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Interfacial Line Defects:

Bridging Structural Information Between Atomic and Continuum Length Scales

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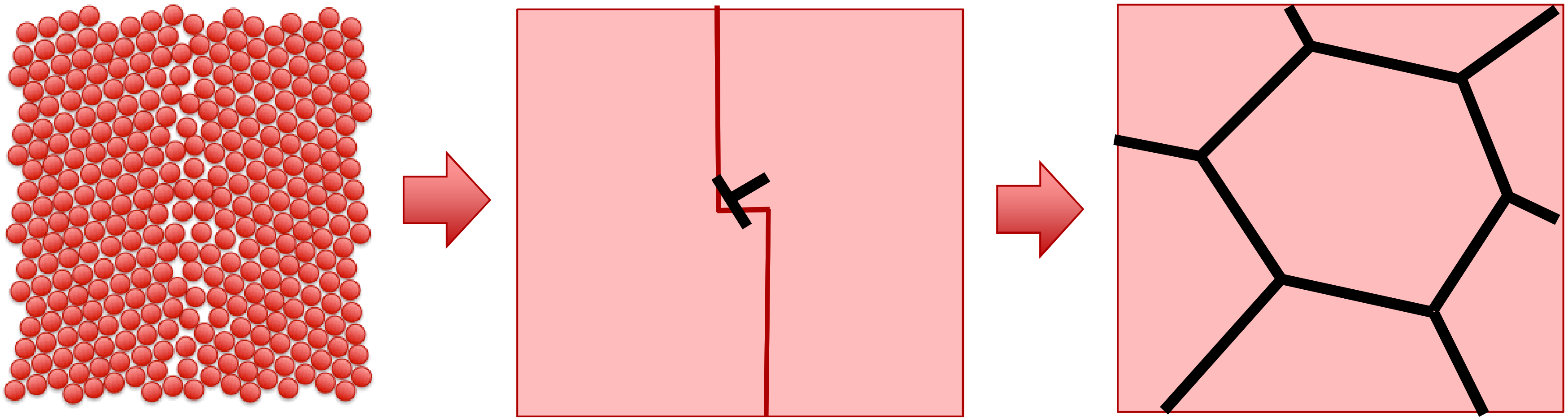
Interfacial Line Defects:
An important bridging concept



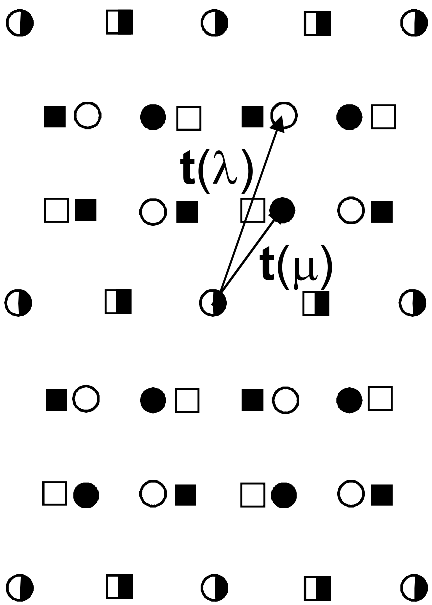
- Connection between details of atomic structure and larger-scale structure and behavior of interfaces.

- Essential to extending from specific boundaries to more general boundaries

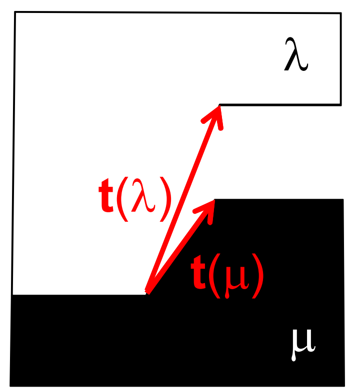
- Clues to essential physics and mechanisms controlling behavior and properties of interfaces.

