SAND2022-2294C

Interactions between interfacial disconnections and facet junctions: implications for faceting and boundary evolution

Douglas L. Medlin[1], Christopher Barr[2,†], James Nathaniel[1], Elton Chen[2], Ping Lu[2], David Adams[2], Rémi Dingreville[2], Brad Boyce[2], Khalid Hattar[2]

[1]Sandia National Laboratories, Livermore, California 94550, USA

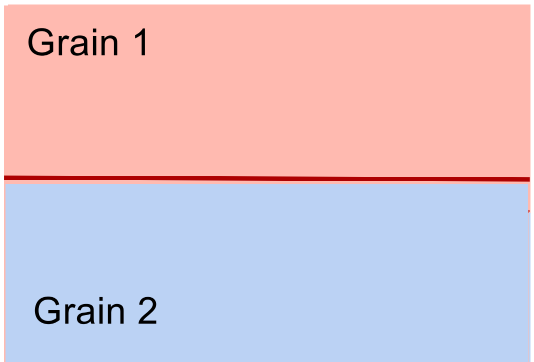
[2]Sandia National Laboratories, Albuquerque, New Mexico 87185, USA

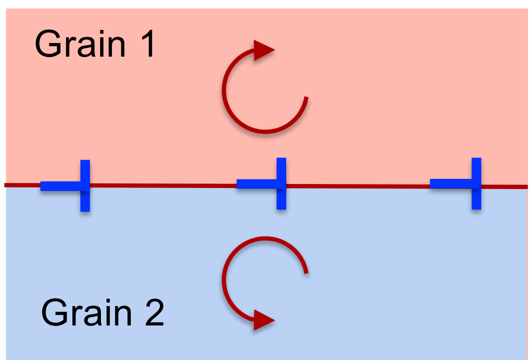
[†]Present address: Naval Nuclear Laboratory, West Mifflin, Pennsylvania 15122, USA

Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and 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.

Facet Junctions and GB Disconnections: Anisotropy in Energy with Inclination and Misorientation





- **Inclination:**
  - **-Reduce energy by faceting on lower energy planes**
  - **-Facet junctions**
    - -**Line forces:** due to discontinuity in interfacial stress
    - **-Dislocation content:**
      -incompatibility of translation states at adjacent facets: $\mathbf{b}=\mathbf{t}_1-\mathbf{t}_2$
      -*"Intrinsic junction dislocations"*
- **Misorientation:**
  - **-Accommodate deviation with interfacial disconnections (steps w/dislocation content)**

Focus of this talk:
Interplay between GB Disconnections and Facet Junctions

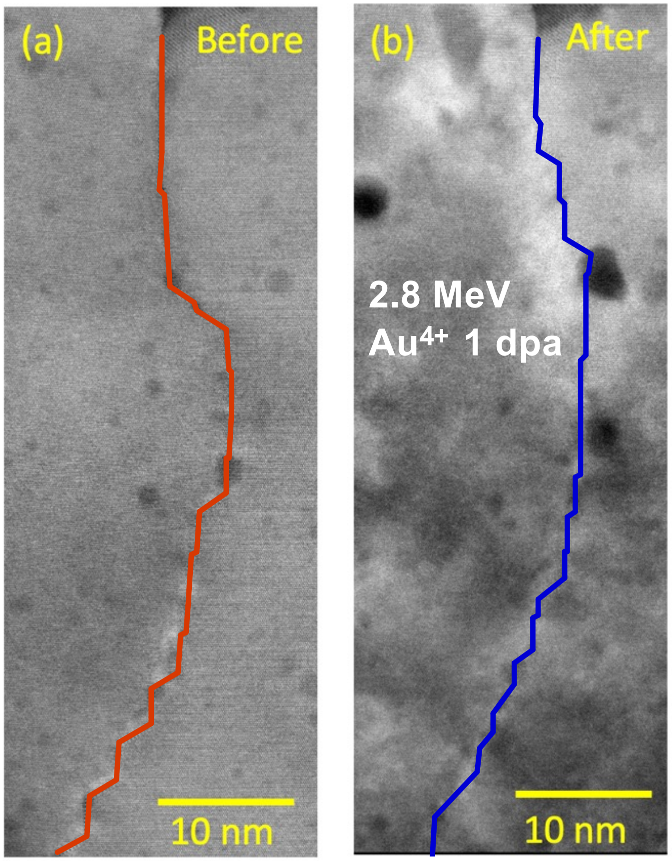
Some Older examples:

- **Σ5 BCC Fe: Disconnections at nanofacets**
- **Σ3 (1/6)<112> Disconnection climb**
  Thermal facet coarsening

Recent work on Ion Irradiation Induced GB evolution:

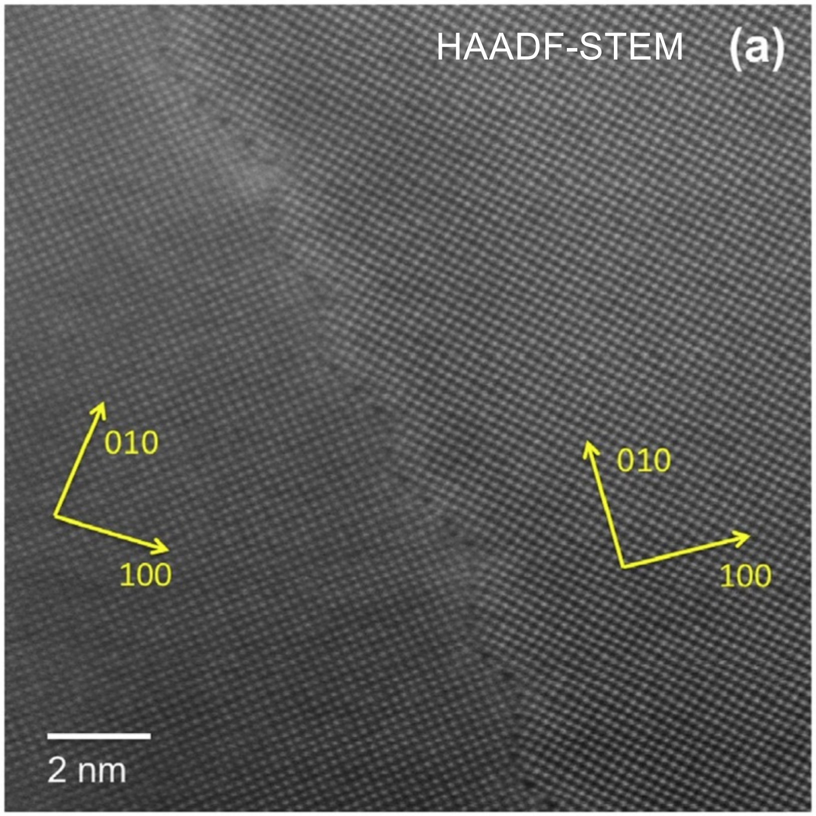
- **Pt Σ3 {112} facet evolution**
- **Molecular Dynamics: insight into roughening and local migration**
- **Dislocation analysis: insight into longer-range interactions.**

C.M. Barr, E.Y. Chen, J.E. Nathaniel II, P. Lu, D.P. Adams, R. Dingreville, K. Hattar, D.L. Medlin, Submitted to Science Advances, 2022



Interaction of GB dislocations and Facet Junctions can dictate faceting length scale

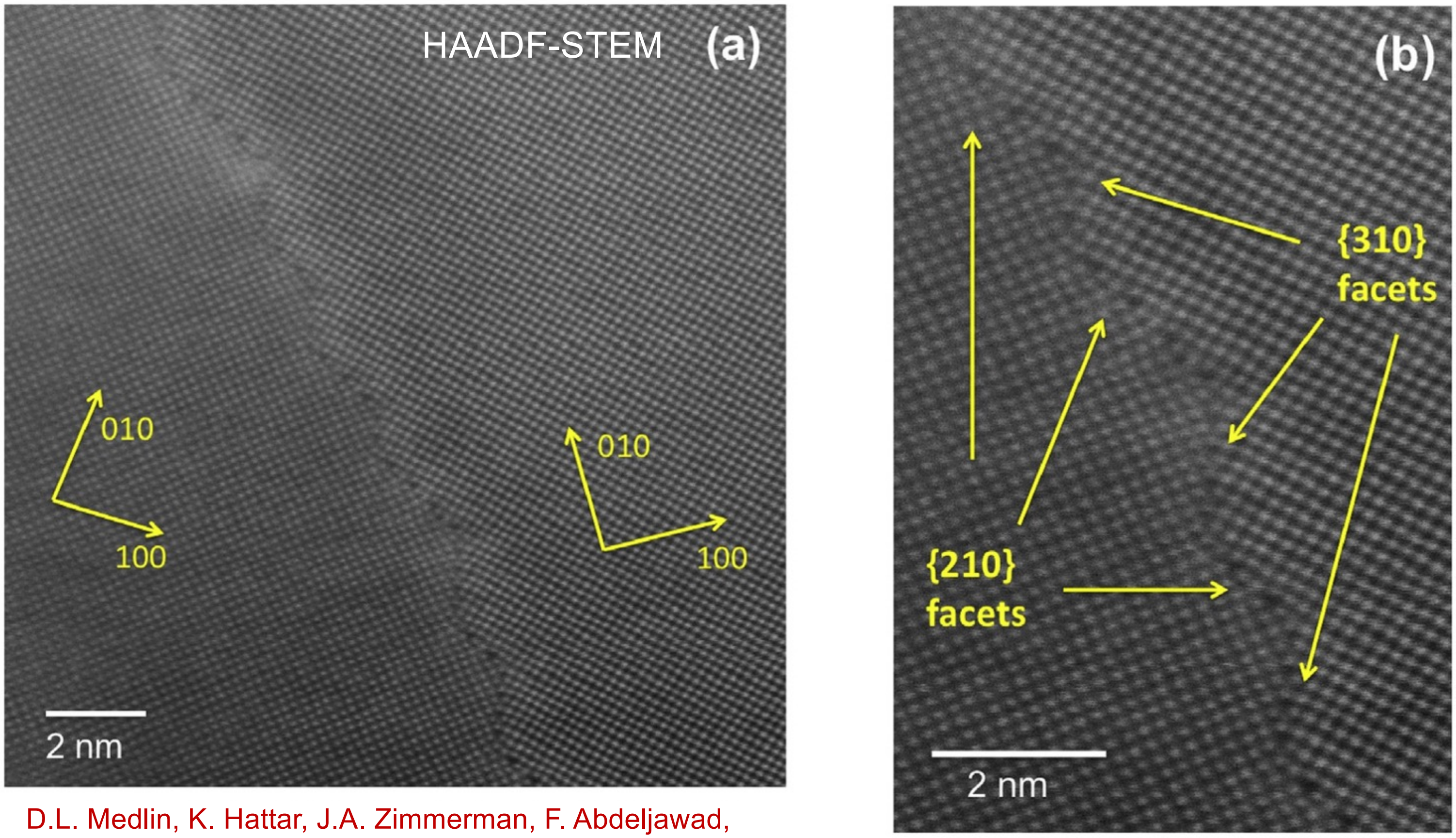
Example: Nanofaceted Σ5 [001] Boundary in BCC Fe

