



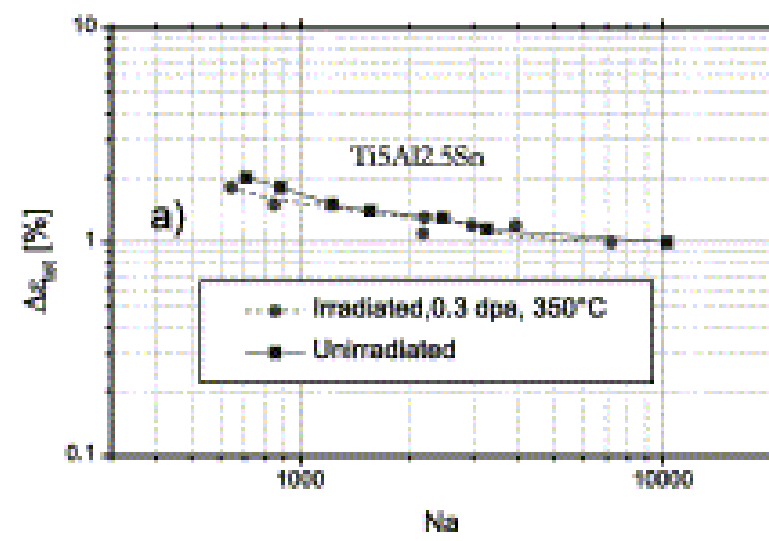
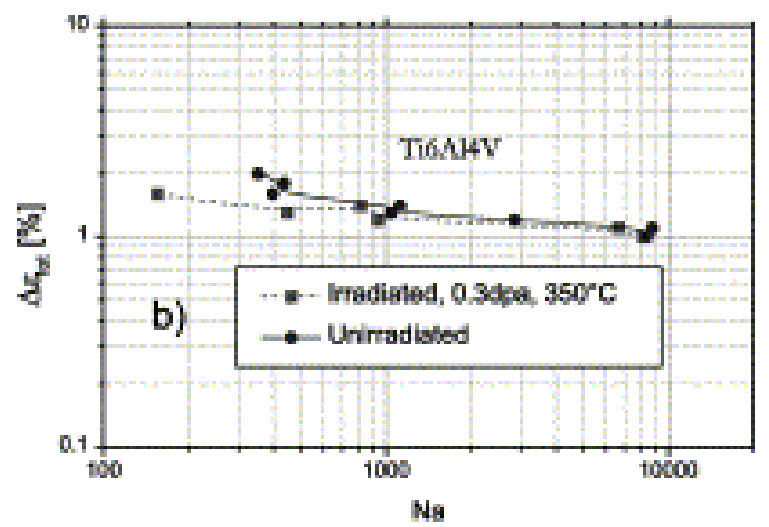
The role of grain boundary migration on irradiation-fatigue

Brad L. Boyce, Chris Barr, Sam Briggs, Elton Chen, Remi Dingreville, Khalid Hattar, Nathan Heckman, Doug Medlin

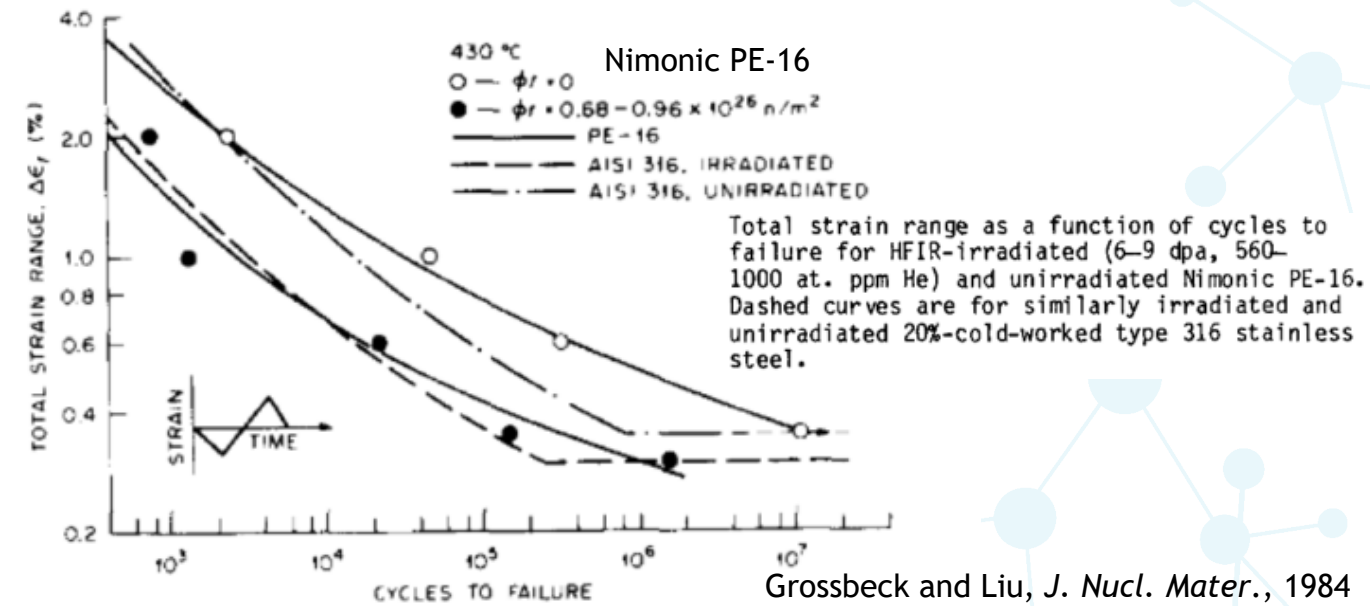
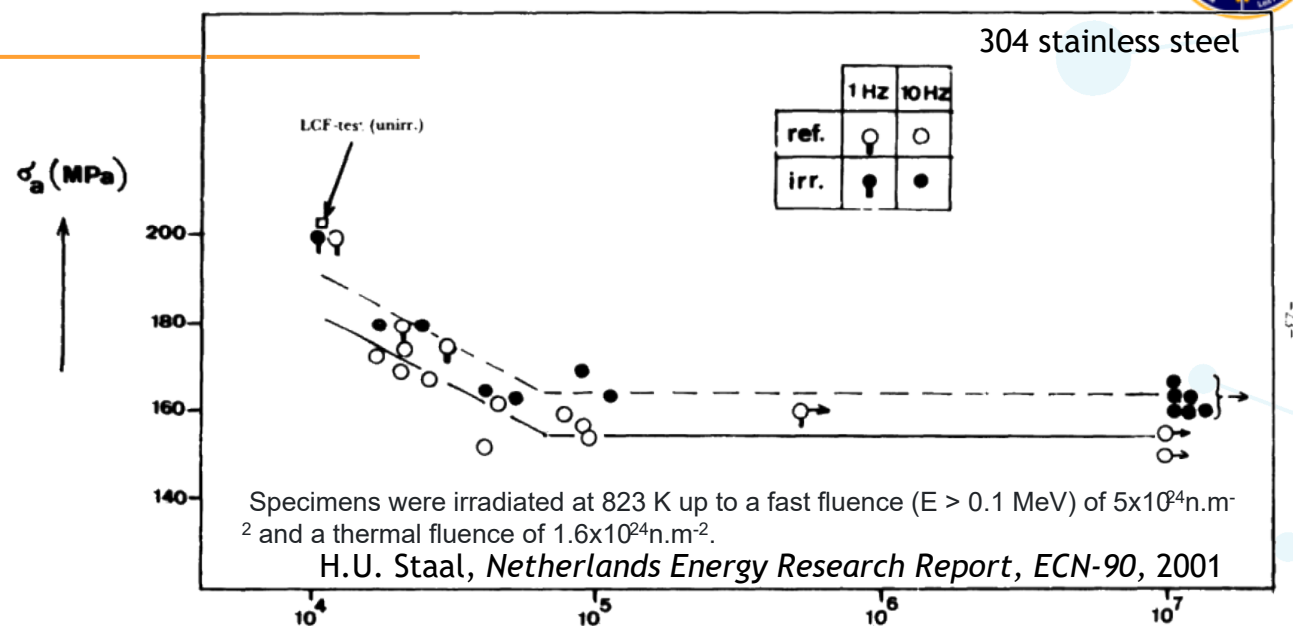
Materials, Chemical, and Physical Sciences Center
Sandia National Laboratories



What do we know about high-cycle fatigue resistance during or after irradiation?