In general interfacial line defects have both dislocation and step content

Dichromatic Pattern



Volterra Operation



$$t(\lambda) = \tfrac{1}{2}[1\bar{2}1]_{\lambda}$$

$$t(\mu) = \tfrac{1}{2}[101]_{\mu}$$

$$\mathbf{b} = \tfrac{1}{3}[1\bar{1}1]_{\lambda}$$

Crystal lattice translation vectors

$$\mathbf{b}_{ij}=\mathbf{t}(\lambda)_{ij}-\mathbf{P}\ \mathbf{t}(\mu)_{ij}$$

Burgers vectors of the set of "admissible" defects

Matrix converts from μ to λ crystal coordinates

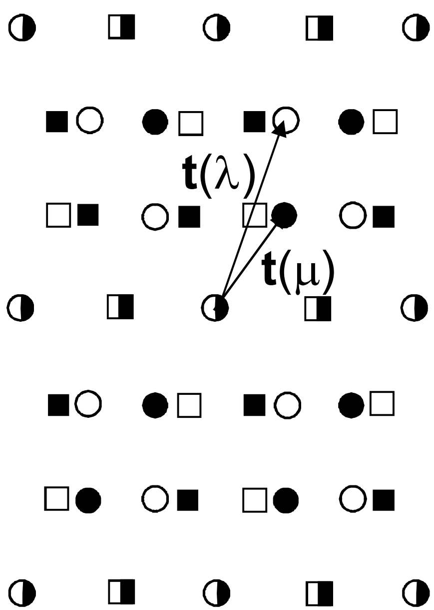
"disconnection" :
both step and dislocation content

Definition of a physically meaningful reference state is critical.

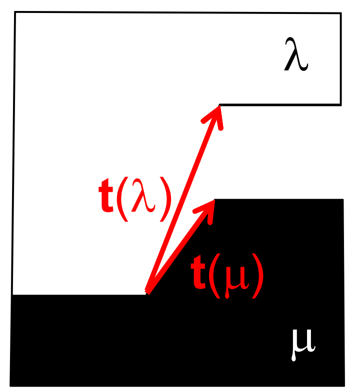
R.C. Pond, Dislocations in Solids, Chapter 38 (1989)
J. Hirth & R.C. Pond, Acta Materialia (1996)