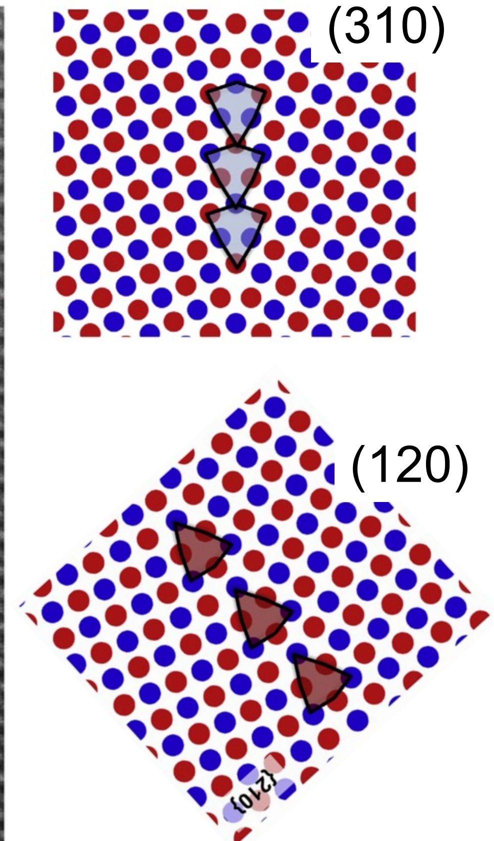


D.L. Medlin, K. Hattar, J.A. Zimmerman, F. Abdeljawad, S.M. Foiles, Acta Materialia (2017)

Interaction of GB dislocations and Facet Junctions can dictate faceting length scale

Example: Nanofaceted Σ5 [001] Boundary in BCC Fe

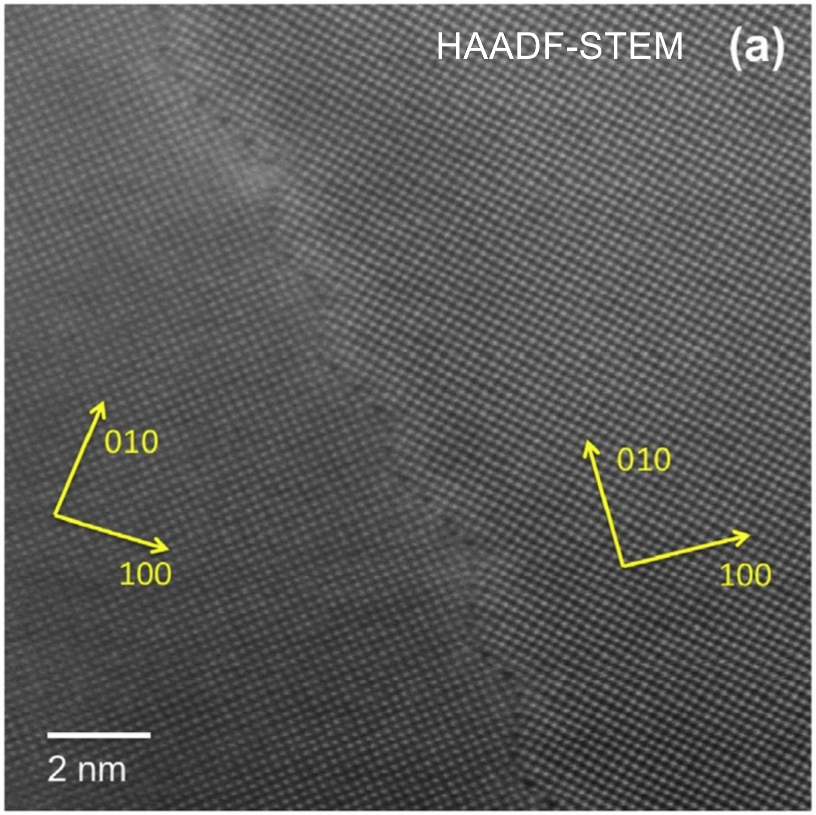




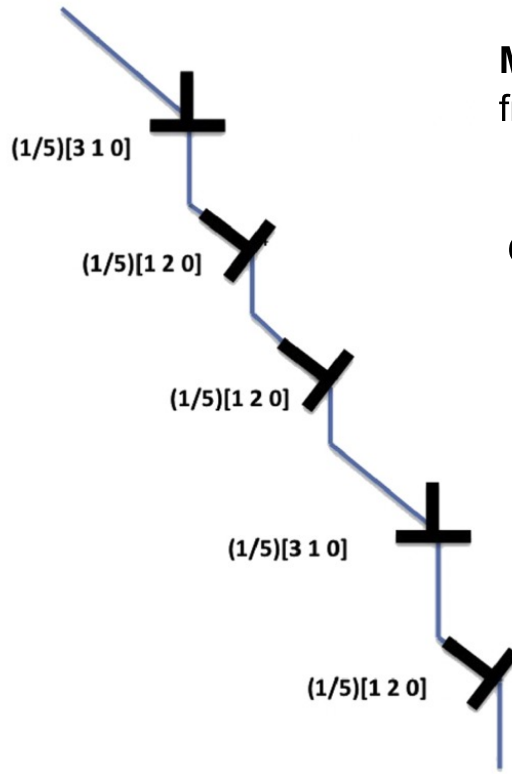
D.L. Medlin, K. Hattar, J.A. Zimmerman, F. Abdeljawad, S.M. Foiles, Acta Materialia (2017)

Interaction of GB dislocations and Facet Junctions can dictate faceting length scale

Example: Nanofaceted Σ5 [001] Boundary in BCC Fe



D.L. Medlin, K. Hattar, J.A. Zimmerman, F. Abdeljawad, S.M. Foiles, Acta Materialia (2017)



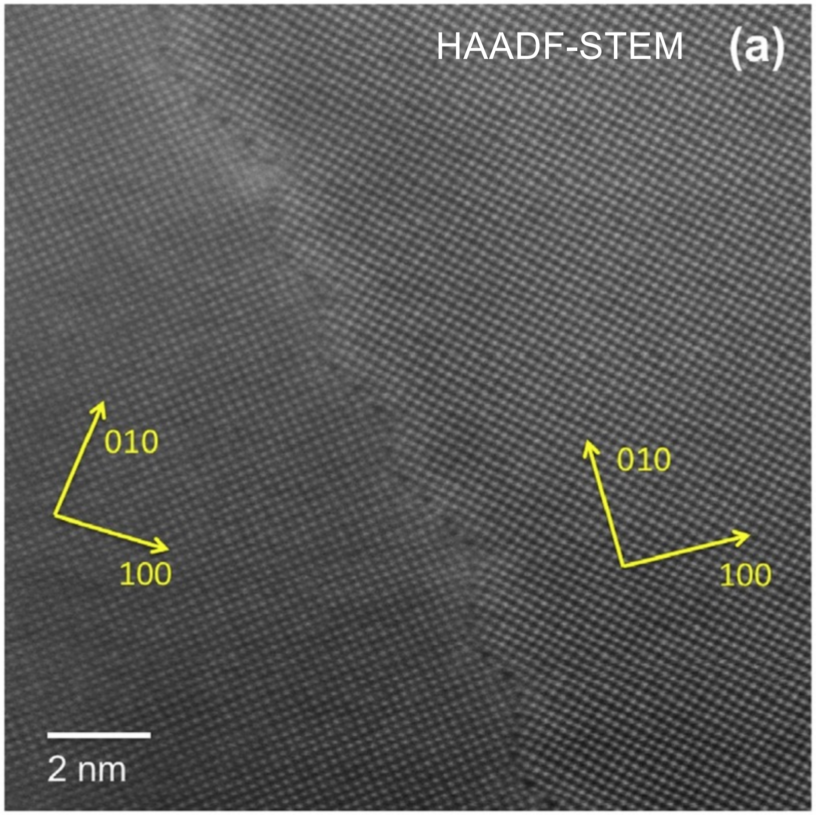
Misorientation 2.38° from exact Σ5 orientation

Circuit Analysis:

GB dislocation content at every junction pair

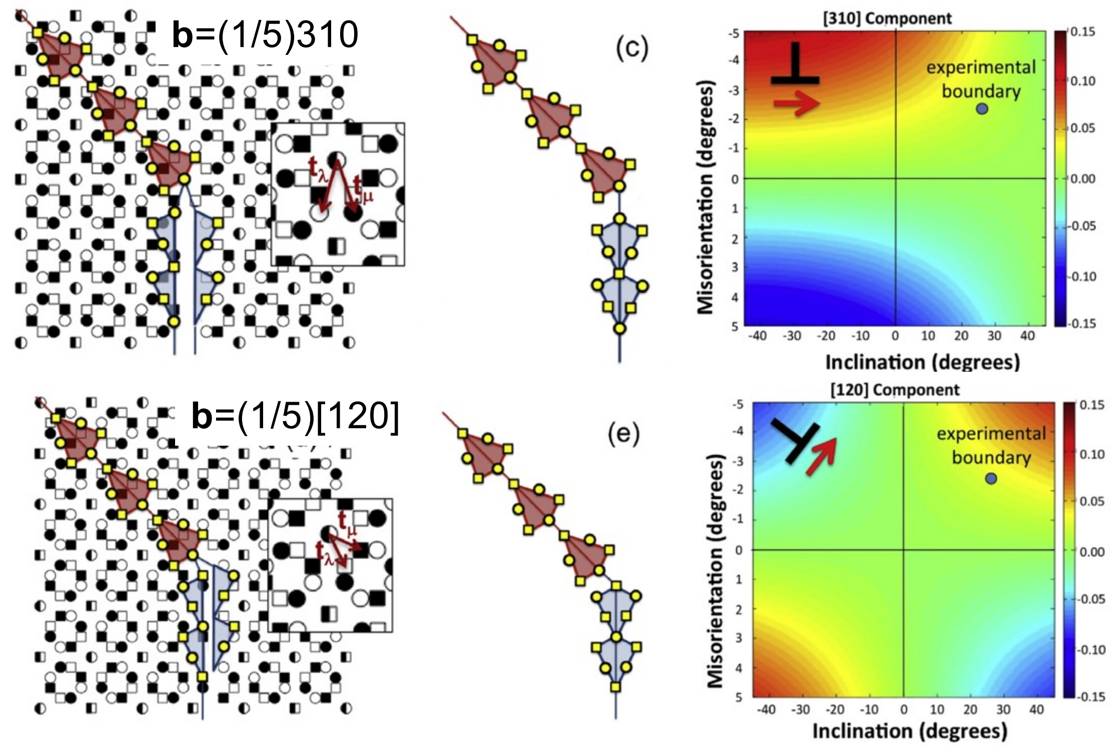
Interaction of GB dislocations and Facet Junctions can dictate faceting length scale

Example: Nanofaceted Σ5 [001] Boundary in BCC Fe



D.L. Medlin, K. Hattar, J.A. Zimmerman, F. Abdeljawad, S.M. Foiles, Acta Materialia (2017)

Defect Distribution Satisfies Frank-Bilby Equation



Accommodates coherency strains due to misorientation from Σ5
Pinning to junctions

→ **faceting length scale linked to misorientation**

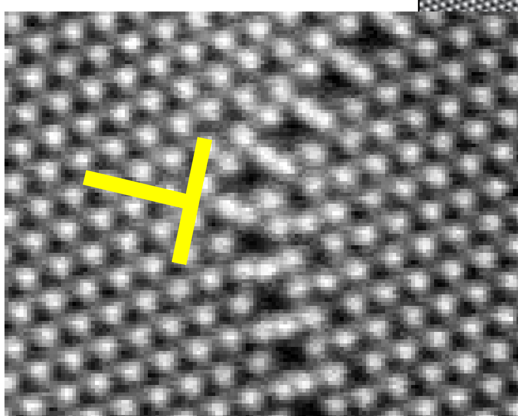
GB disconnection at facet junction: Au Σ3 {112}