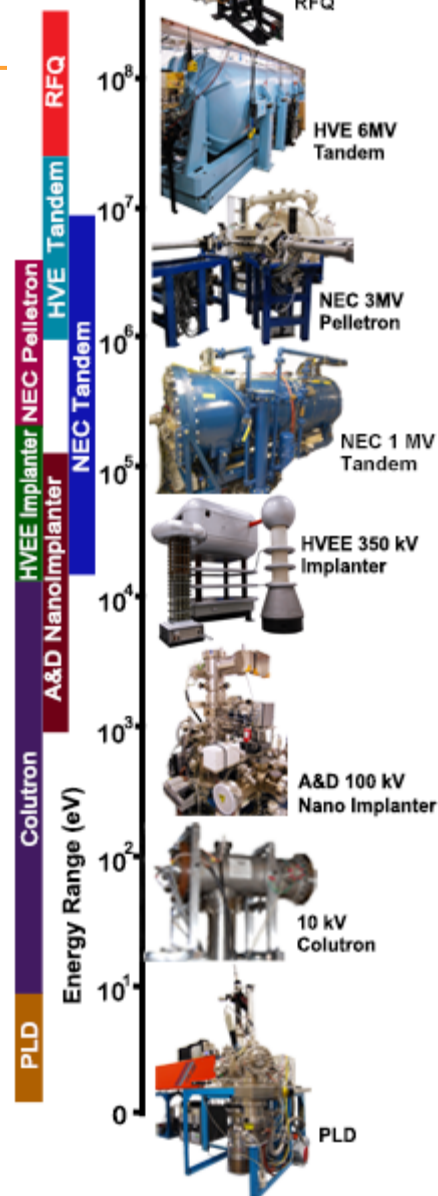


Marmy and Leguey, *J. Nucl. Mater.*, 2001

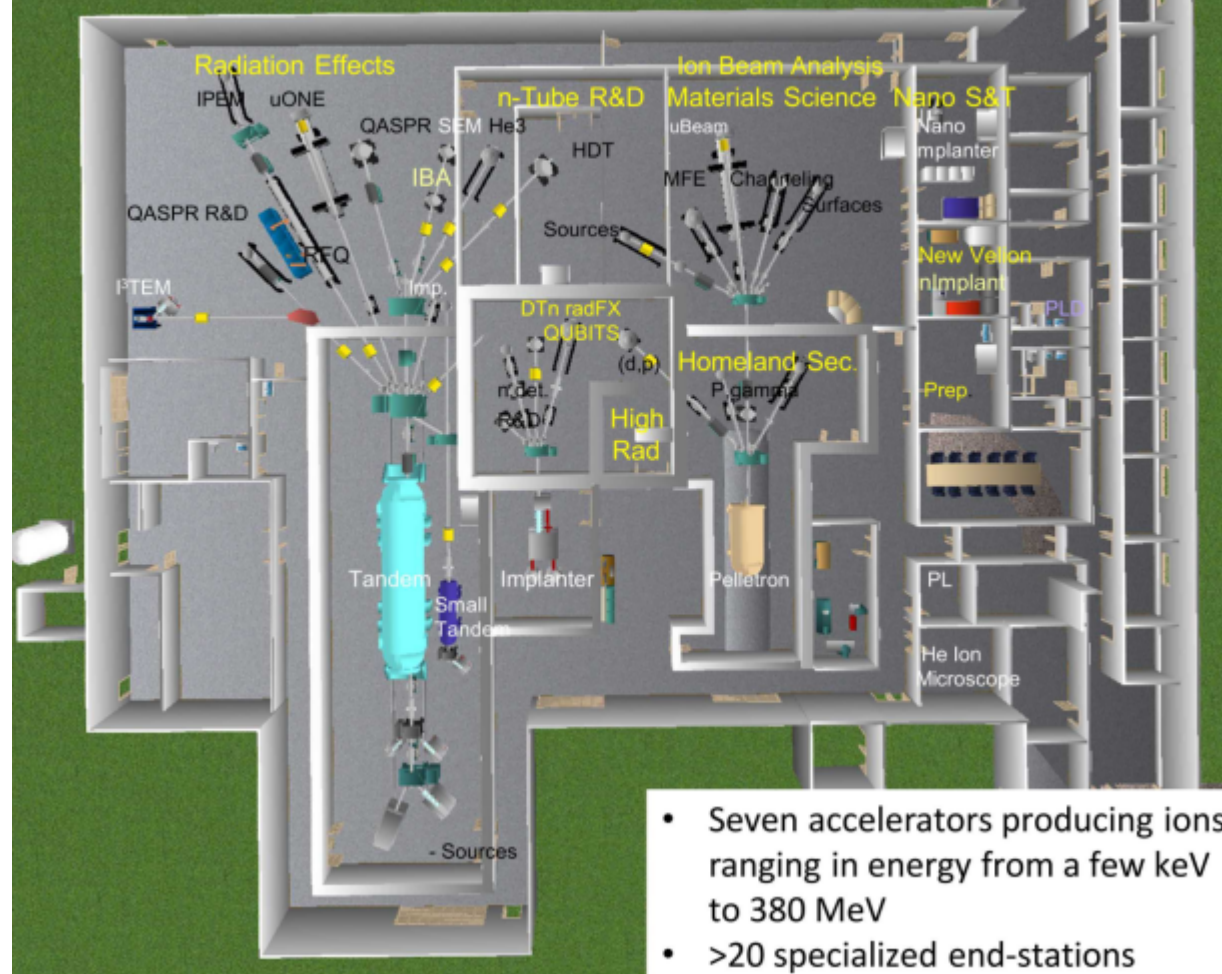


Grossbeck and Liu, *J. Nucl. Mater.*, 1984

Sandia's Ion Beam Laboratory



Sandia's Ion Beam Laboratory (IBL)

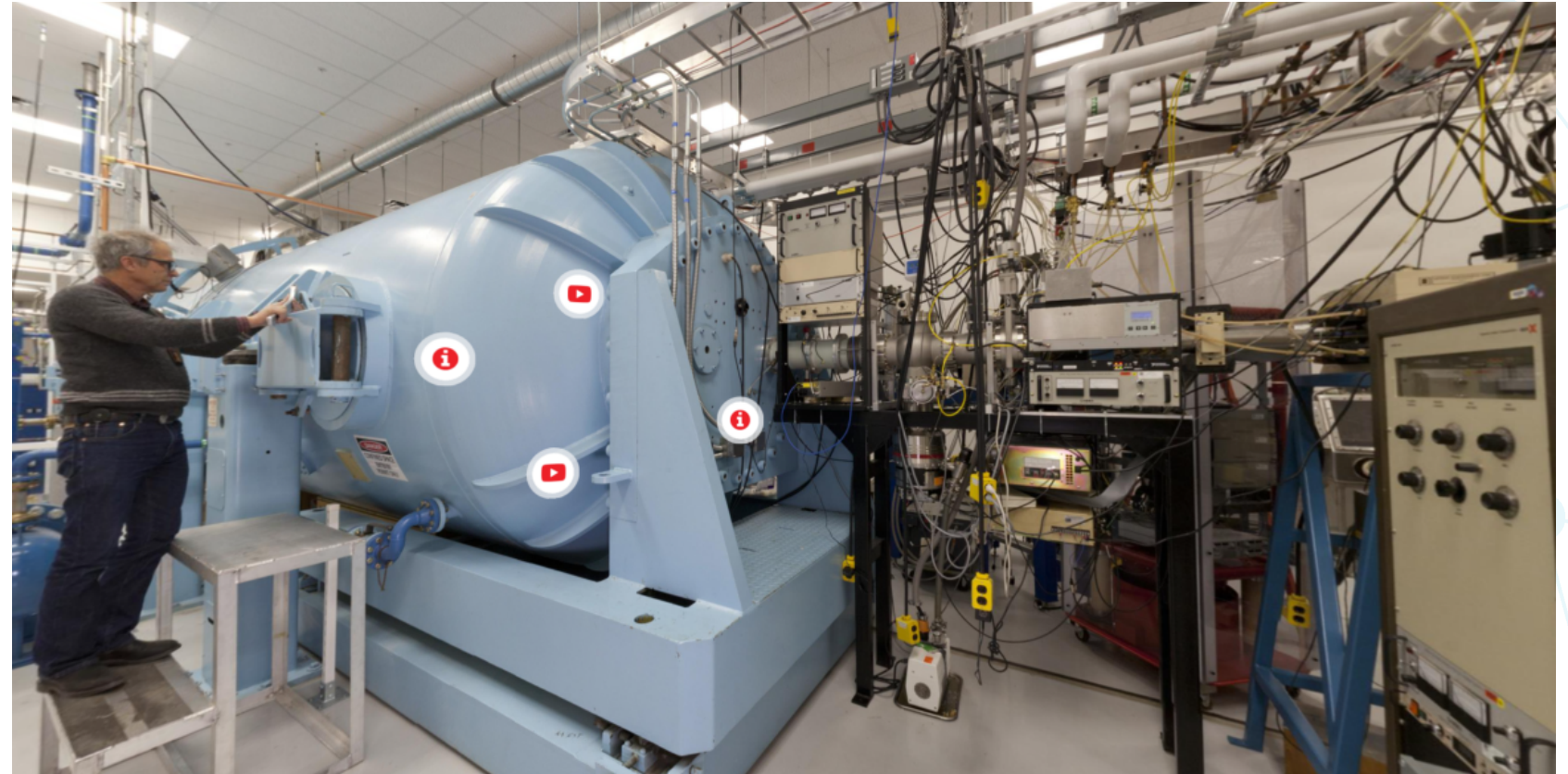


- Seven accelerators producing ions ranging in energy from a few keV to 380 MeV
- >20 specialized end-stations

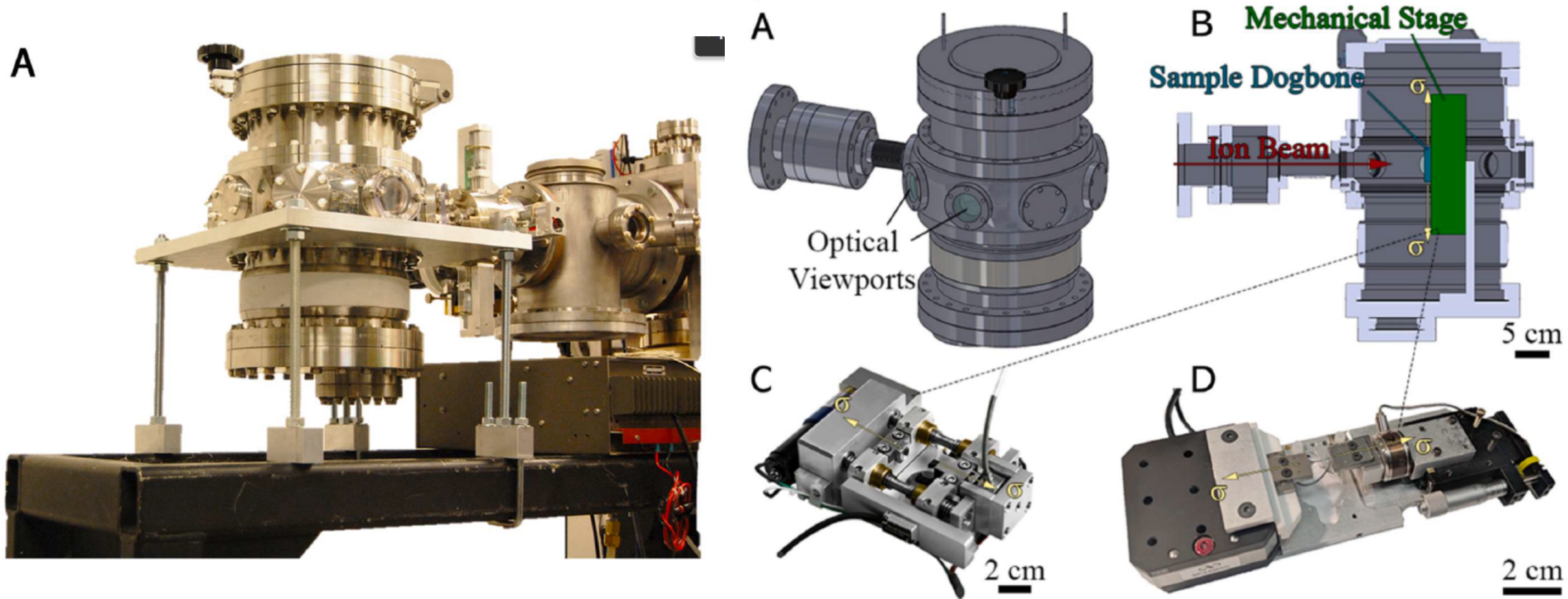
6 MeV Tandem Accelerator @ Sandia's Ion Beam Lab

Ions from protons to Au

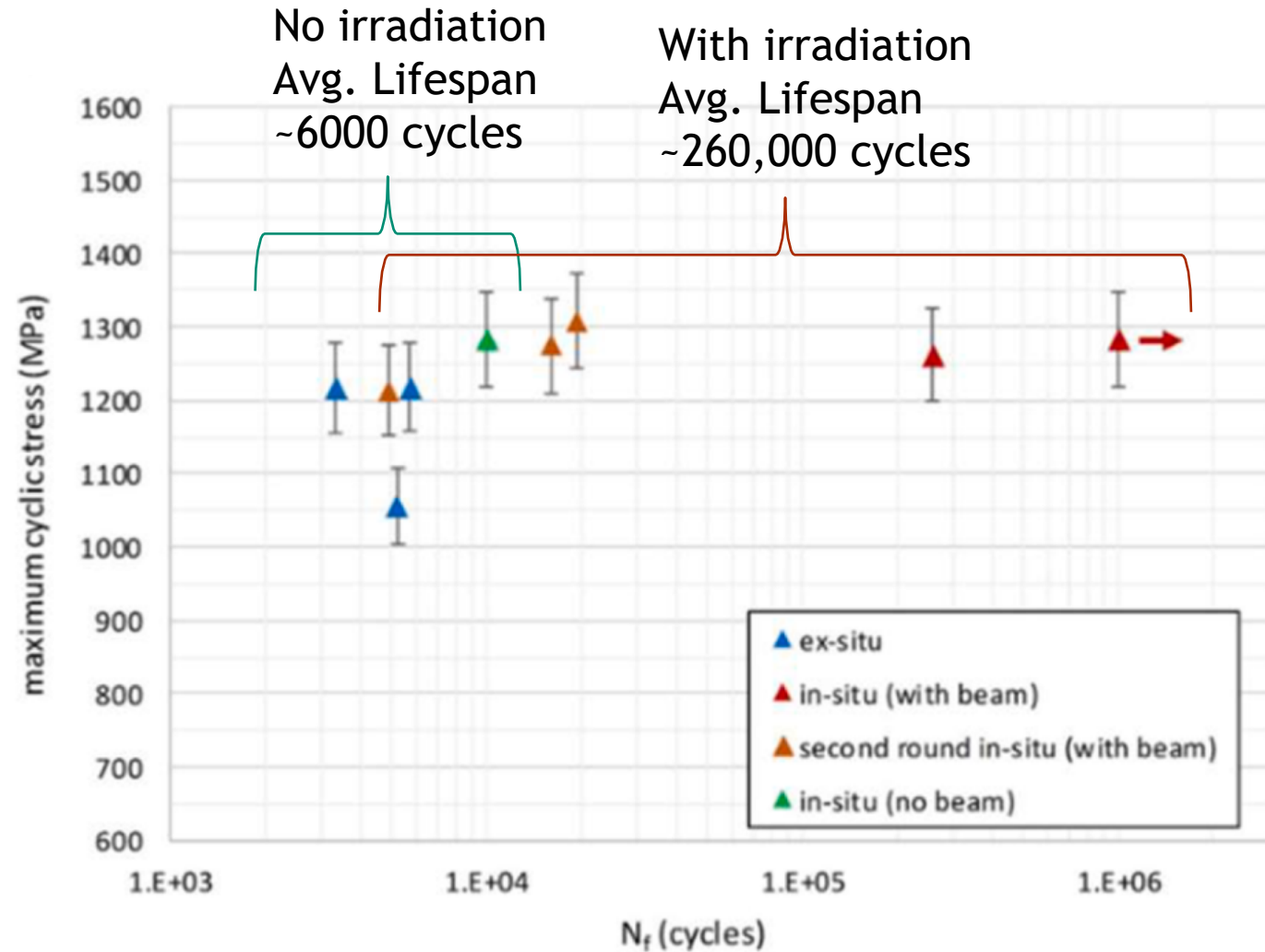
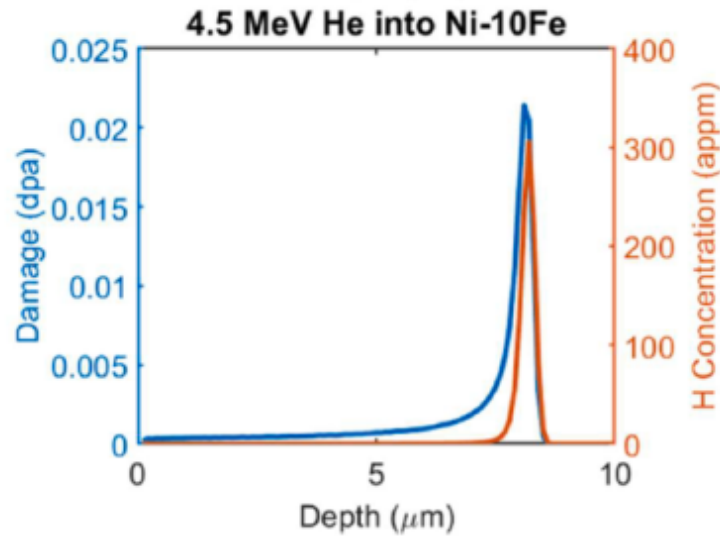
Energy:
10-100 keV; 800 keV-100 MeV.