In general interfacial line defects have both dislocation and step content

Dichromatic Pattern



Volterra Operation

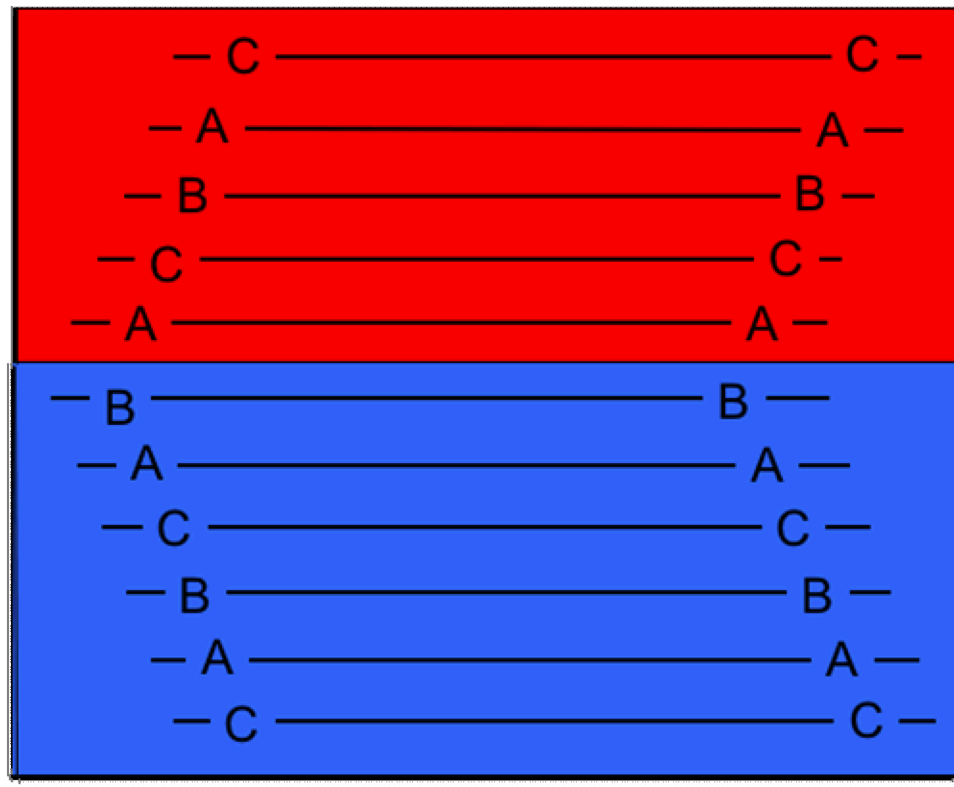


$$t(\lambda) = \tfrac{1}{2}[1\bar{2}1]_\lambda$$

$$t(\mu) = \tfrac{1}{2}[101]_\mu$$

$$\mathbf{b} = \tfrac{1}{3}[1\bar{1}1]_\lambda$$

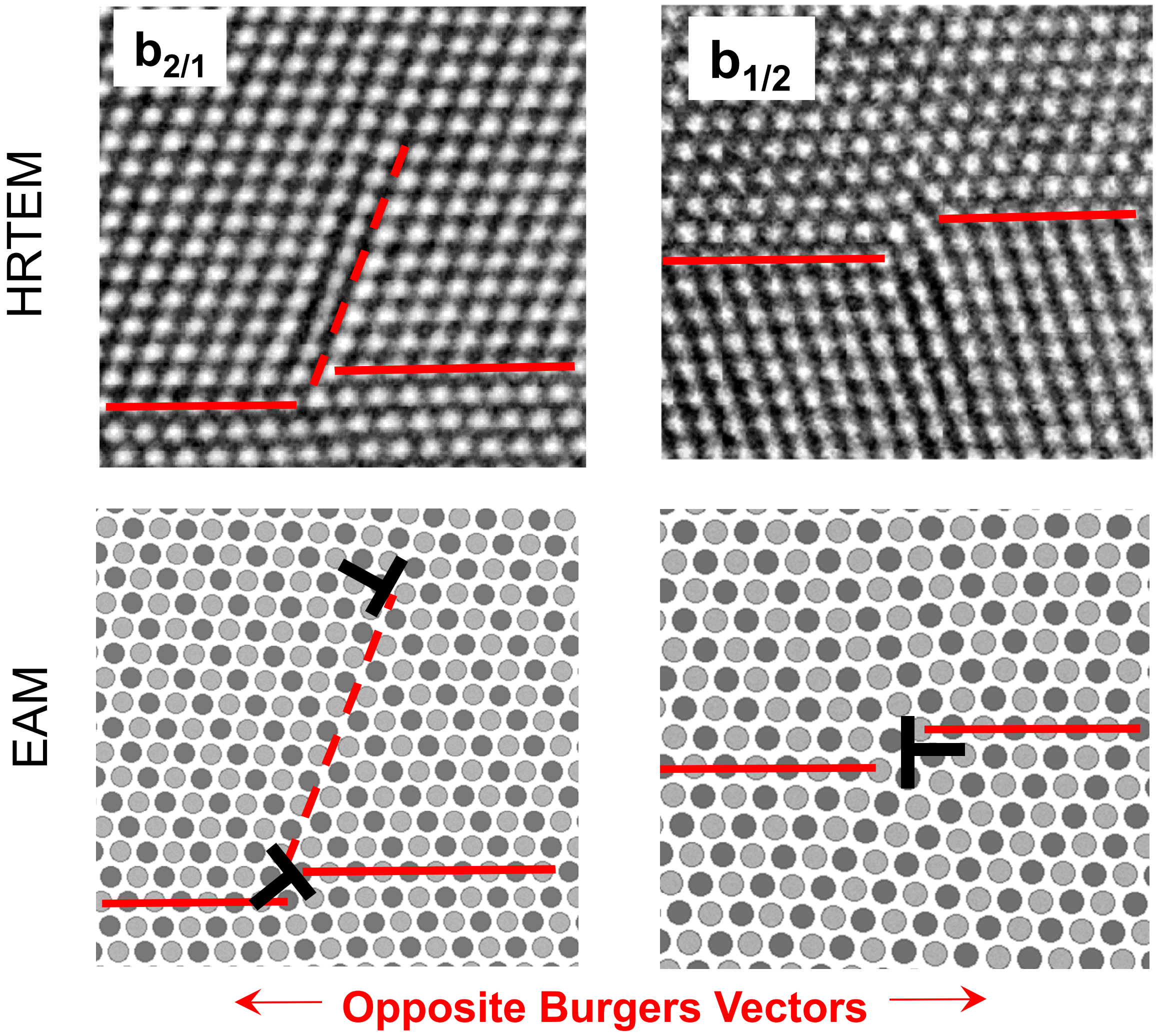
Example: (1/3)<111> disconnection:
FCC {111} twin boundary (Σ=3)