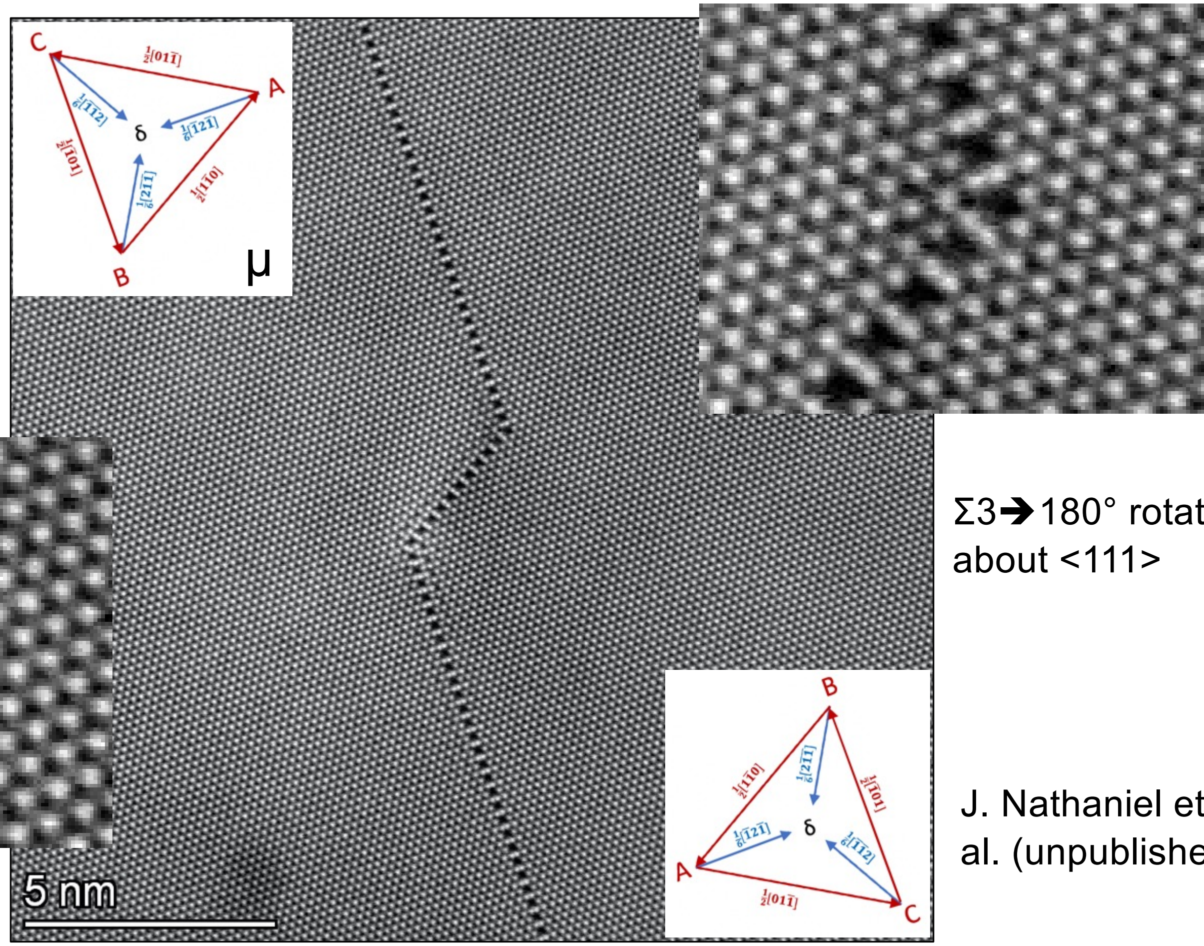
HAADF-STEM

Au. <111> projection

Circuit analysis identifies 1/6)<112> dislocation at facet junction

$$\boldsymbol{b} = \boldsymbol{B\delta} = \left(\frac{\mathbf{1}}{\mathbf{6}}\right)[\mathbf{2\bar{1}\bar{1}}]_{\boldsymbol{\lambda}}$$

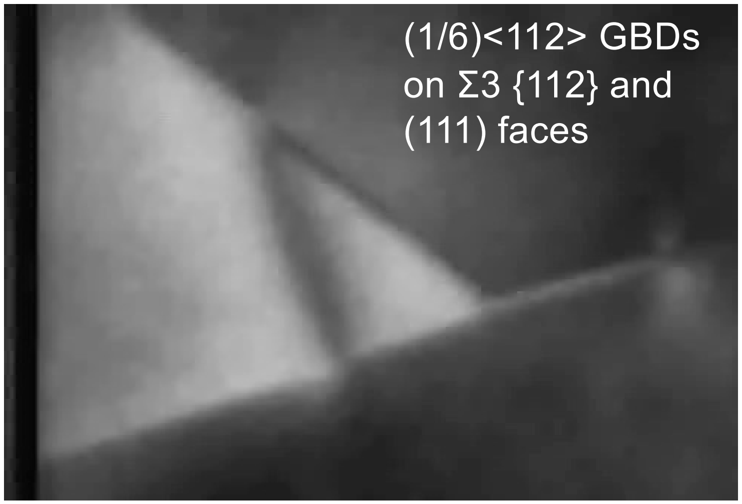




Σ3➔180° rotation about <111>

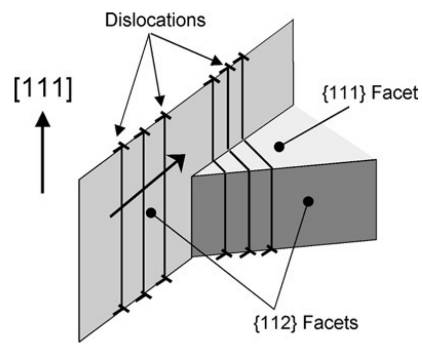
J. Nathaniel et al. (unpublished)

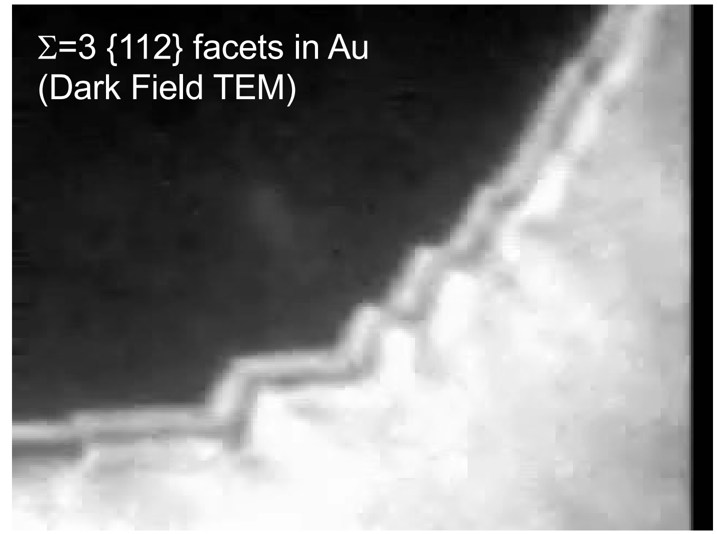
GBD Climb and facet coarsening at elevated temperature



T=550° Δt=400 sec
Movie is repeated

20 nm





50 nm T=490°C 185 minutes

-(1/6)<112> dislocations climb on Σ=3 {112} facets

-Segments on horizontal {111} facets move by glide.

-Climb is driven by repulsive elastic interactions between the dislocations

-Finite tilt wall, un-relaxed long-range stresses

G. Lucadamo and D.L. Medlin, Acta Materialia 50 (2002)

Coordinated motion of Σ3 facet

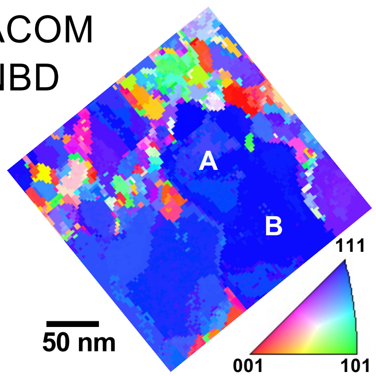
-Elastic interactions between disconnections at facet junctions

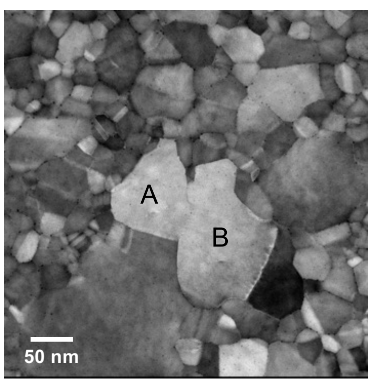
-Eventual coarsening of the facets

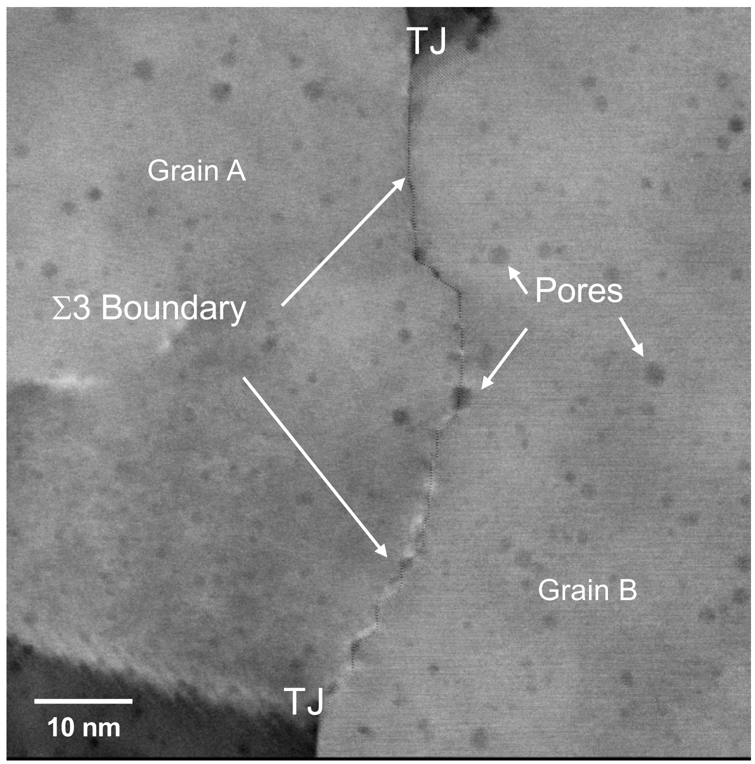
D.L. Medlin and G. Lucadamo, MRS Symp 252 (2001)