Sandia Ion Beam Lab's thermomechanical end station

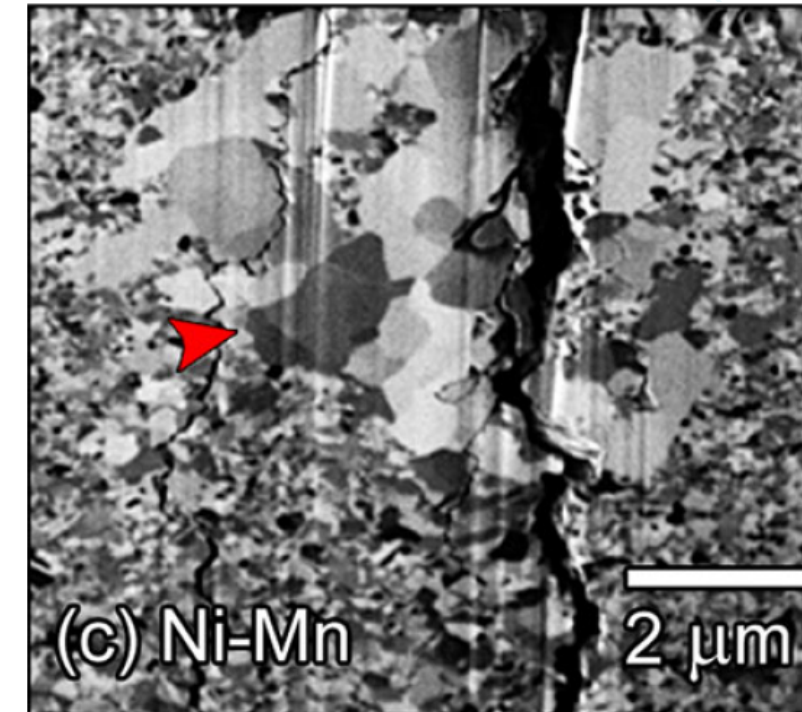
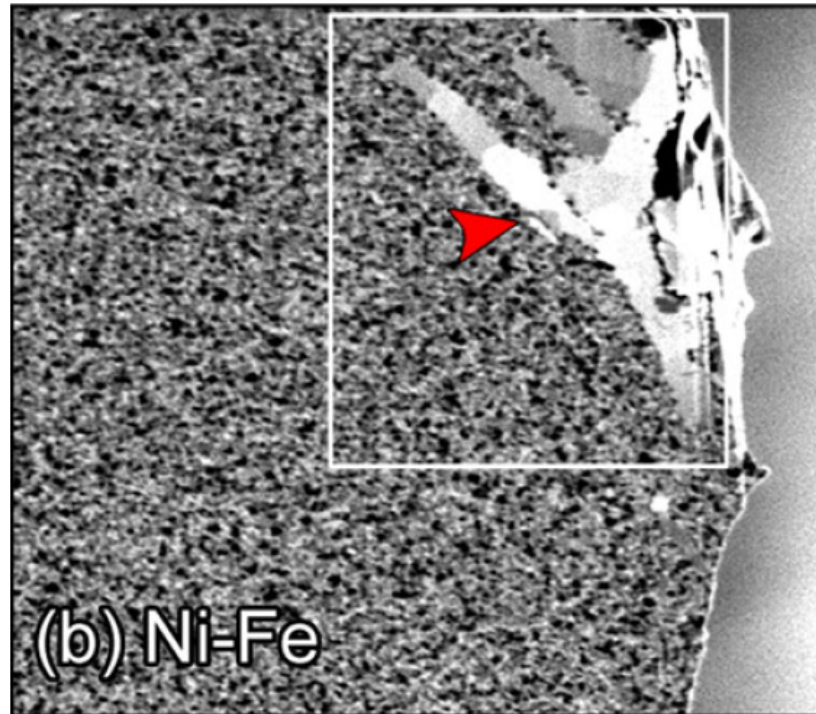
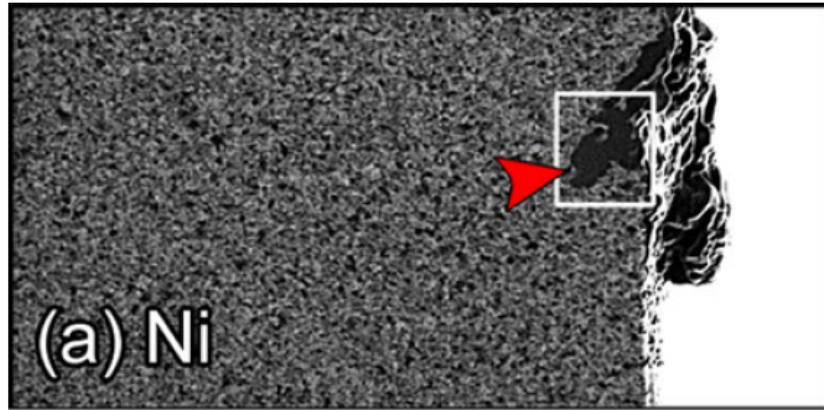


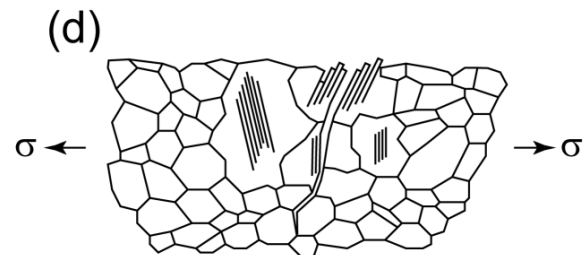
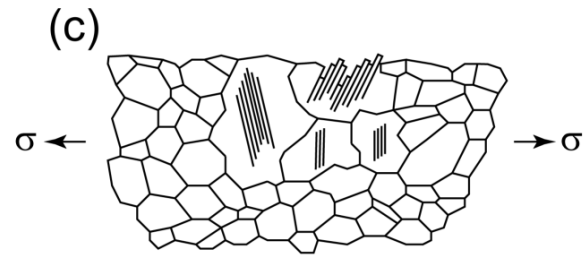
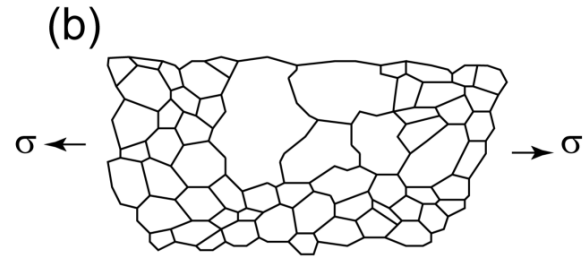
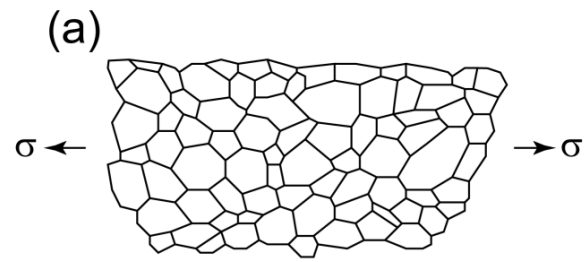
Bottom line up front: enhanced fatigue resistance under irradiation?



What do we know about the high-cycle fatigue process in nanocrystalline metals?

Localized grain growth precedes fatigue-crack initiation





We posit that in nanocrystalline metals ($d_{gb} < \sim 70$ nm), the fatigue process induces grain growth as a precursor to gross slip and eventual crack initiation

- a. Can fatigue really cause grain growth? **YES**
- b. Does the grain growth precede crack initiation? **YES**
- c. Does the crack initiate at the site of grain growth? **YES**

For more details, our work:

