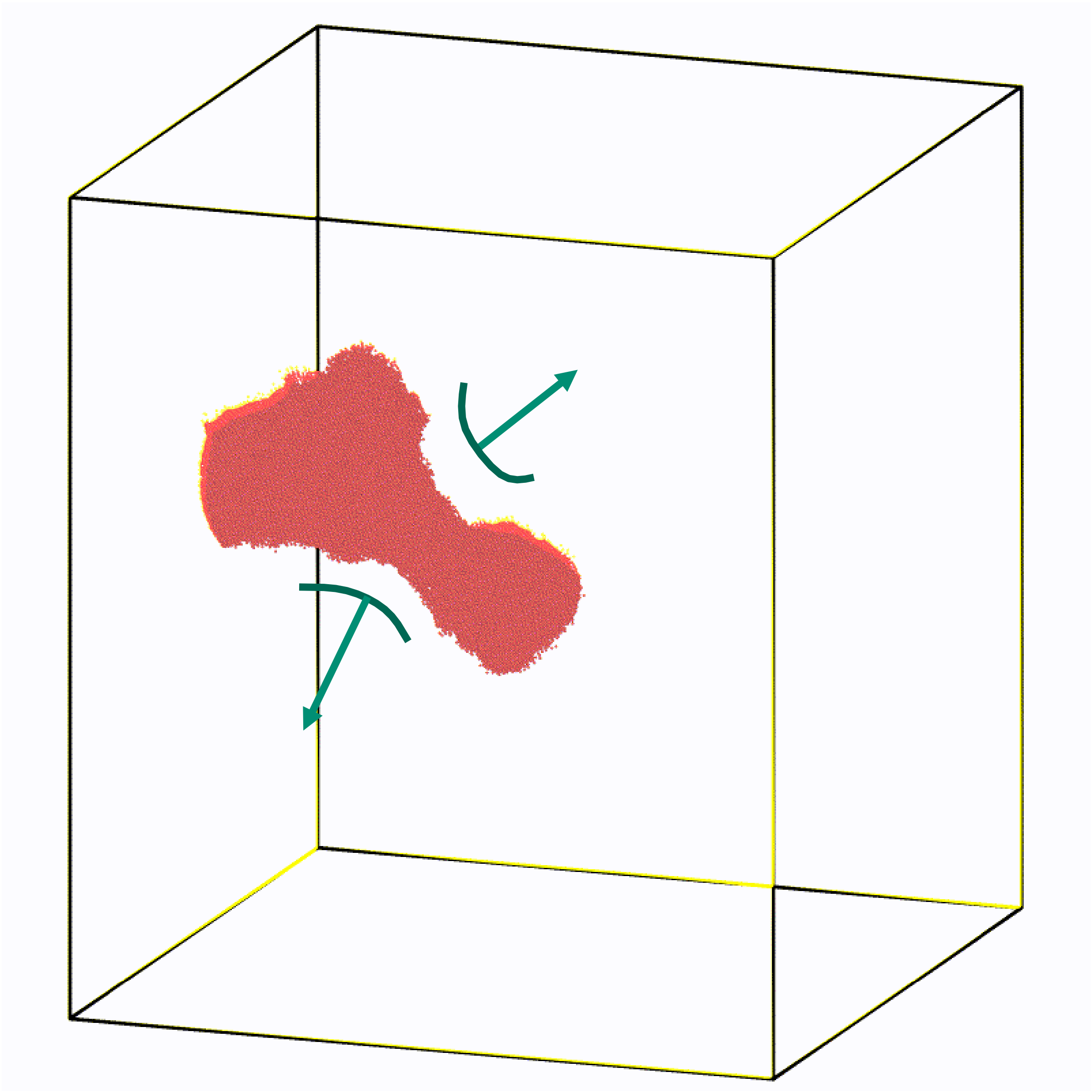
E.Y. Chen et al., submitted

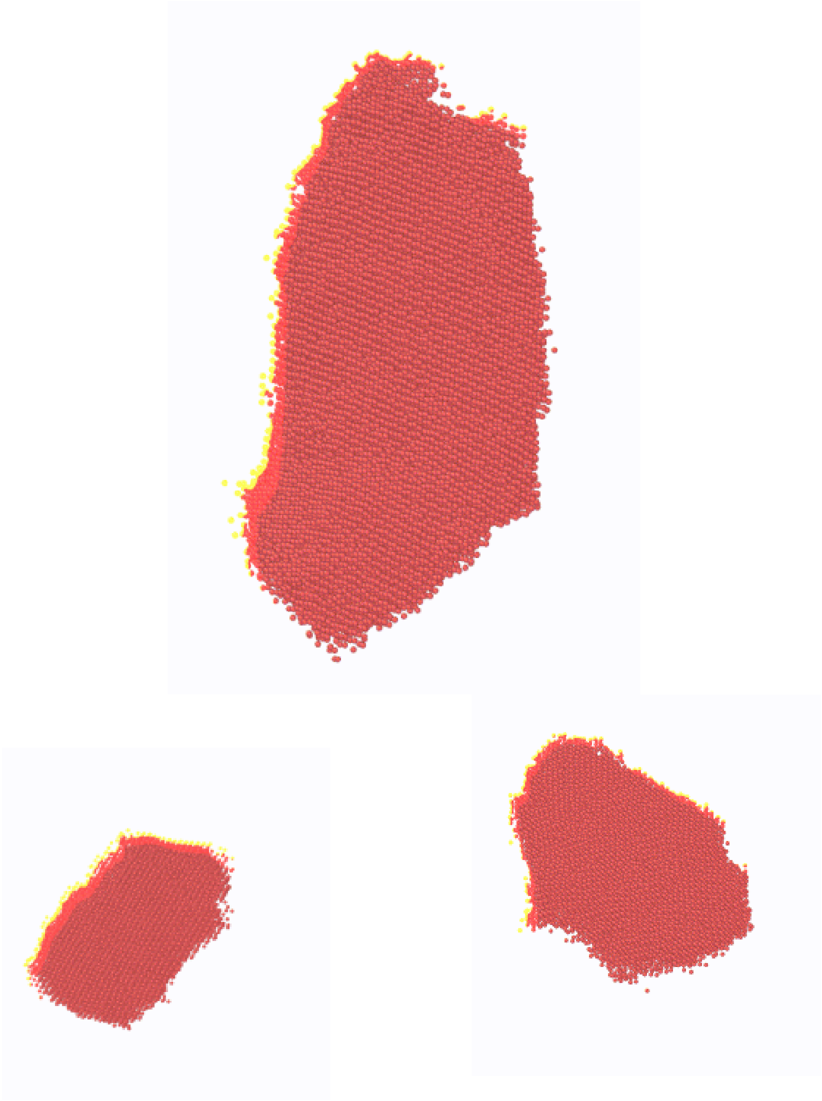
Defected defects: facet junctions as a network of dislocations



E.Y. Chen et al., submitted

The complexity of grain growth…





E.Y. Chen et al., submitted