Nanocrystalline Pt Irradiation Study: Initial state

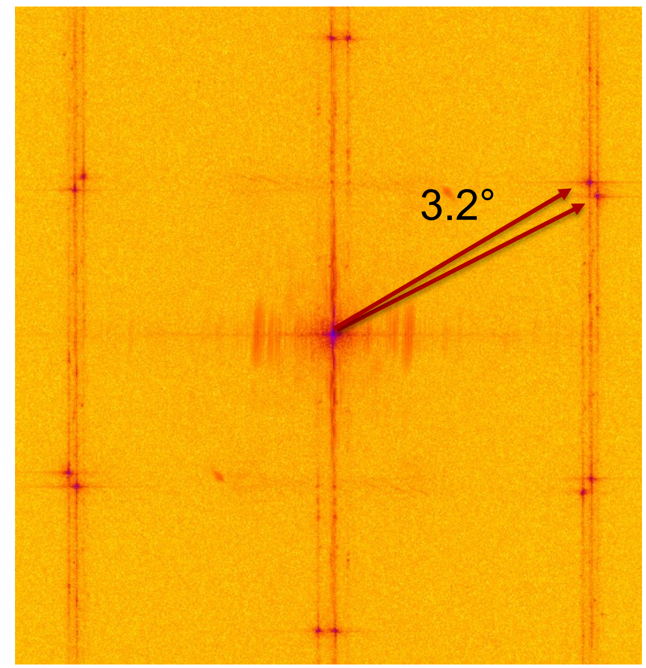
ACOM
NBD







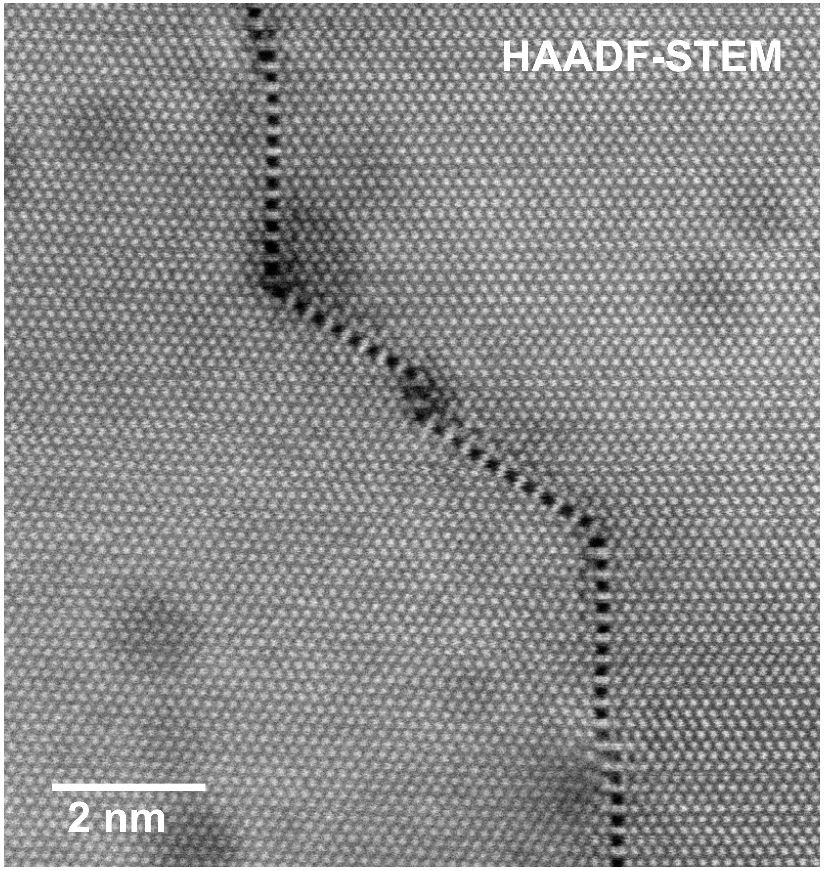
Boundary close to Σ3

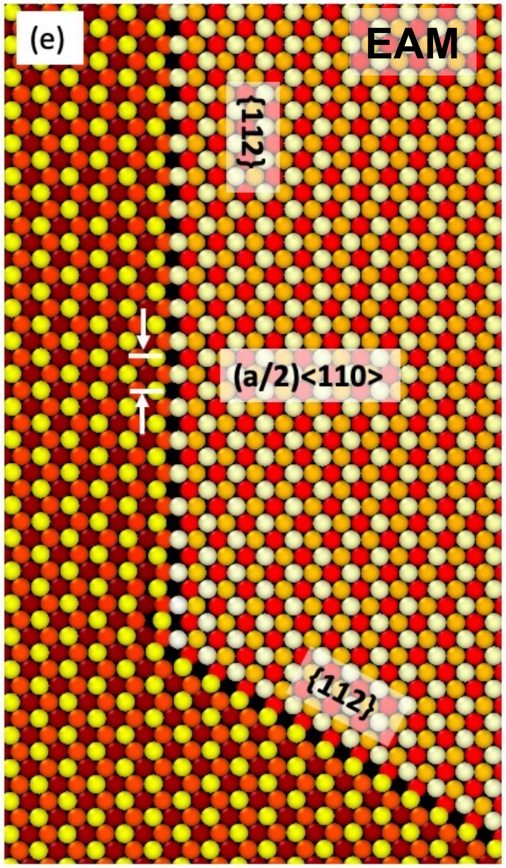


3.2° rotation about <111>
from exact Σ3

Irradiation in Sandia I^{3}TEM: **2.8 MeV Au^{4+} 1 dpa**

Initial state of Pt GB (prior to irradiation):



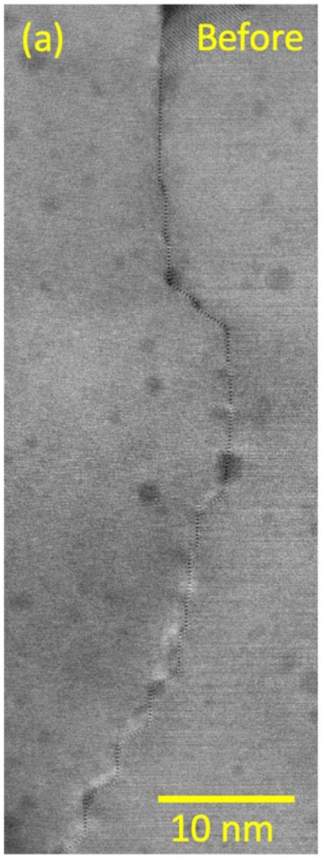


Σ3 {112} Facets meet 120° angles

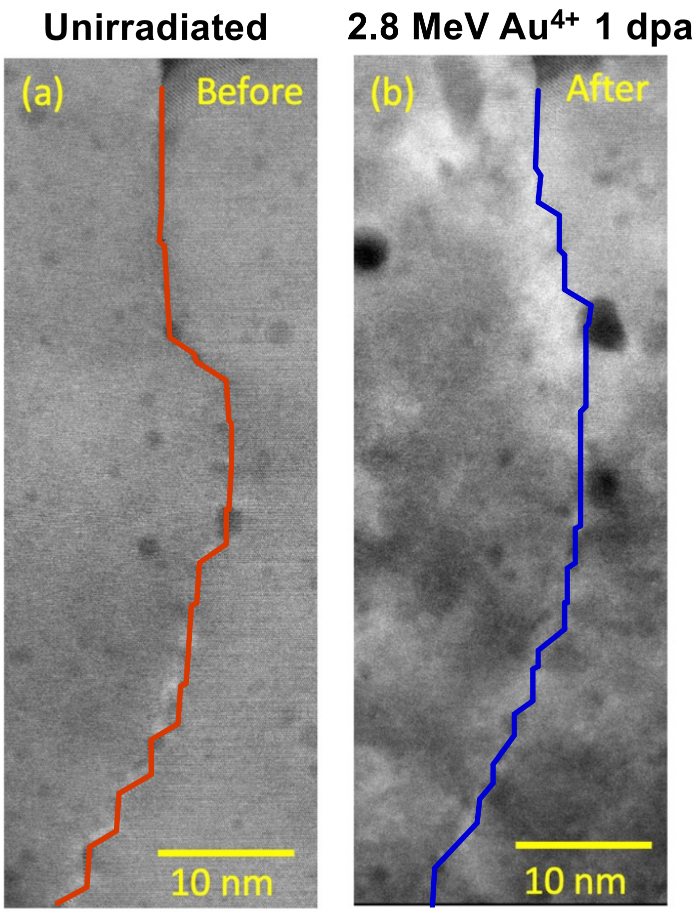
In this projection we resolve all 3 (ABC) stackings stacking positions of the {111} planes

Irradiated Pt boundary: Evolution of facets

Unirradiated

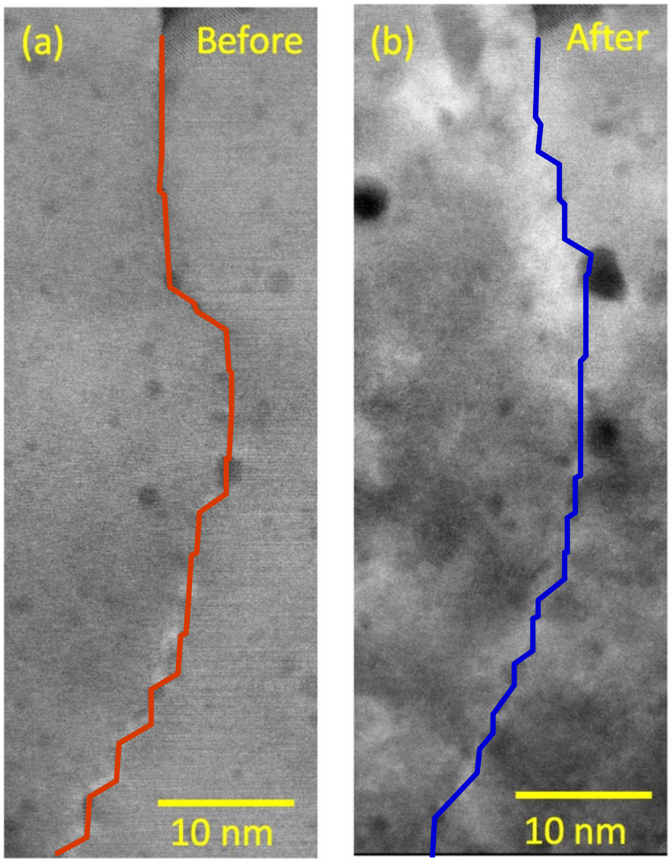


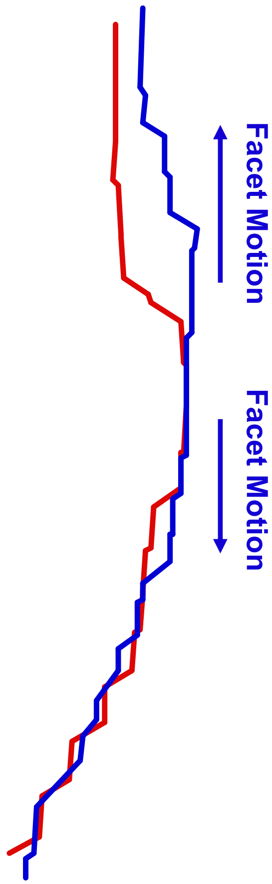
Irradiated Pt boundary: Evolution of facets