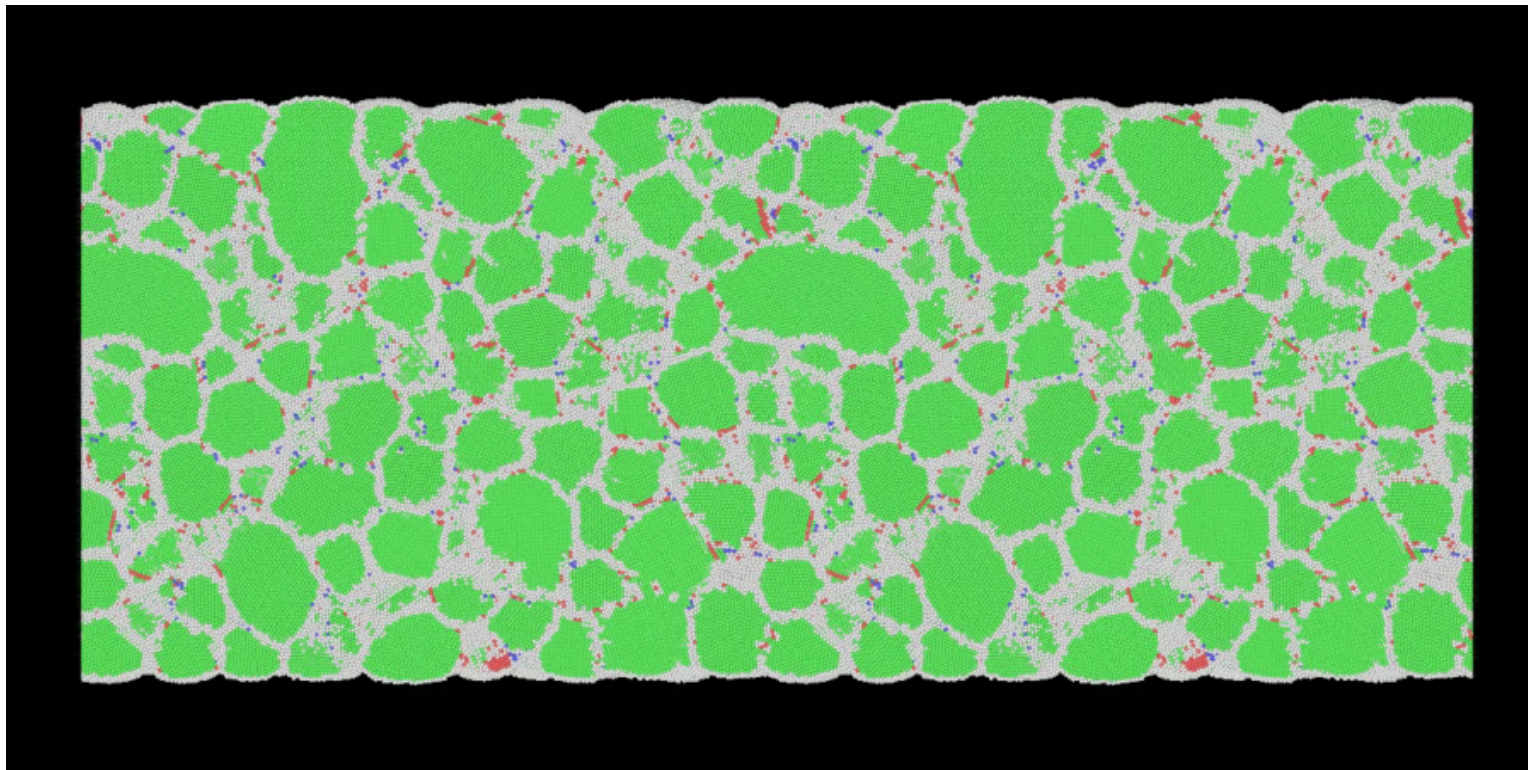
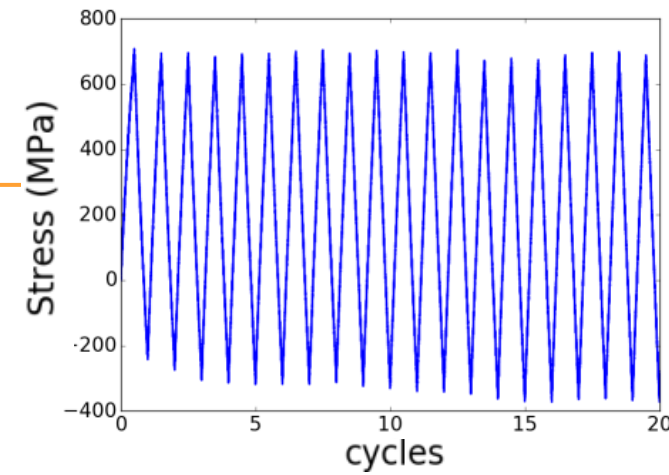
Padilla and Boyce, *Exper. Mech.*, 2010
Boyce and Padilla, *Metall. Trans. A*, 2011
Bufford et al., *Nano Letters*, 2016
Furnish et al., *J. Mater. Sci.*, 2017
Furnish et al., *Scripta Mater.*, 2018
Foiles et al., *Model. Sim. Mater. Sci. Eng.*, 2019
Heckman et al., *Int. J. Fatigue*, 2020
Heckman et al., *Acta Mater.*, 2022

Others as well, e.g.,

Luo, Zhu, Zhang, *Nature Comm*, 2014
Kobayashi, Kamata, Watanabe, *Acta Mater*, 2015
Kapp, Renk, Leitner, Ghosh, Yang, Pippin, *J. Mater. Res.* 2017
Goswami, Feng, Qadri, Pande, *Sci. Reports*, 2017
Zhao, Chen, Kelleher, Yuan, Guan, Zhang, Tu, *Acta Mater*, 2019
Zheng, Luo, Zhang, *J. Mater. Res.*, 2020
Zhang, Zeng, Cheng, Wang, *J. Mater. Sci. Tech.*, 2021

Molecular dynamics simulation of fatigue-induced grain growth

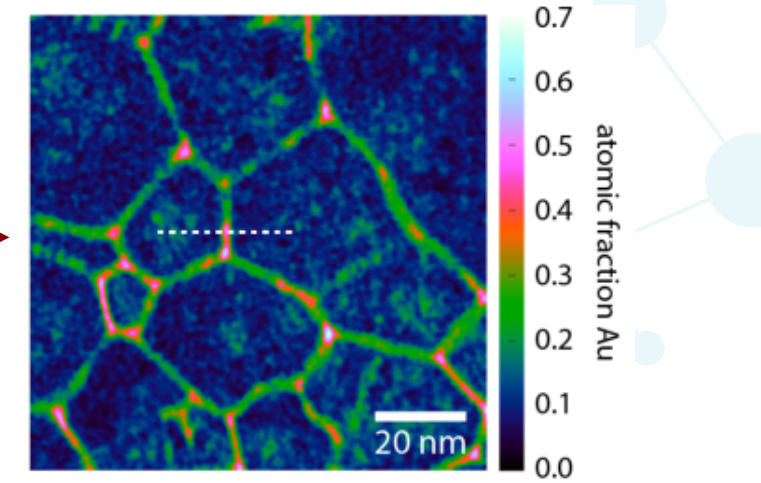
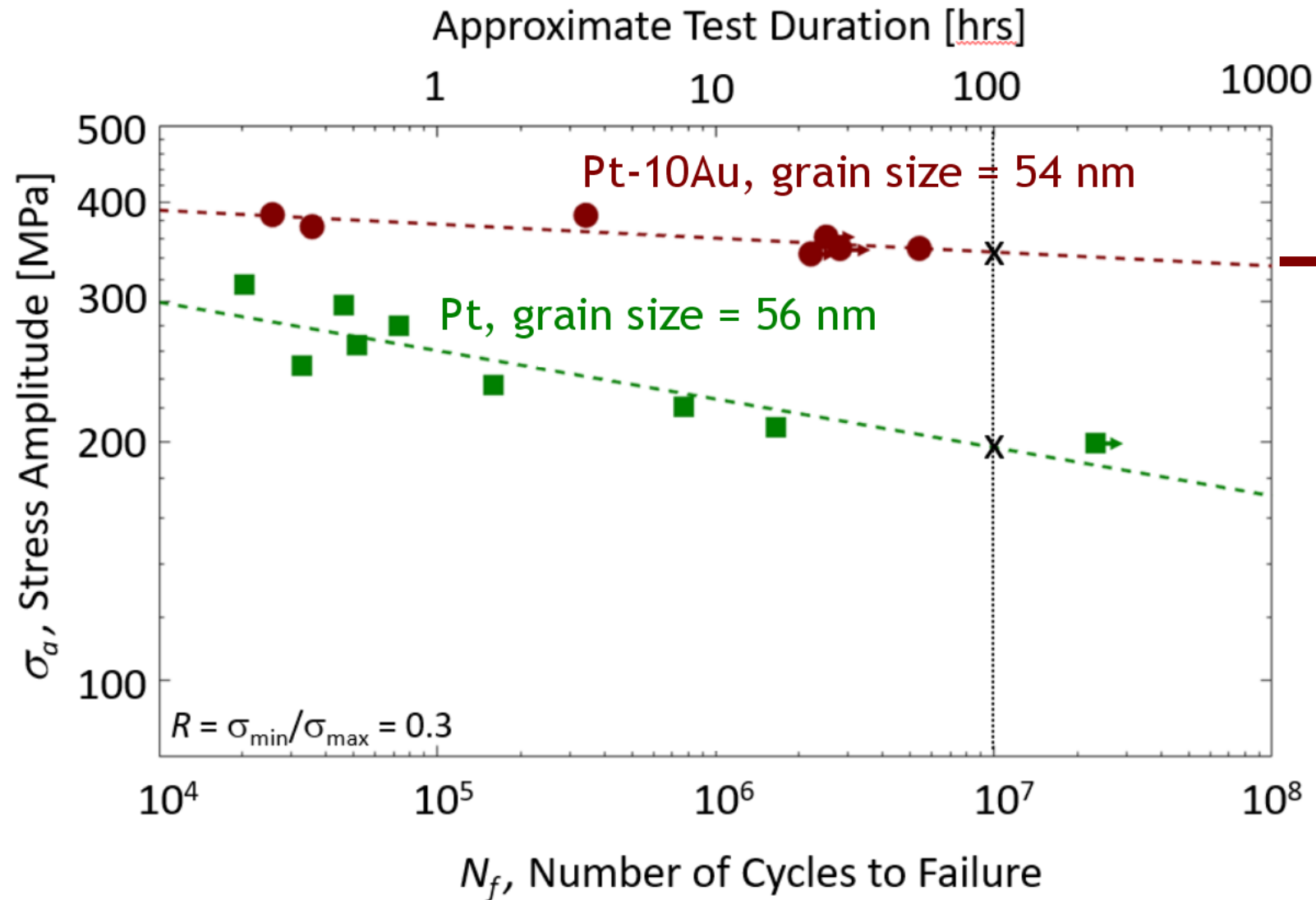
20 cycles, 2 ns/cycle, 1% strain
Simulation: 110,000 cpu-hours



- fcc
- twin/fault
- other

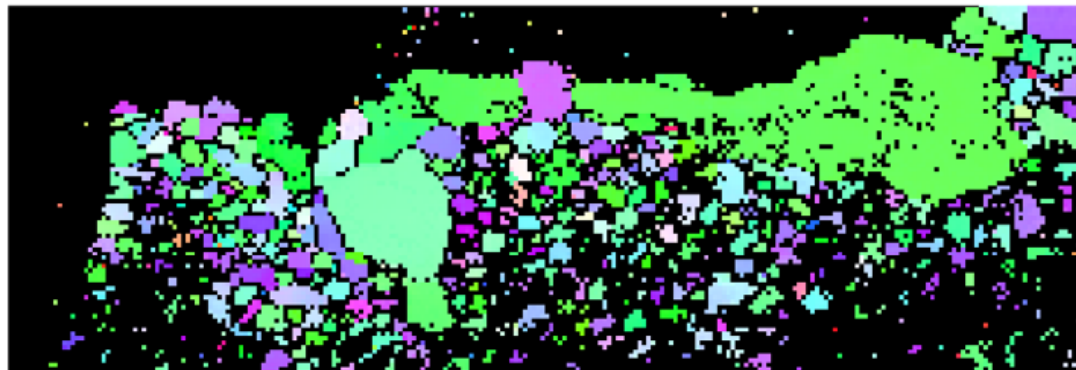
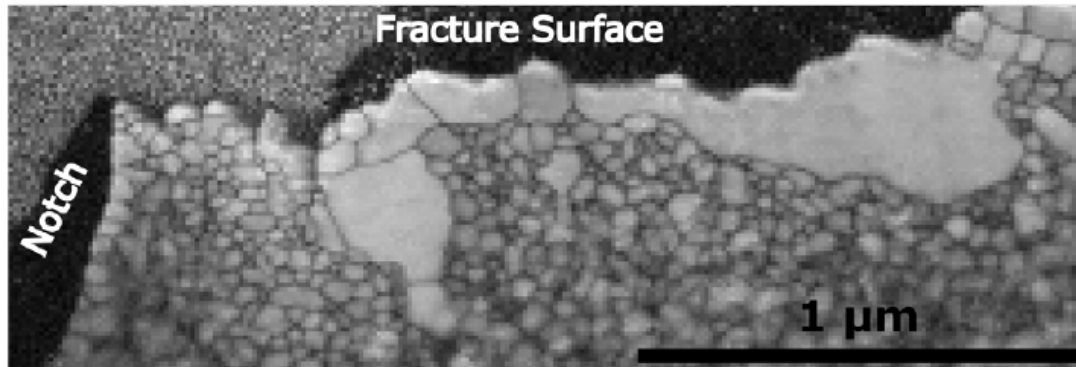
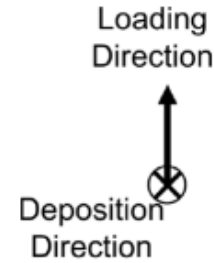
5 nm

Ok, so is stabilized Pt-Au more fatigue resistant?