"disconnection" :
both step and dislocation content

R.C. Pond, Dislocations in Solids, Chapter 38 (1989)
J. Hirth & R.C. Pond, Acta Materialia (1996)

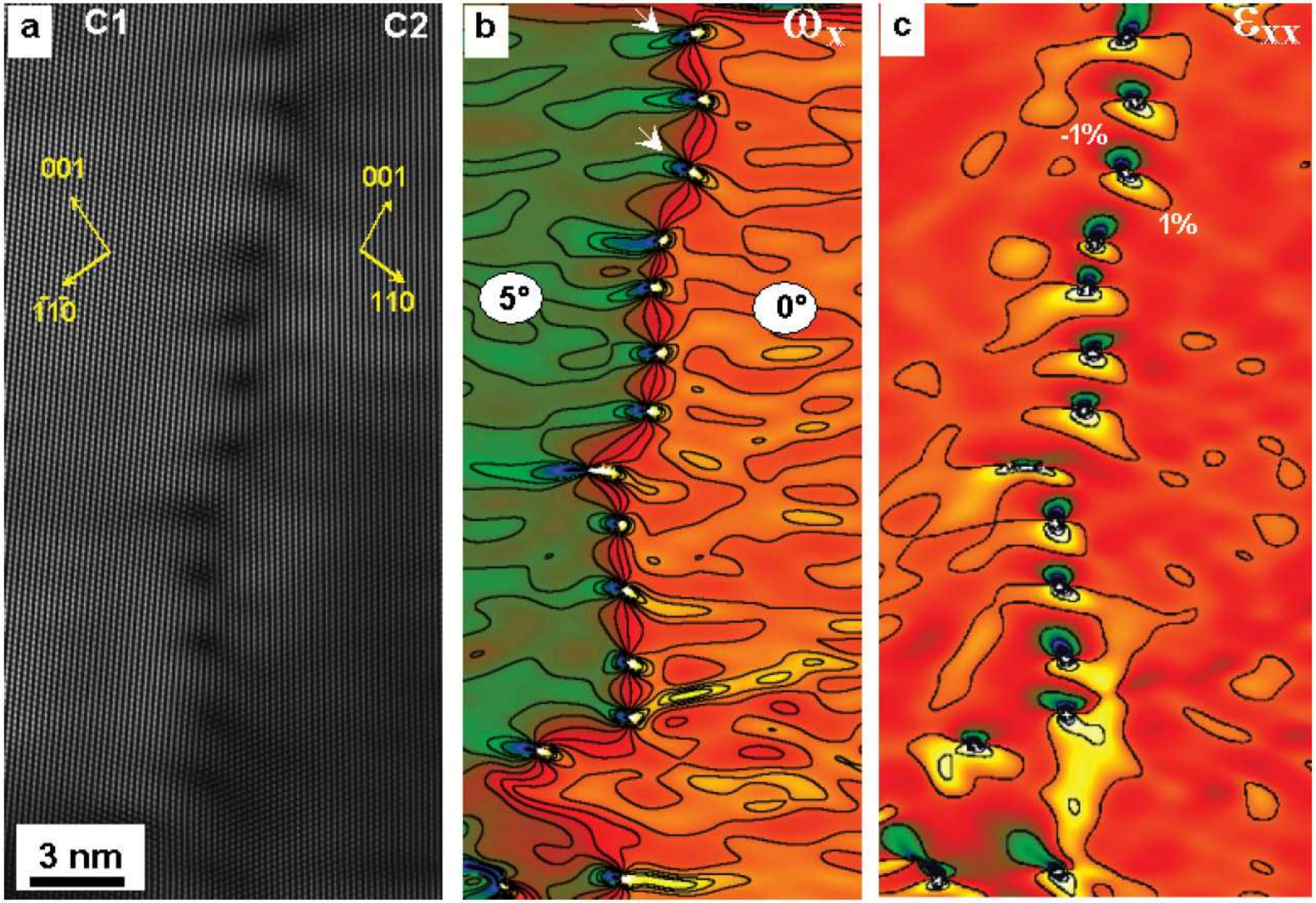
(1/3) <111> Disconnection at twin in Au: Core-relaxation by stacking fault emission