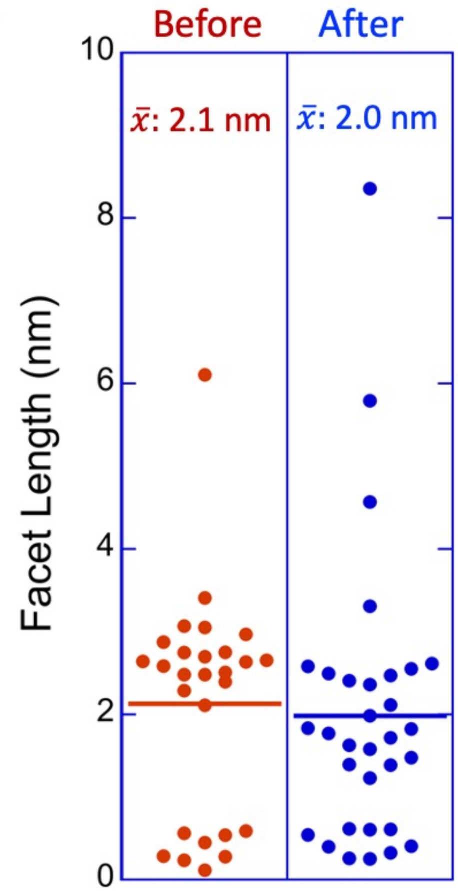
Irradiated Pt boundary: Evolution of facets

Unirradiated **2.8 MeV Au^{4+} 1 dpa**





Facet Length Distributions



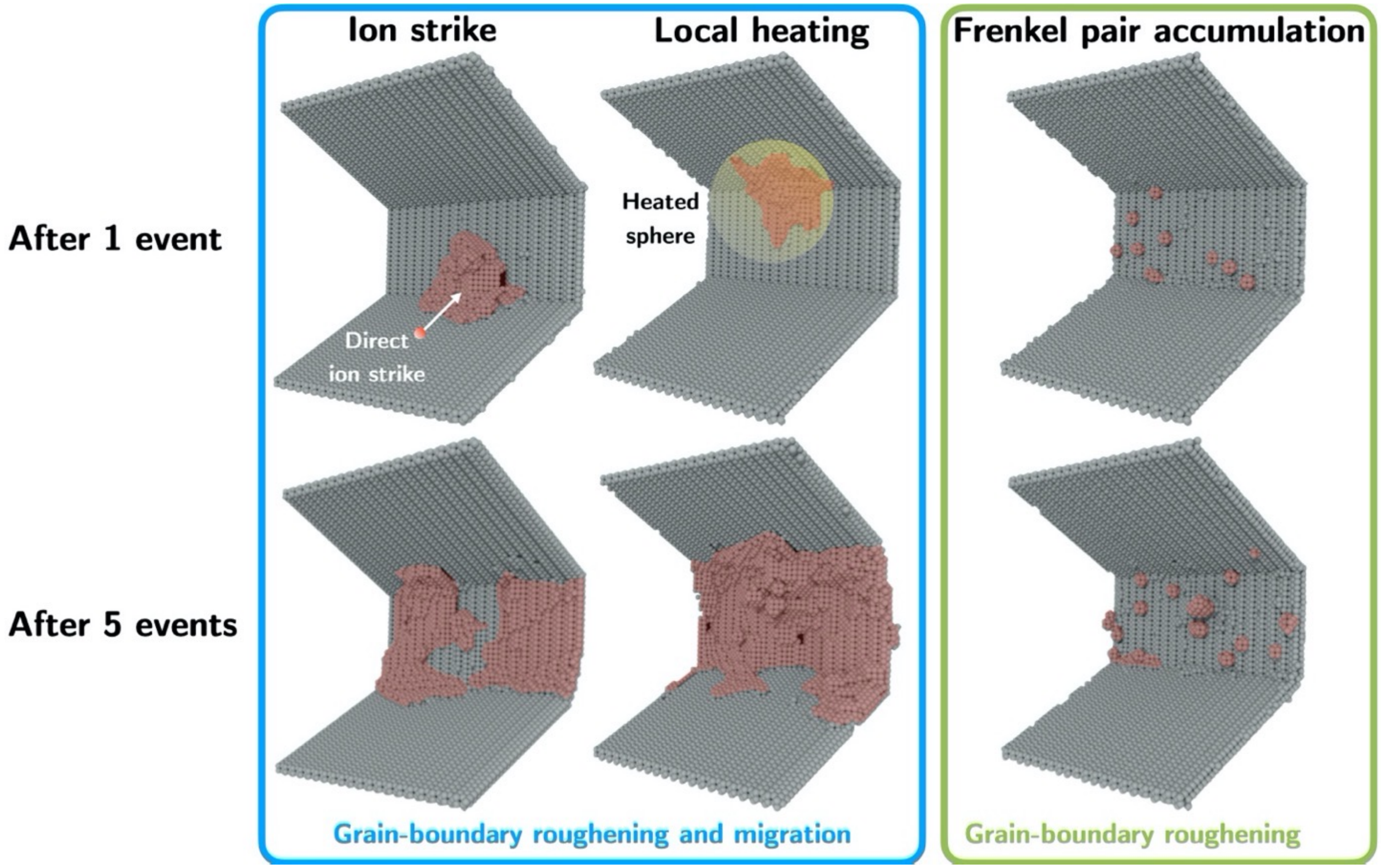
Average facet length stays same

Distribution changes

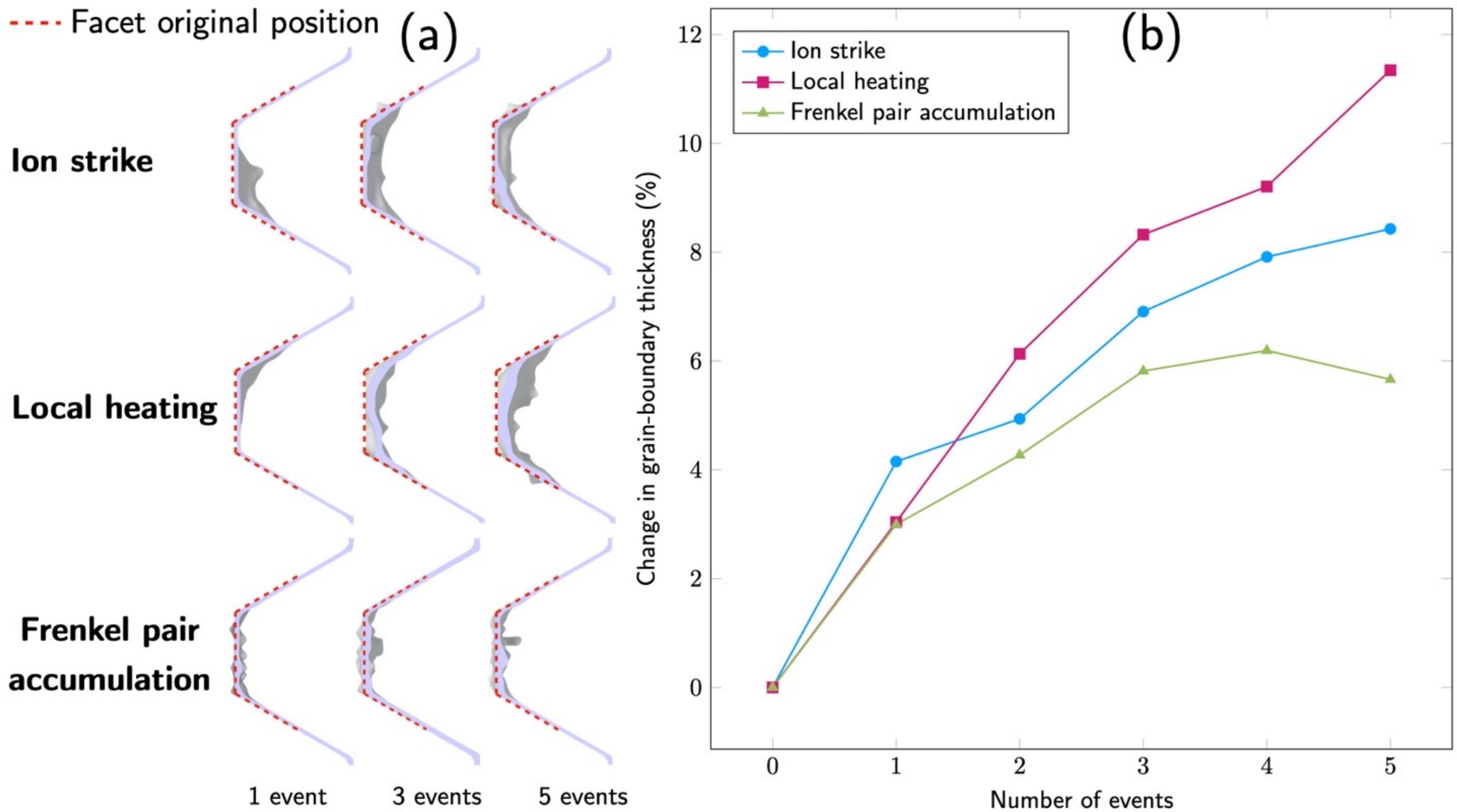
Coarsening

Increase in small facet population

Molecular Dynamics:
Irradiation induced GB roughening and local migration



Molecular Dynamics:
Irradiation induced GB roughening and local migration



C.M. Barr, E.Y. Chen, J.E. Nathaniel II, P. Lu, D.P. Adams, R. Dingreville, K. Hattar, D.L. Medlin, Submitted to Science Advances, 2022

Interfacial Dislocation Content

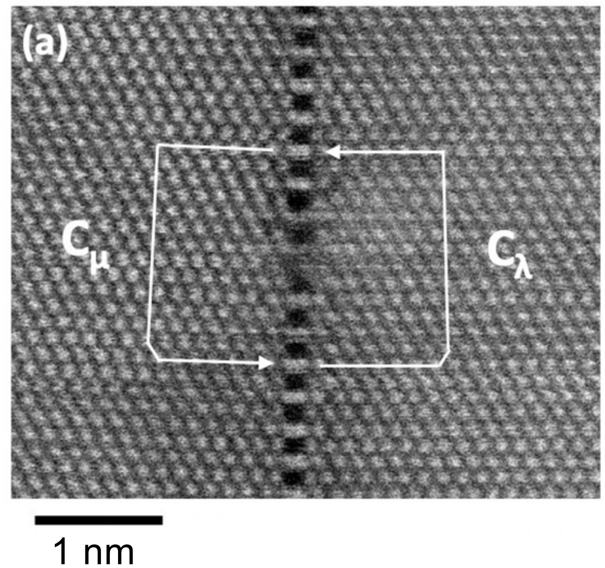
Circuit analyses at each disconnection and pair of facet junctions in pre-irradiated boundary

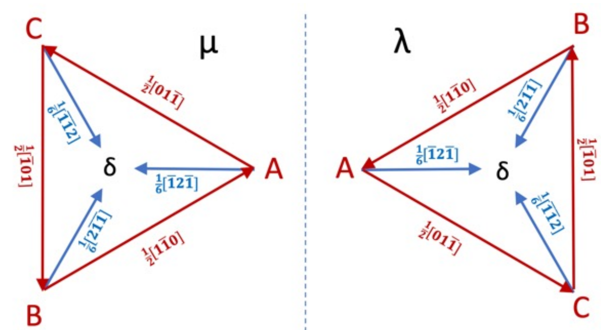
Circuit paths in two crystals

$$\boldsymbol{b} = -(\boldsymbol{C}_\lambda + \mathbf{P}\boldsymbol{C}_\mu)$$

Crystal coordinate transformation

$$\mathbf{P} = \frac{1}{3}\begin{pmatrix} -1 & 2 & 2 \\ 2 & -1 & 2 \\ 2 & 2 & -1 \end{pmatrix}$$