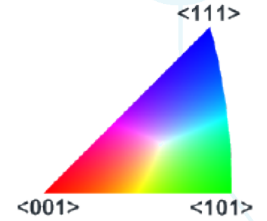
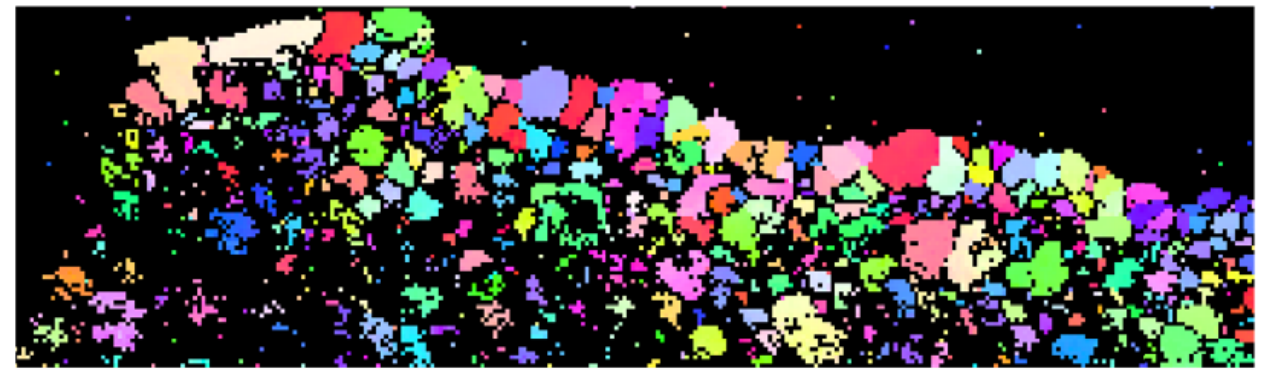
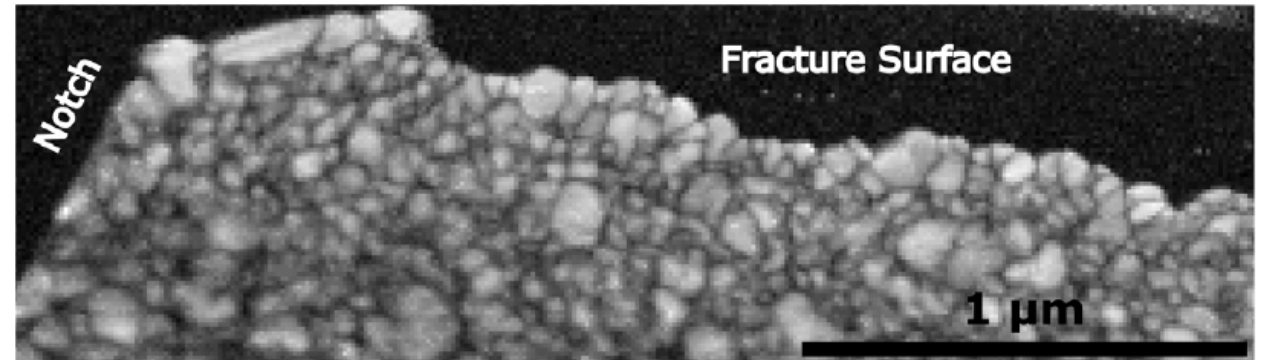


Did the Pt-Au actually resist fatigue-induced grain growth?

Pt
 $N_f = 8.5 \times 10^5$ cycles
 $\sigma_a = 104$ MPa



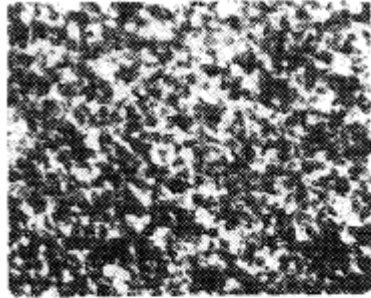
Pt-10Au
 $N_f = 7.1 \times 10^5$ cycles
 $\sigma_a = 126$ MPa



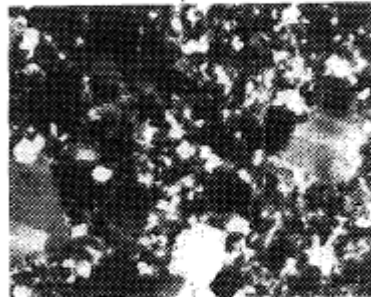
How do grain boundaries respond to irradiation???

Radiation-enhanced grain growth in metals...

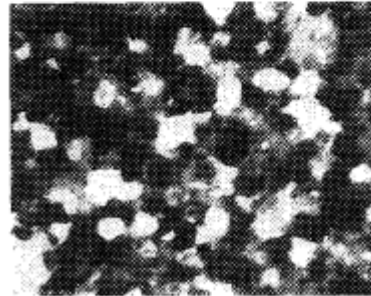
560-keV Xe⁺² into nanocrystalline Pd



As Deposited



200°C Annealed



$1 \times 10^{15} \text{ Xe/cm}^2$

100 nm

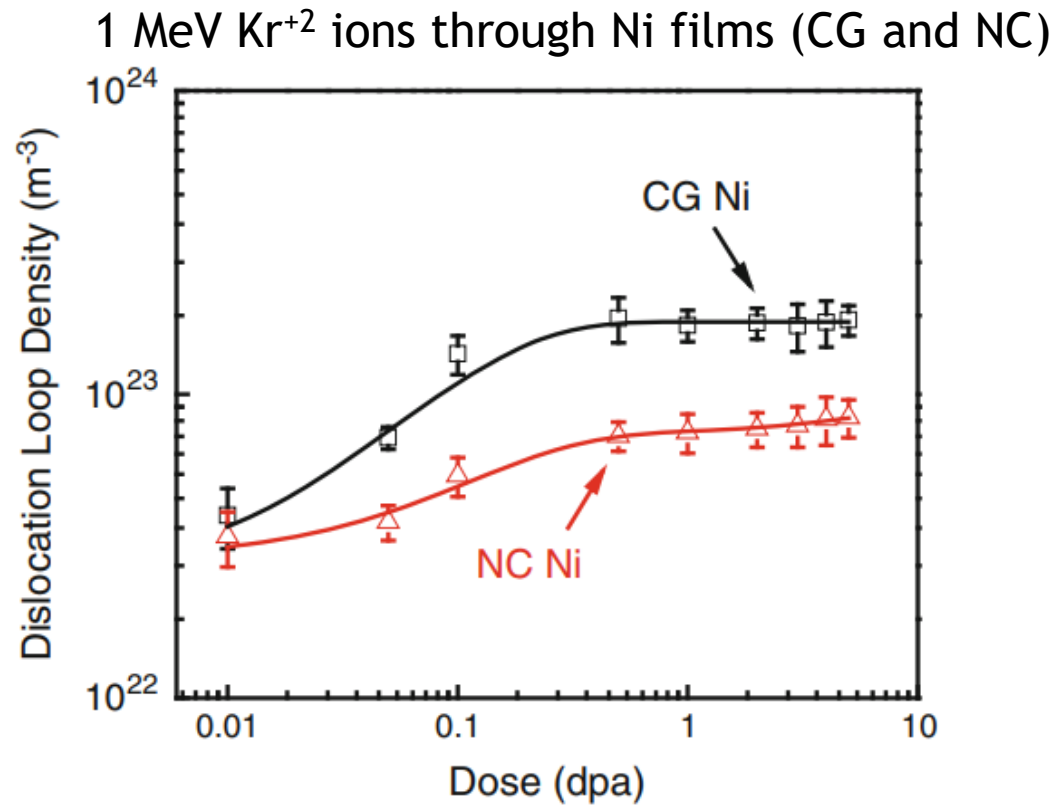
Some studies rationalize the grain growth on the basis of thermal spikes alone:

Liu, Li, and Mayer, *J. Appl. Phys.*, 1989

Kaoumi, Motta, Birtcher, *J. Appl. Phys.*, 2008

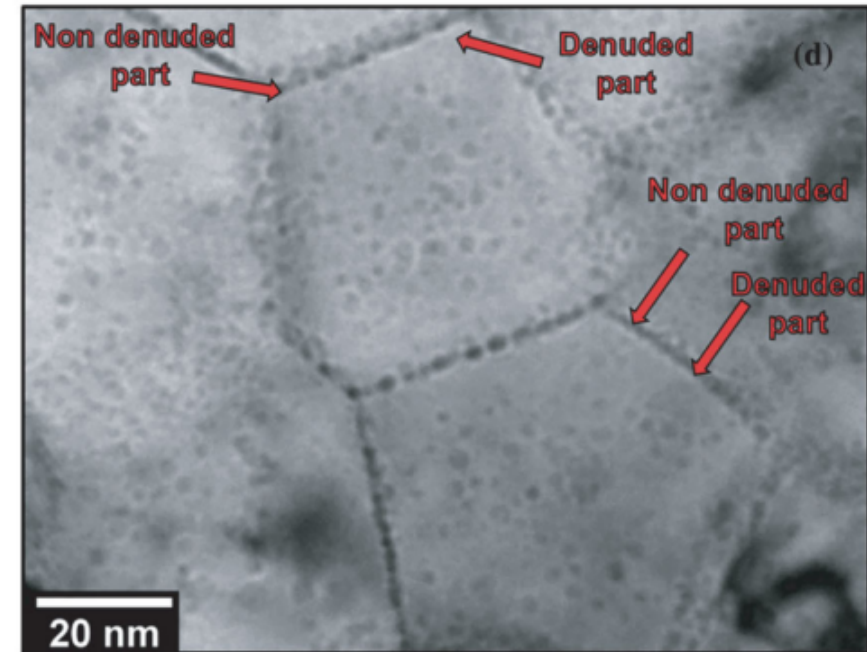
Liu, Nastasi and Mayer, *J. Appl. Phys.*, 1987

Generally, GBs are thought of radiation defect sinks



C. Sun et al., *Metall. Mater. Trans A*, 2013

Denuded zone of He bubbles near GBs

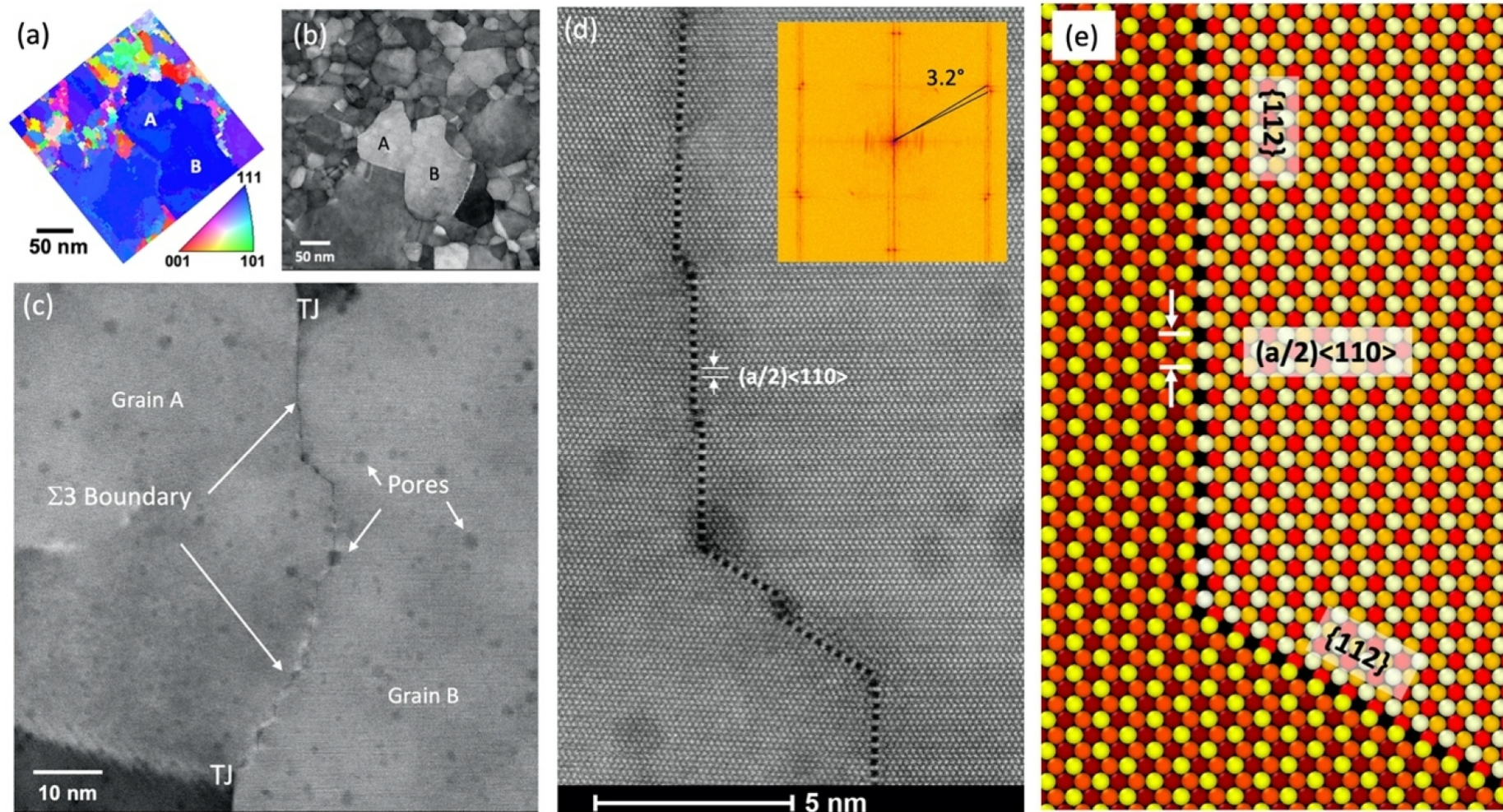


10 keV helium ions into nanocrystalline Fe

El-Atwani et al., *Mater. Res. Lett.*, 2017

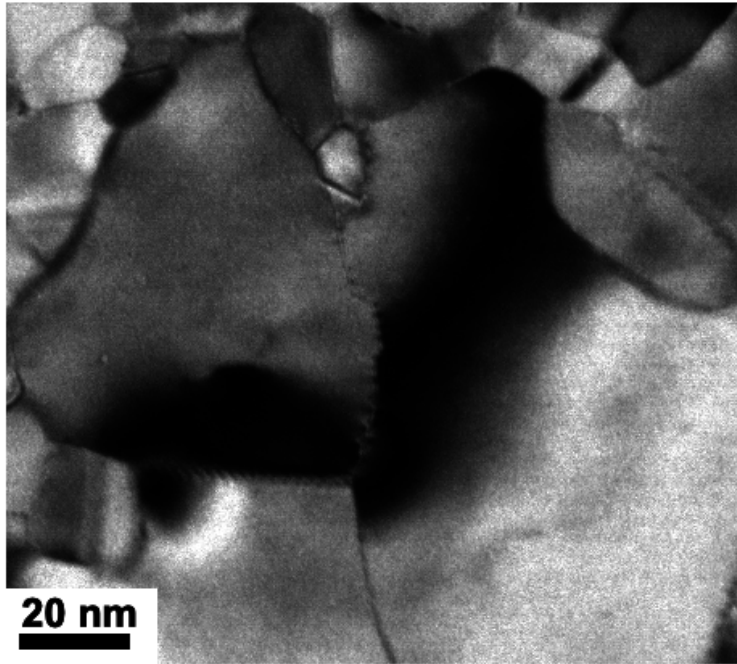
Radiation response of a faceted $\Sigma 3$ $\{112\}$ boundary w/ 120° junctions

Pt polycrystal

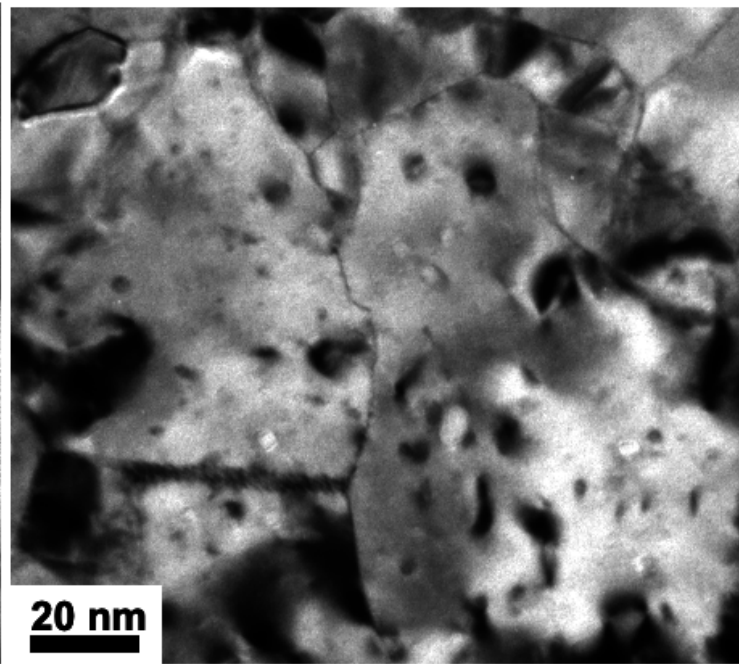


Irradiated with 2.8 MeV Au⁴⁺

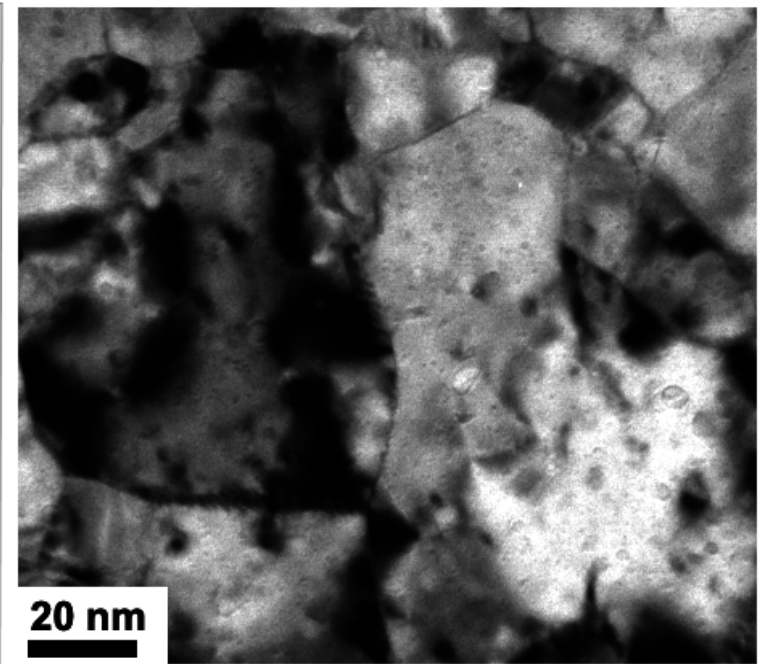
(a) Pre-irradiation



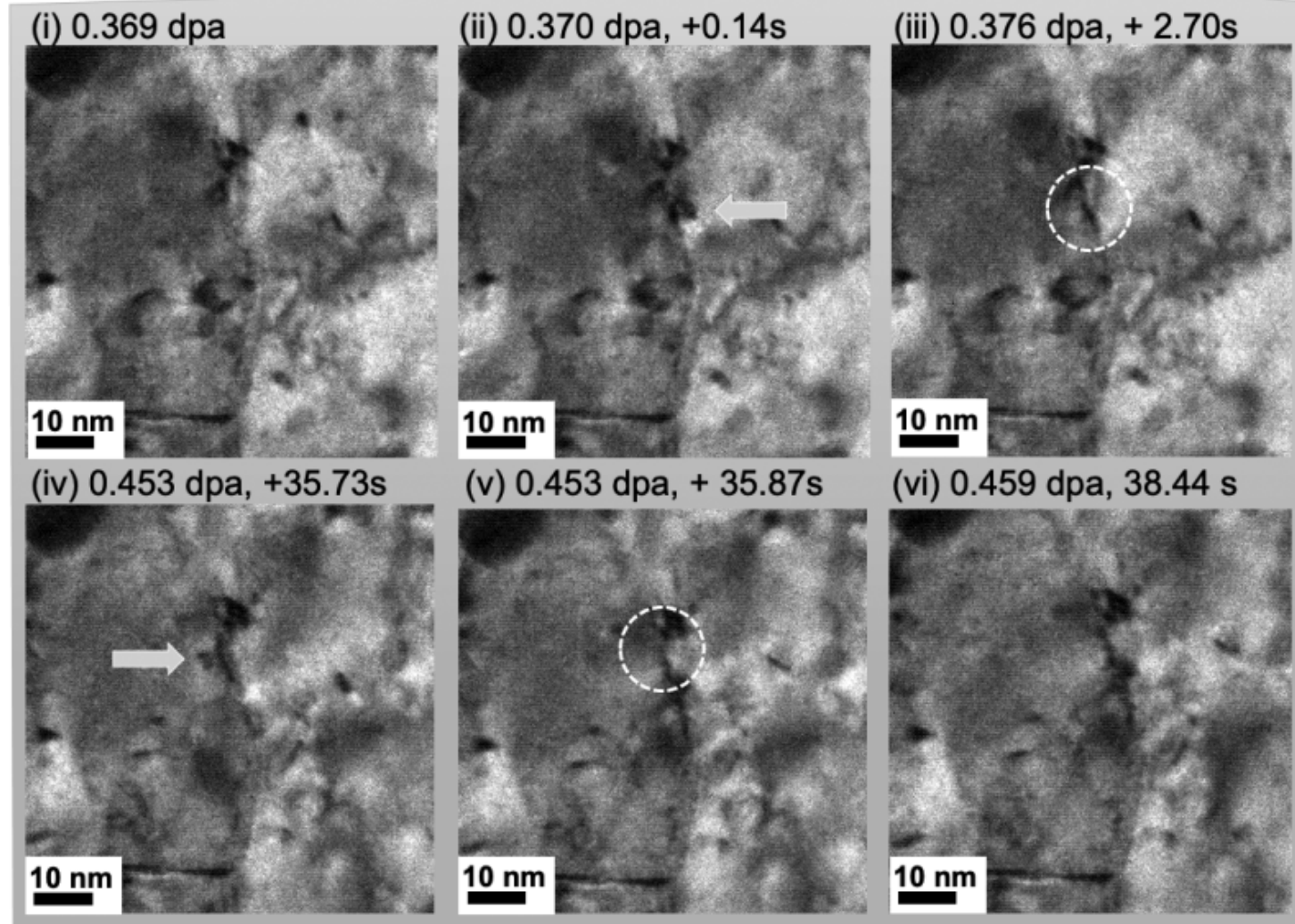
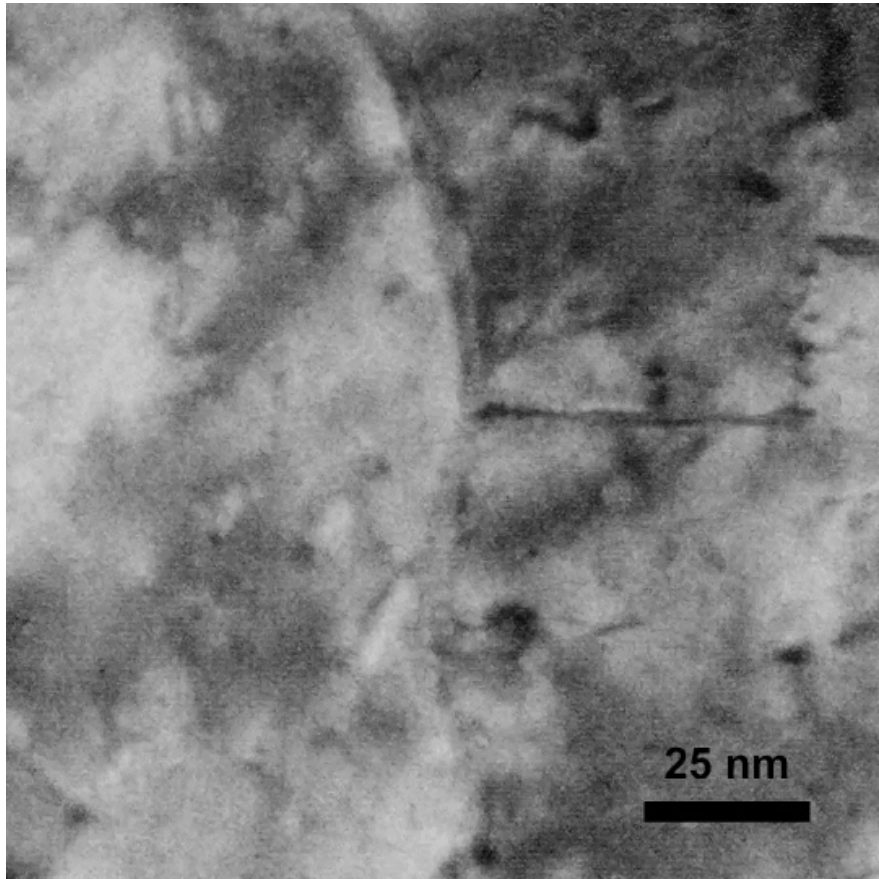
(b) 0.3 dpa