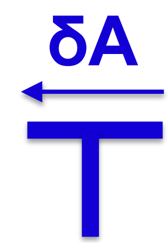


Dislocation and step content character

$$\boldsymbol{b} = \tfrac{1}{6}[1,-2,1] = \boldsymbol{\delta A}$$

$$h(\mu) = +1\ d_{224}$$

$$h(\lambda) = -1\ d_{224}$$



C.M. Barr, E.Y. Chen, J.E. Nathaniel II, P. Lu, D.P. Adams, R. Dingreville, K. Hattar, D.L. Medlin, Submitted to Science Advances, 2022

Interfacial Dislocation Content

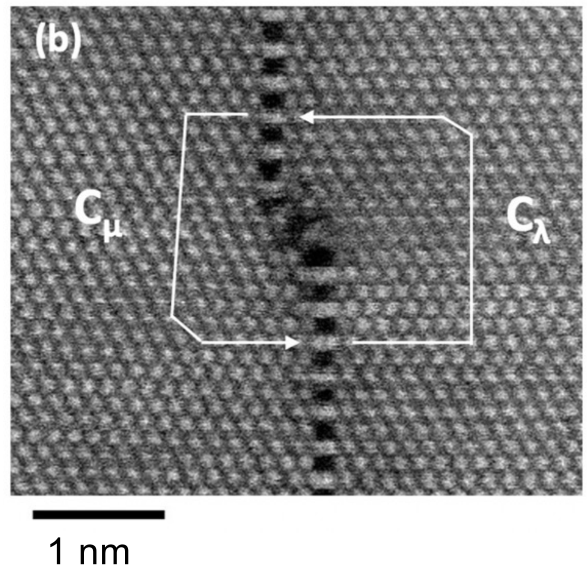
Circuit analyses at each disconnection and pair of facet junctions in pre-irradiated boundary

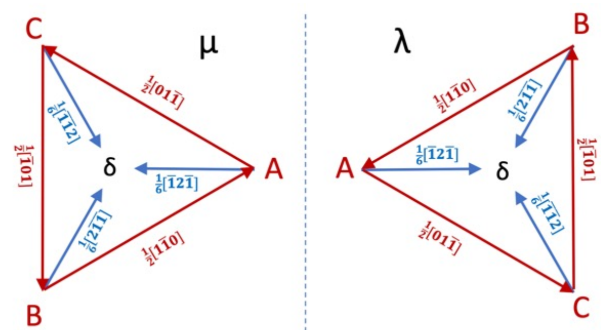
Circuit paths in two crystals

$$\boldsymbol{b} = -(\boldsymbol{C}_\lambda + \mathbf{P}\boldsymbol{C}_\mu)$$

Crystal coordinate transformation

$$\mathbf{P} = \frac{1}{3}\begin{pmatrix} -1 & 2 & 2 \\ 2 & -1 & 2 \\ 2 & 2 & -1 \end{pmatrix}$$



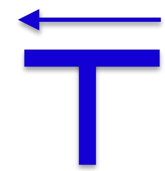


Dislocation and step content character

$$\boldsymbol{b} = \tfrac{1}{6}[1,-2,1] = \boldsymbol{\delta A}$$

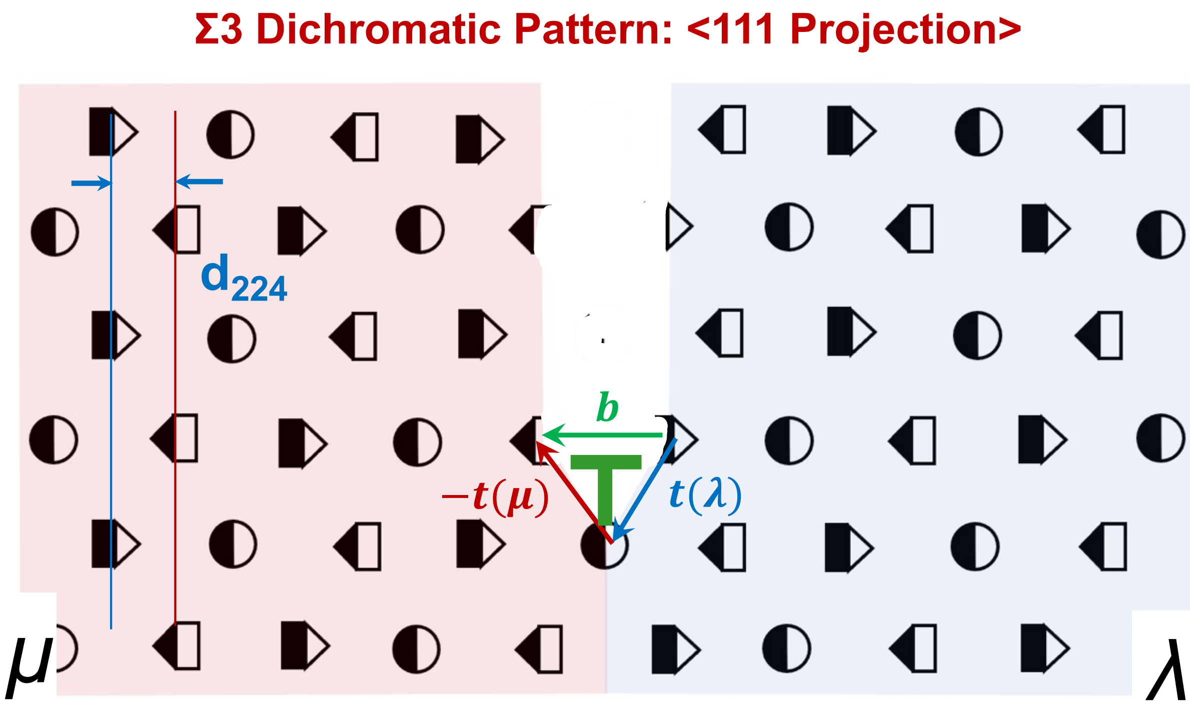
$$h(\mu) = +7\, d_{224}$$

$$h(\lambda) = +5\, d_{224}$$



C.M. Barr, E.Y. Chen, J.E. Nathaniel II, P. Lu, D.P. Adams, R. Dingreville, K. Hattar, D.L. Medlin, Submitted to Science Advances, 2022

Bicrystallography: (1/6)<112> disconnections on {112} facet



Burgers vector: A Difference of Lattice Translation Vectors

Crystalline coordinate transformation

$$\boldsymbol{b} = \boldsymbol{t}(\boldsymbol{\lambda}) - \boldsymbol{P}\boldsymbol{t}(\boldsymbol{\mu})$$

Crystal translation vectors

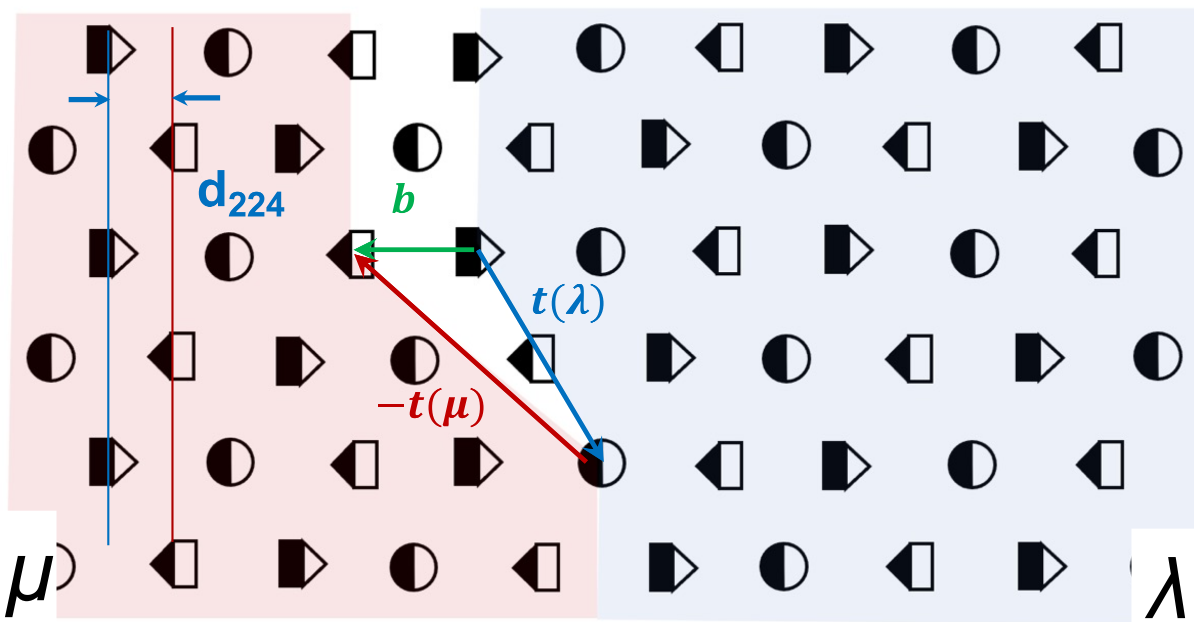
Hirth & Pond, Acta Mat, 1996

$\boldsymbol{t}(\mu) = \frac{1}{2}[\bar{1}\bar{1}0]$ $\quad h(\mu) = +1\, d_{224}$

$\boldsymbol{t}(\lambda) = \frac{1}{2}[0\bar{1}\bar{1}]$ $\quad h(\lambda) = -1\, d_{224}$

Bicrystallography: (1/6)<112> disconnections on {112} facet

Σ3 Dichromatic Pattern: <111 Projection>



Burgers vector: A Difference of Lattice Translation Vectors

Crystalline coordinate transformation

$$\boldsymbol{b} = \boldsymbol{t}(\boldsymbol{\lambda}) - \boldsymbol{P}\boldsymbol{t}(\boldsymbol{\mu})$$

Crystal translation vectors

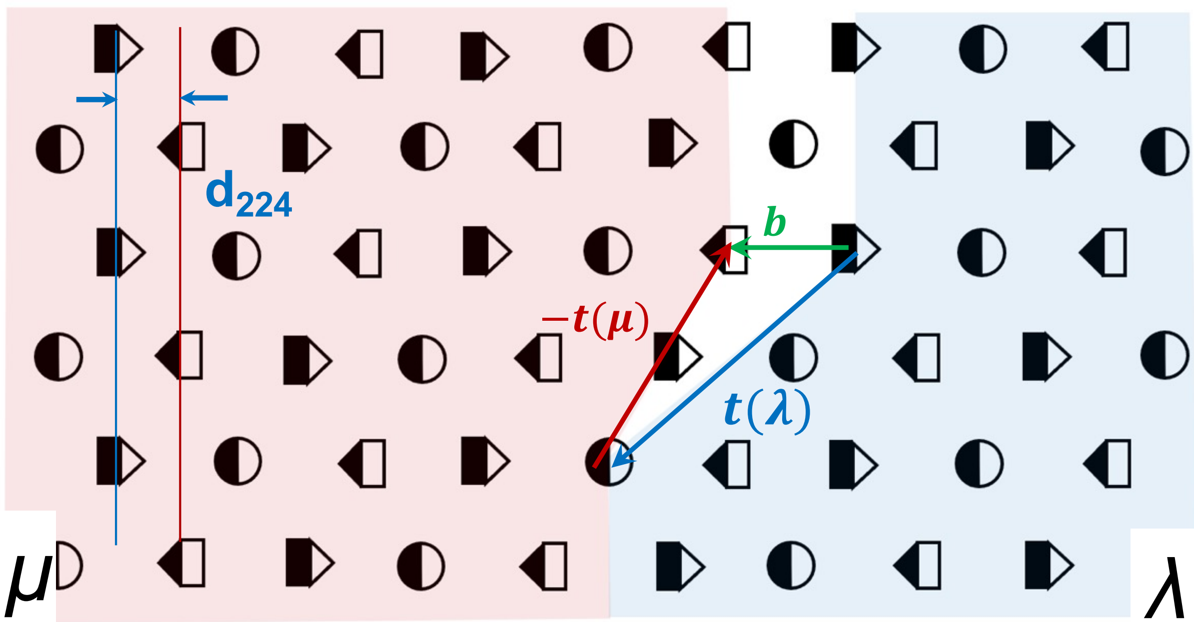
Hirth & Pond, Acta Mat, 1996

$\boldsymbol{t}(\mu) = \frac{1}{2}[\bar{1}\bar{2}1]$	$h(\lambda) = +2\ d_{224}$
$\boldsymbol{t}(\lambda) = [0\ 0\ \bar{1}]$	$h(\mu) = +4\ d_{224}$

Different Step Heights, but same Burgers vector

Bicrystallography: (1/6)<112> disconnections on {112} facet

Σ3 Dichromatic Pattern: <111 Projection>



Burgers vector: A Difference of Lattice Translation Vectors

Crystalline coordinate transformation

$$b = t(\lambda) - Pt(\mu)$$

Crystal translation vectors

Hirth & Pond, Acta Mat, 1996

$t(\mu) = [\bar{1}\ 0\ 0]$ $\quad h(\mu) = -2\ d_{224}$

$t(\lambda) = \frac{1}{2}[1\bar{2}\bar{1}]$ $\quad h(\lambda) = -4\ d_{224}$

Different Step Heights, but same Burgers vector

C.M. Barr, E.Y. Chen, J.E. Nathaniel II, P. Lu, D.P. Adams, R. Dingreville, K. Hattar, D.L. Medlin, Submitted to Science Advances, 2022

Interfacial Dislocation Content

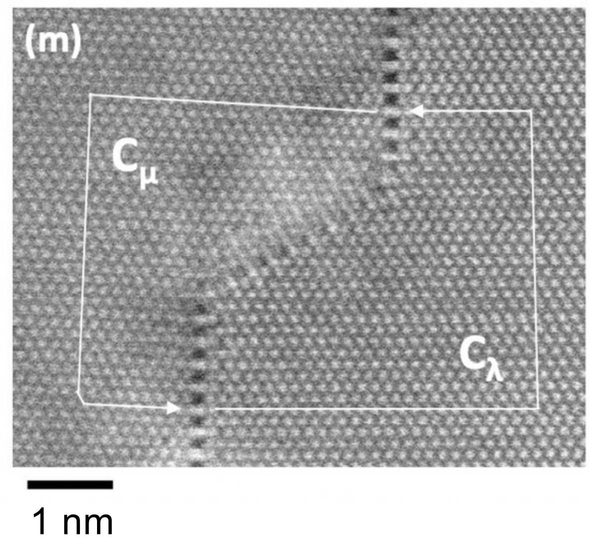
Circuit analyses at each disconnection and pair of facet junctions in pre-irradiated boundary

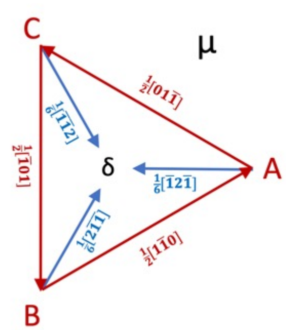
Circuit paths in two crystals

$$\boldsymbol{b} = -(\boldsymbol{C}_\lambda + \mathbf{P}\boldsymbol{C}_\mu)$$

Crystal coordinate transformation

$$\mathbf{P} = \frac{1}{3}\begin{pmatrix} -1 & 2 & 2 \\ 2 & -1 & 2 \\ 2 & 2 & -1 \end{pmatrix}$$





Dislocation and step content character

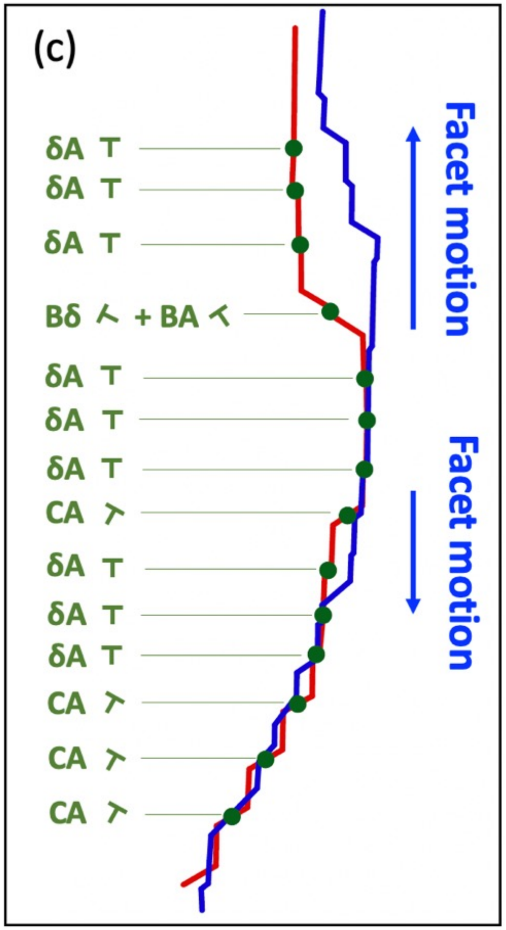
$$\boldsymbol{b} = \tfrac{1}{2}[0,-1,1] = \mathbf{CA}$$

$$h(\mu) = -27\, d_{224}$$

$$h(\lambda) = -30\, d_{224}$$

C.M. Barr, E.Y. Chen, J.E. Nathaniel II, P. Lu, D.P. Adams, R. Dingreville, K. Hattar, D.L. Medlin, Submitted to Science Advances, 2022

Defect distribution: Accommodates misorientation from Σ3



Misorientation from Σ3 : **3.2°± 0.1°** before and after irradiation

➔ **Net Burgers vector density remains constant**

Estimated misorientation based on dislocation distribution:

$$\theta \approx 2\sin^{-1}((b/L)/2) \approx 3.8°$$

approximating L as average vertical separation; b as normal component

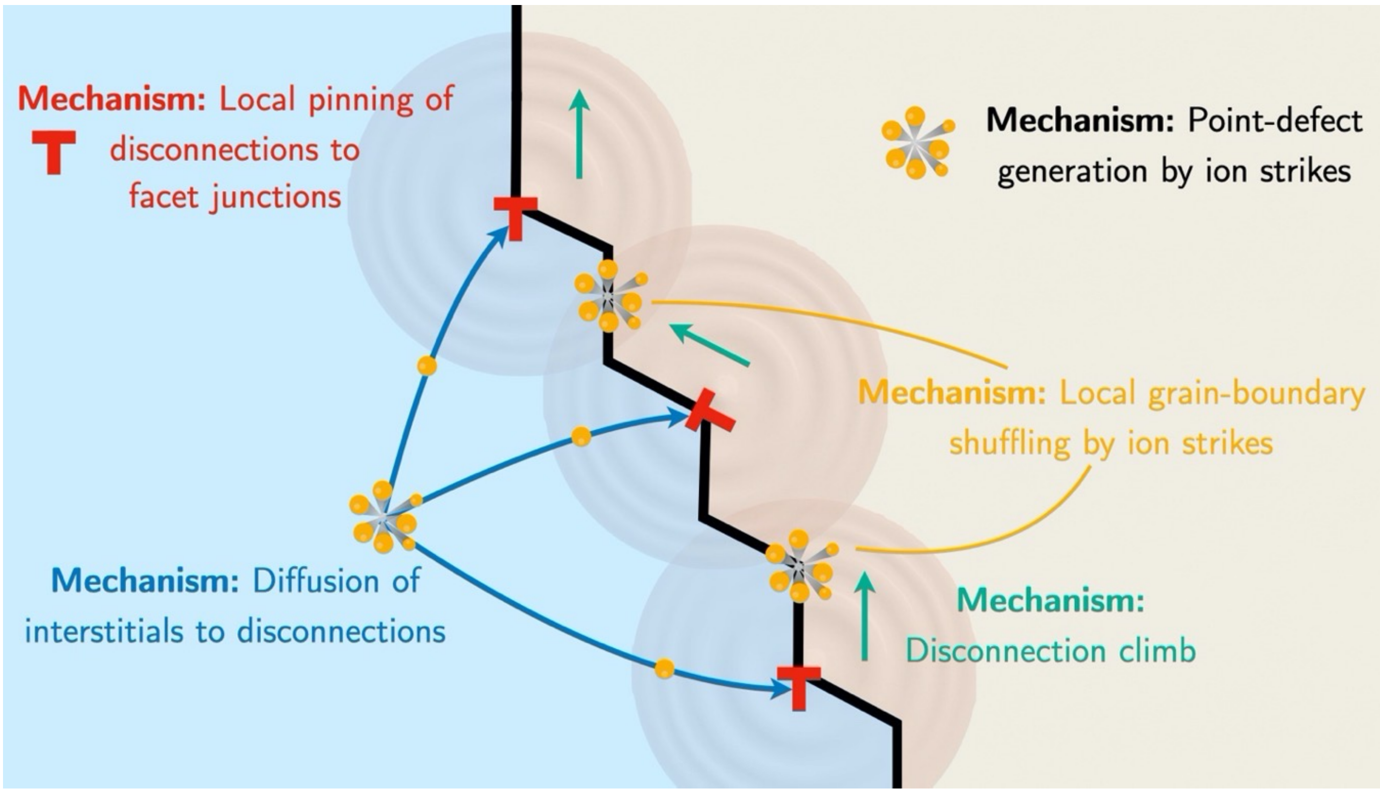
➔ **Coherency strains associated with misorientation being accommodated by disconnection distribution**

Every pair of junctions is associated with disconnection.