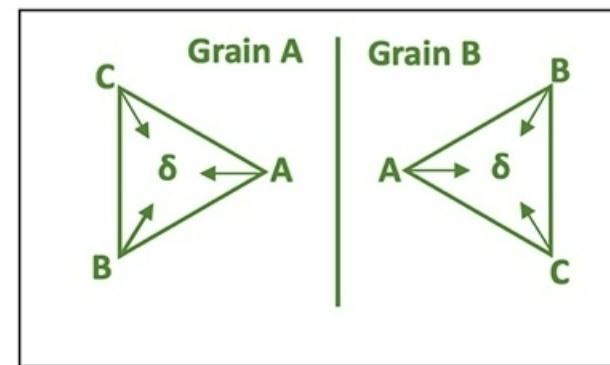
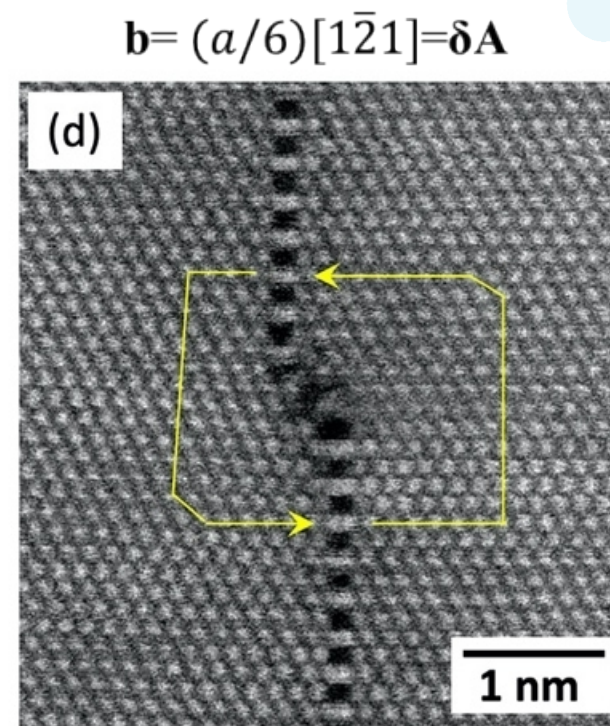
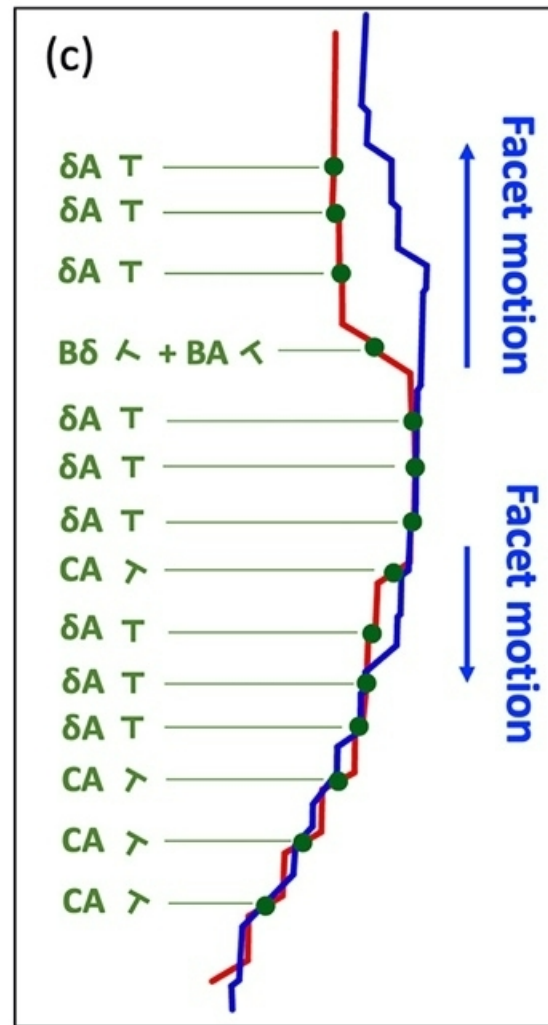
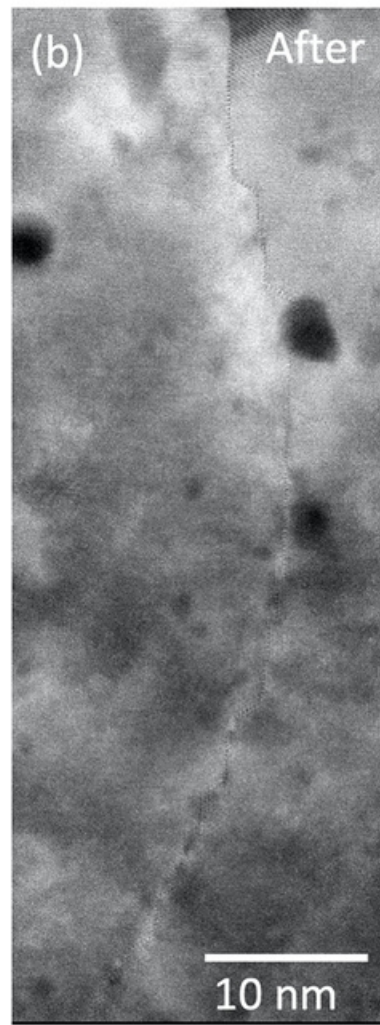
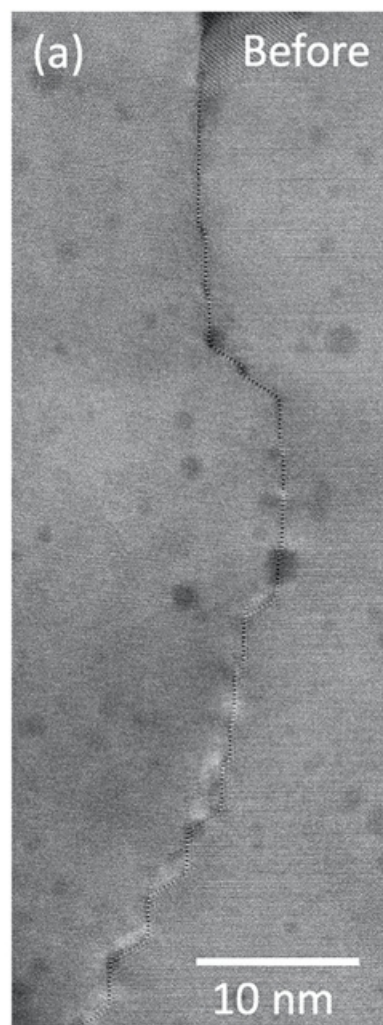
(c) 1 dpa



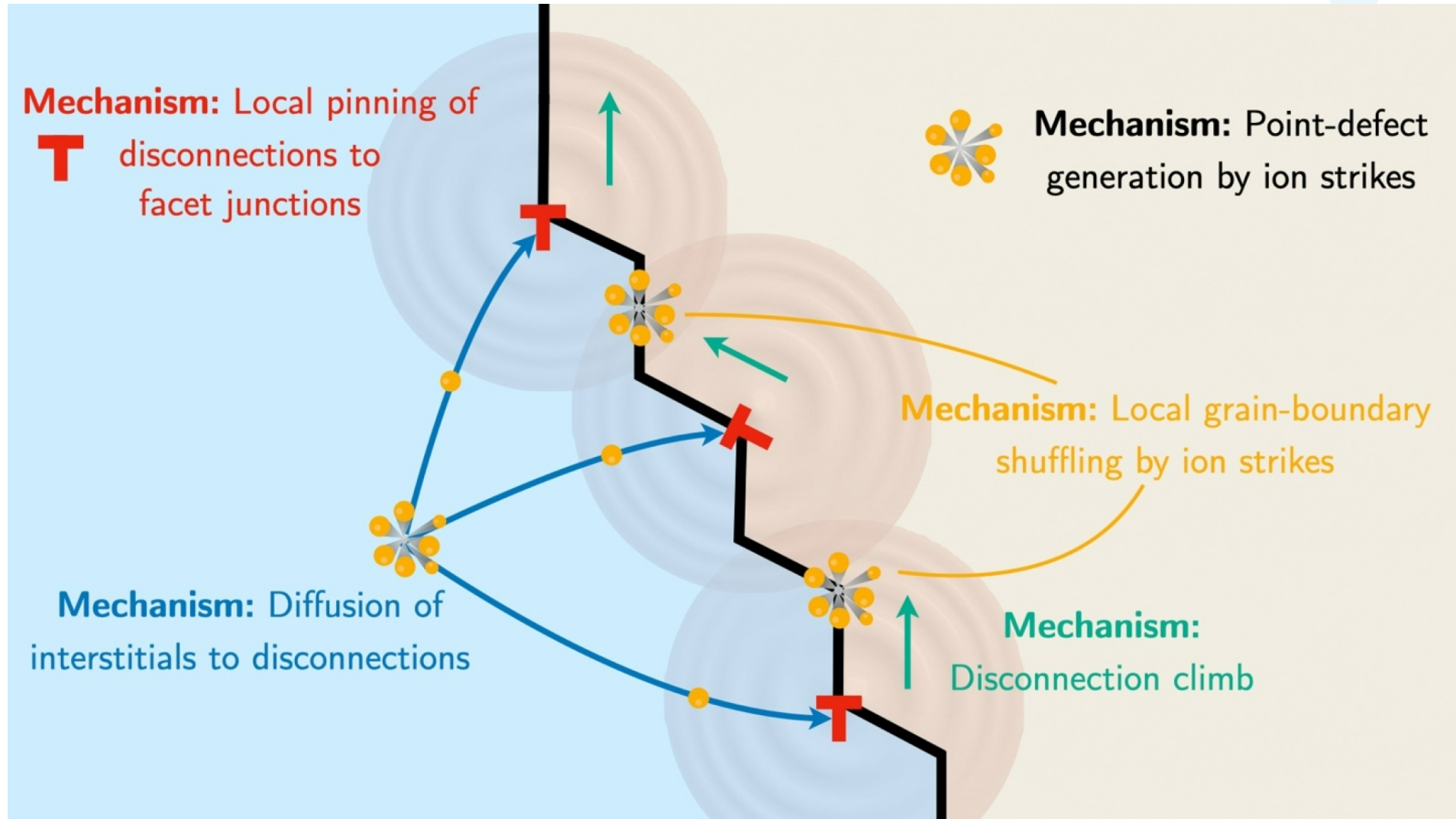
Watching the evolution *in situ*



Detailed analysis of facet junction character & facet motion



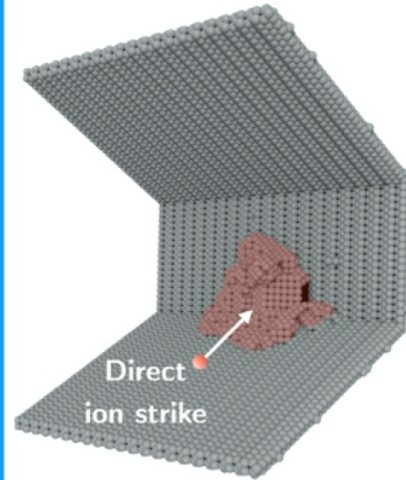
What unit mechanism(s) cause migration?



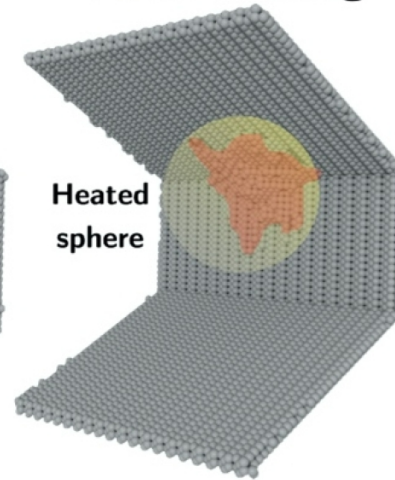
Atomistic simulation

After 1 event

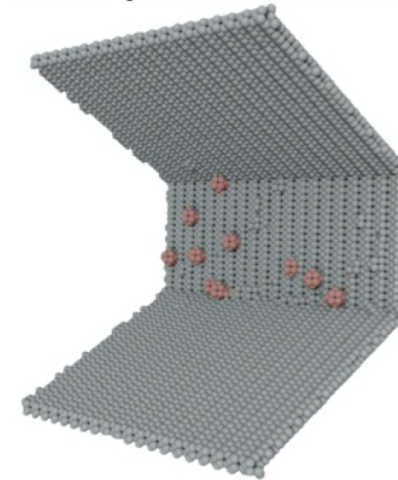
Ion strike



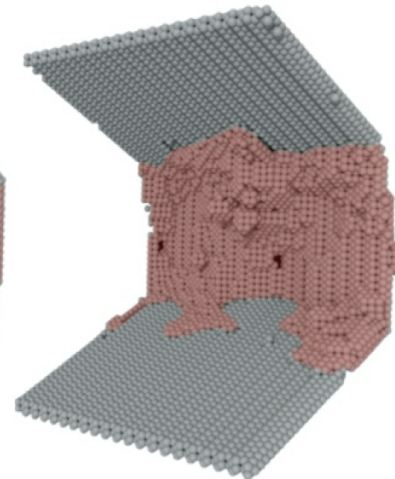
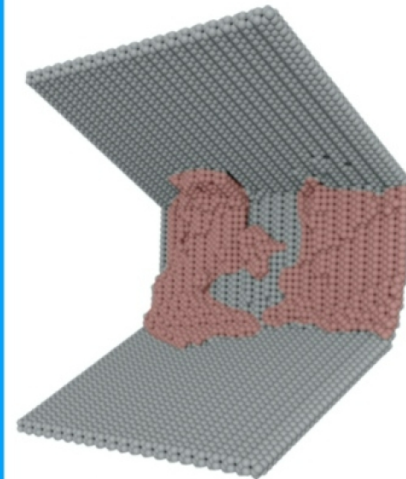
Local heating



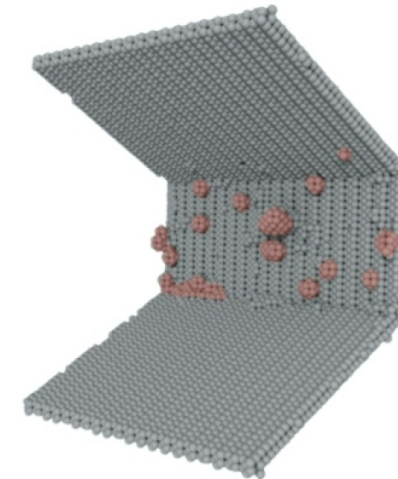
Frenkel pair accumulation



After 5 events

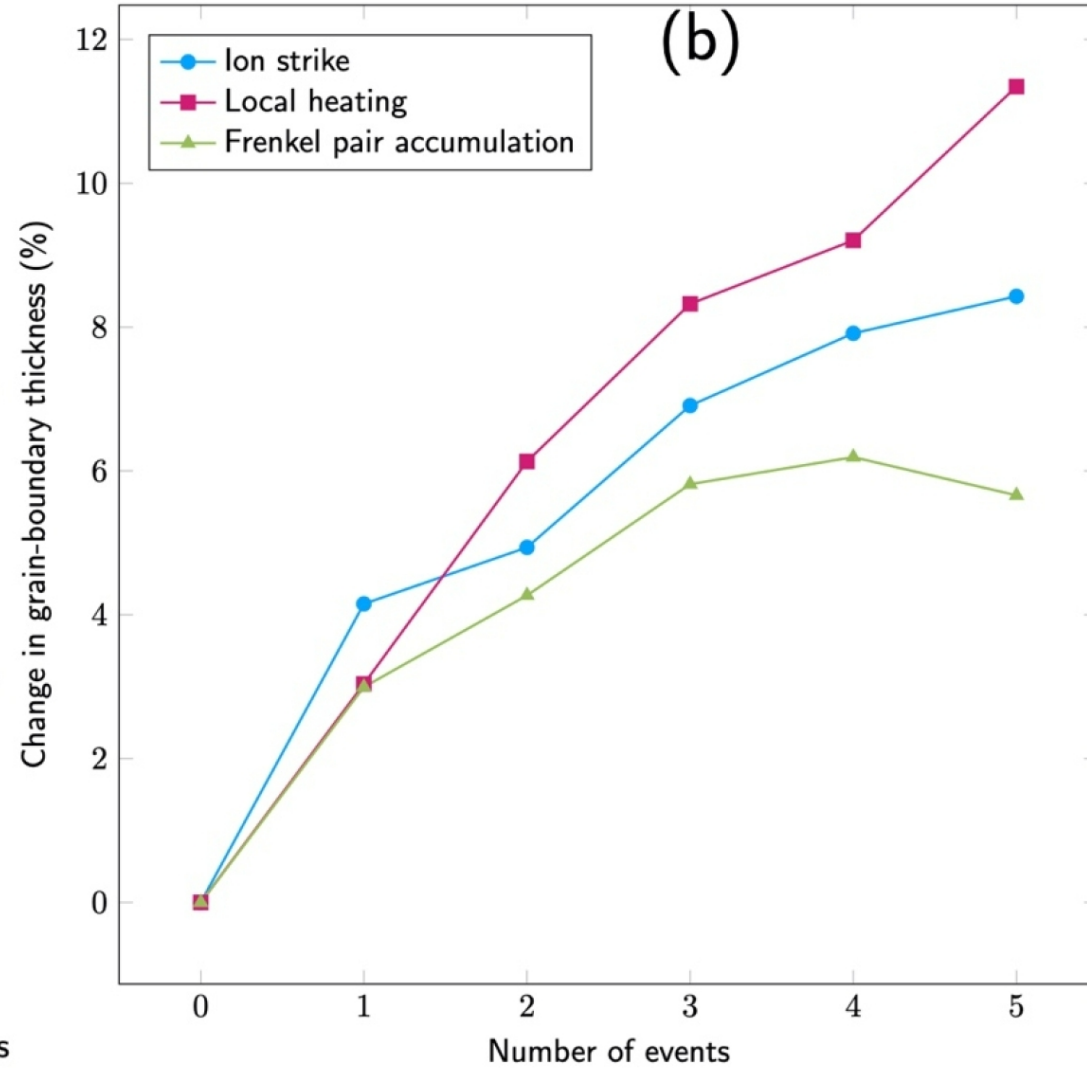
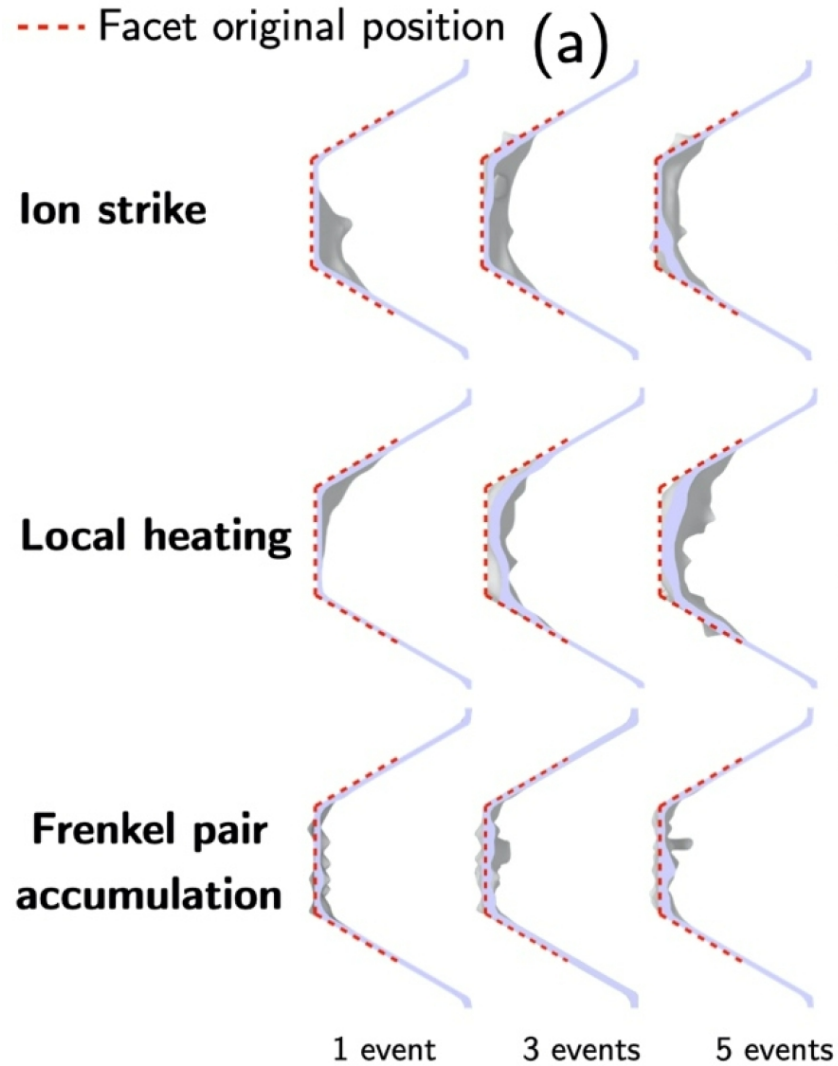


Grain-boundary roughening and migration



Grain-boundary roughening

Atomistic simulation

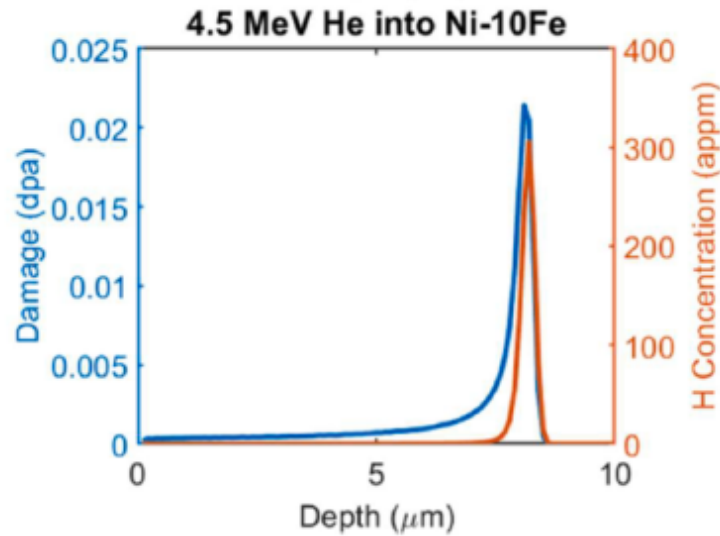


Summary...

High-cycle fatigue, and in particular crack initiation, of nanocrystalline metals seems to be facilitated by grain growth

In general, non-depositing radiation damage serves to heat a GB and induce defects, seemingly stimulating boundary motion and grain growth

Bottom line up front: enhanced fatigue resistance under irradiation?



What else?

Compressive residual stress?

Radiation-induced strengthening?

Complex defect-interactions?