➔ **Localization of disconnections to facet junctions**

Orientation of Burgers vectors ➔ any net motion along facets is non-conservative (climb)

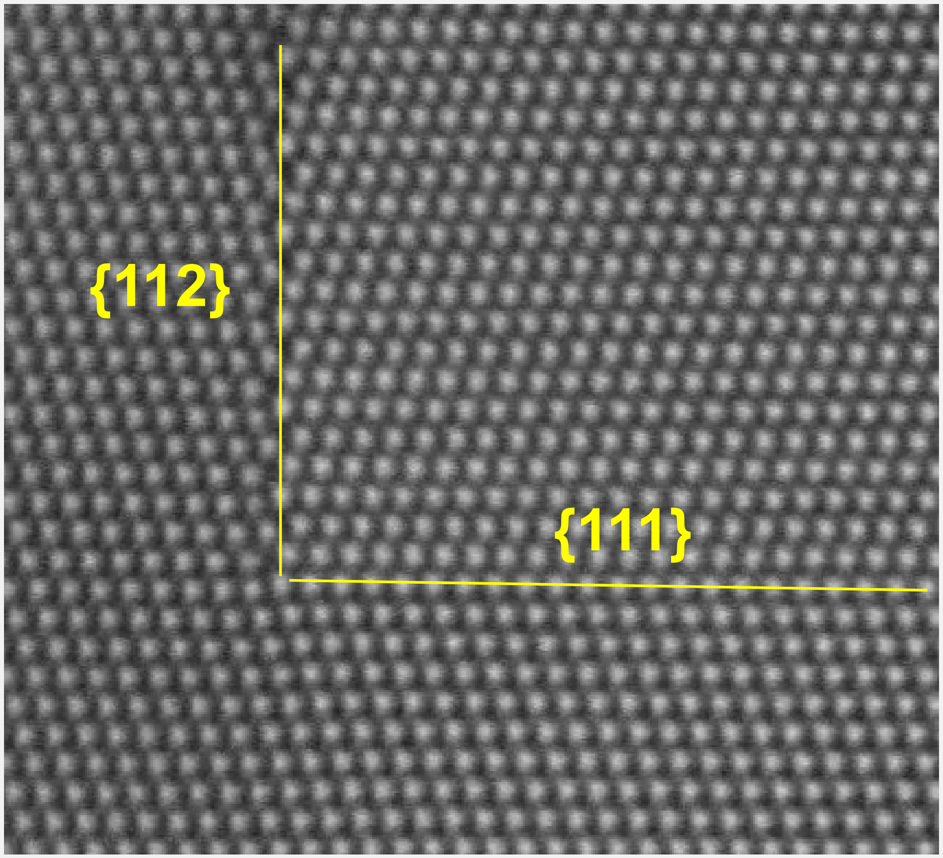
Summary: Coupled multi-scale mechanisms control grain boundary facet evolution under irradiation

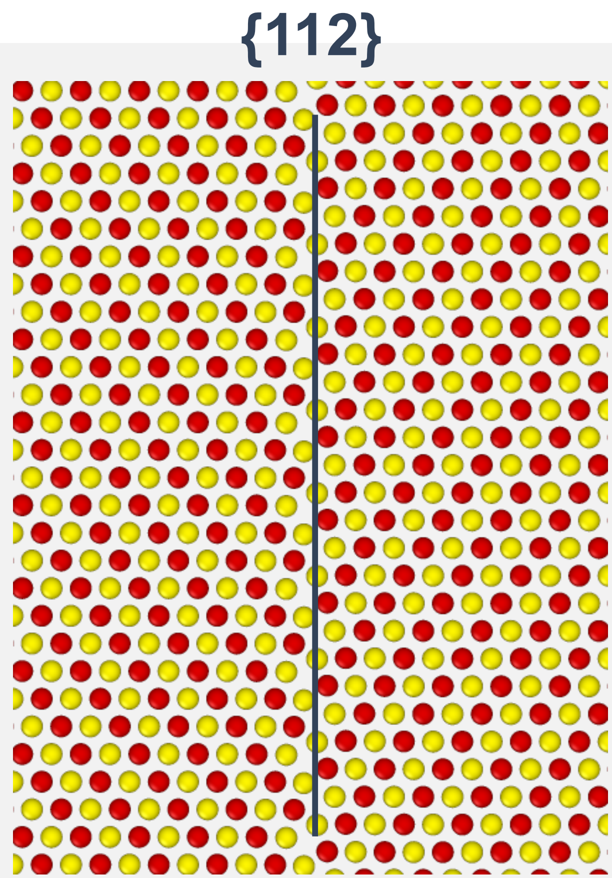


EXTRA

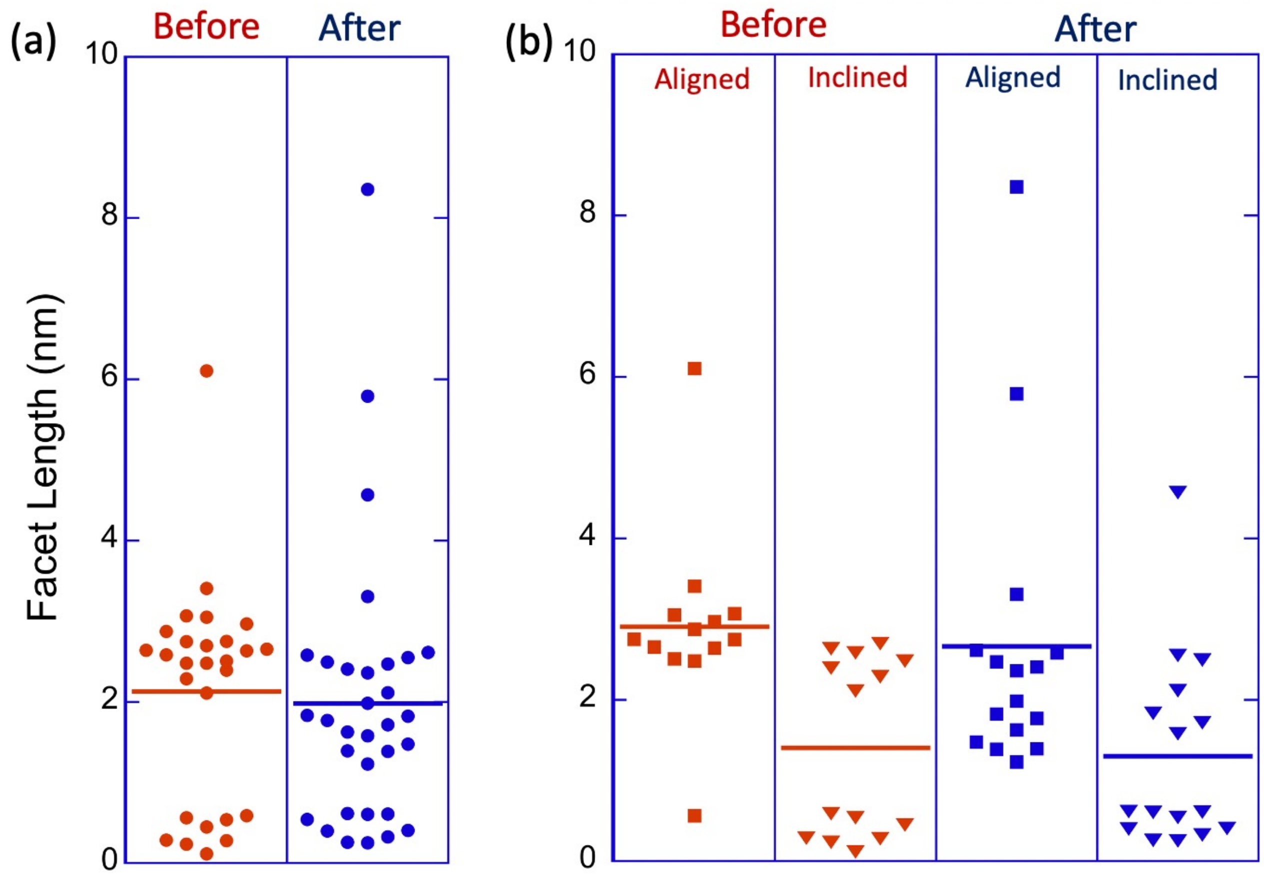
Σ3 Bicrystallography: Projection along <110>

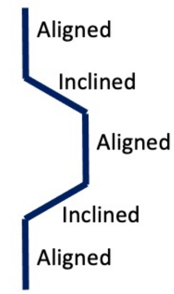
Example: HAADF-STEM Σ3 {111}/{112} facet junction in Au





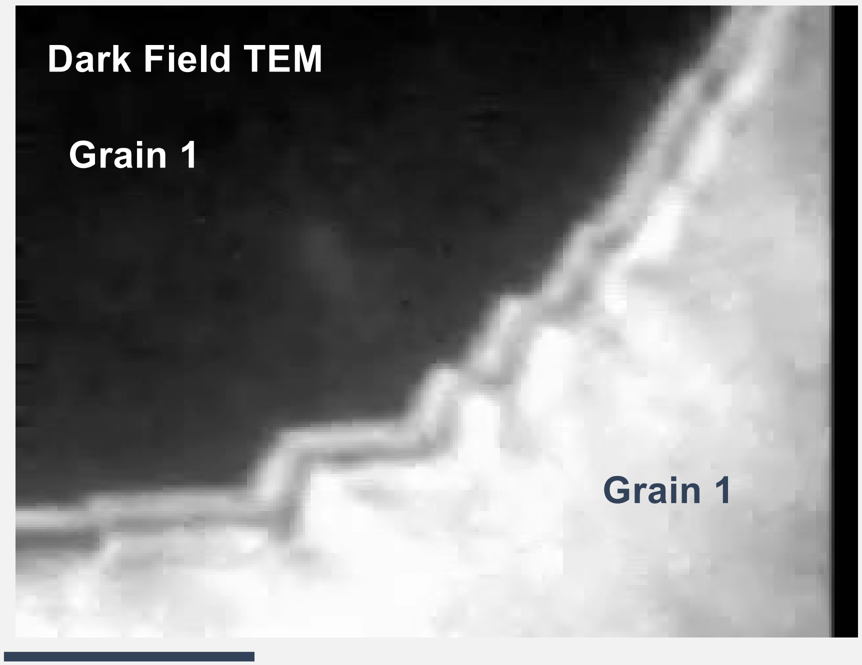
Irradiated Pt boundary: Facet Length Distribution





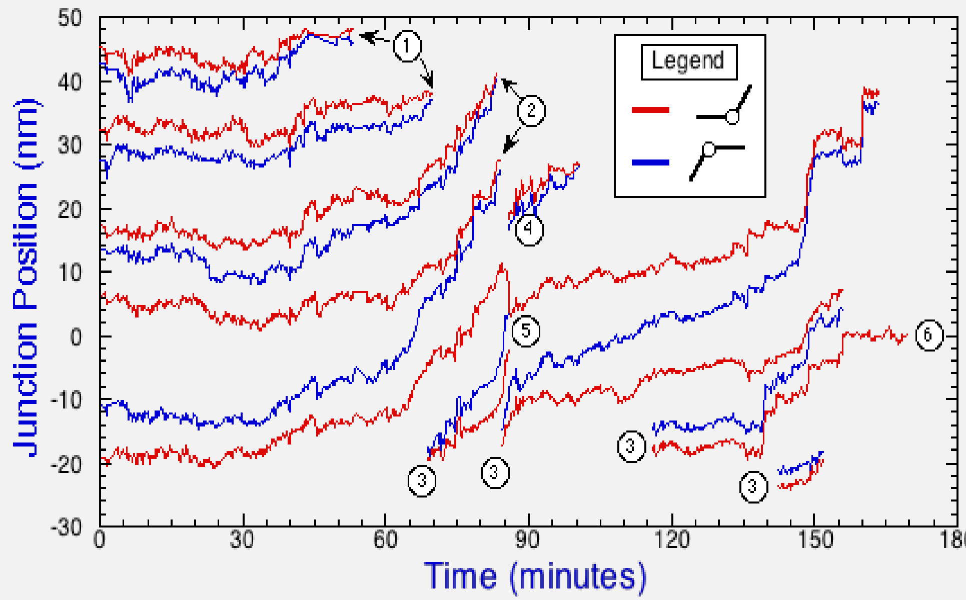
Thermal evolution: Coarsening of facet lengths

Example: Thermal Evolution of Σ3 {112} facets in Au



50 nm

T=490°C
185 minutes



- **Coordinated, biased motion**
- **Strain interactions:**
  GB dislocations at facet junctions

D.L. Medlin and G. Lucadamo, MRS Symp 252 (2001)