- Interface breaks symmetry of dislocation.
- $b_{2/1}$ reduces strain energy by dissociating into Shockley and stair rod dislocations.
- $b_{1/2}$ disconnection cannot dissociate without creating unfavorable "AA" stacking.

E.A. Marquis and D.L. Medlin, Phil. Mag. Letters (2005).

(1/3)<111> dislocations accommodating misorientation at Σ=3 twin boundary



Deformed Ultra Fine Grained (UFG) Copper

HRTEM Strain analysis from Geometric Phase Analysis (GPA)

M. Sennour,S. Lartigue-Korinek, Y. Champion, M.J. Hÿtch, Phil Mag (2007)

Grain Boundary Structural Transition: dissociation of (1/3)<111> disconnections with compact core

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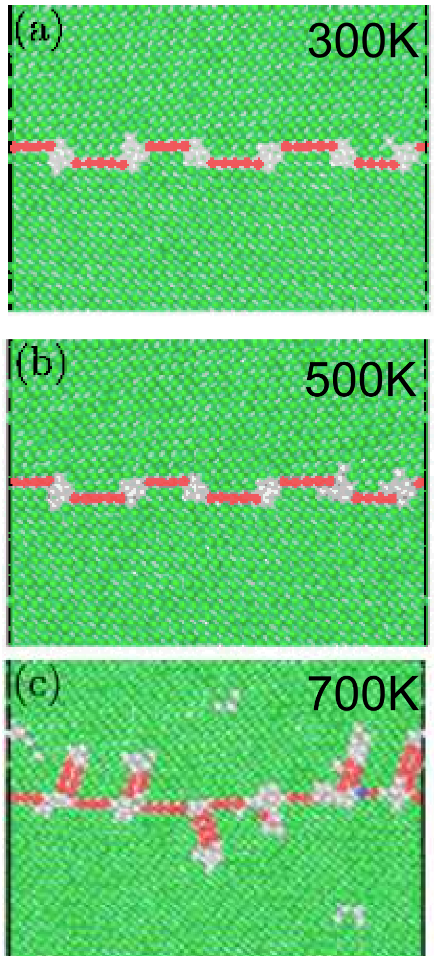
(1/3)<111> Disconnections
Δθ=+8.98° from exact Σ=3

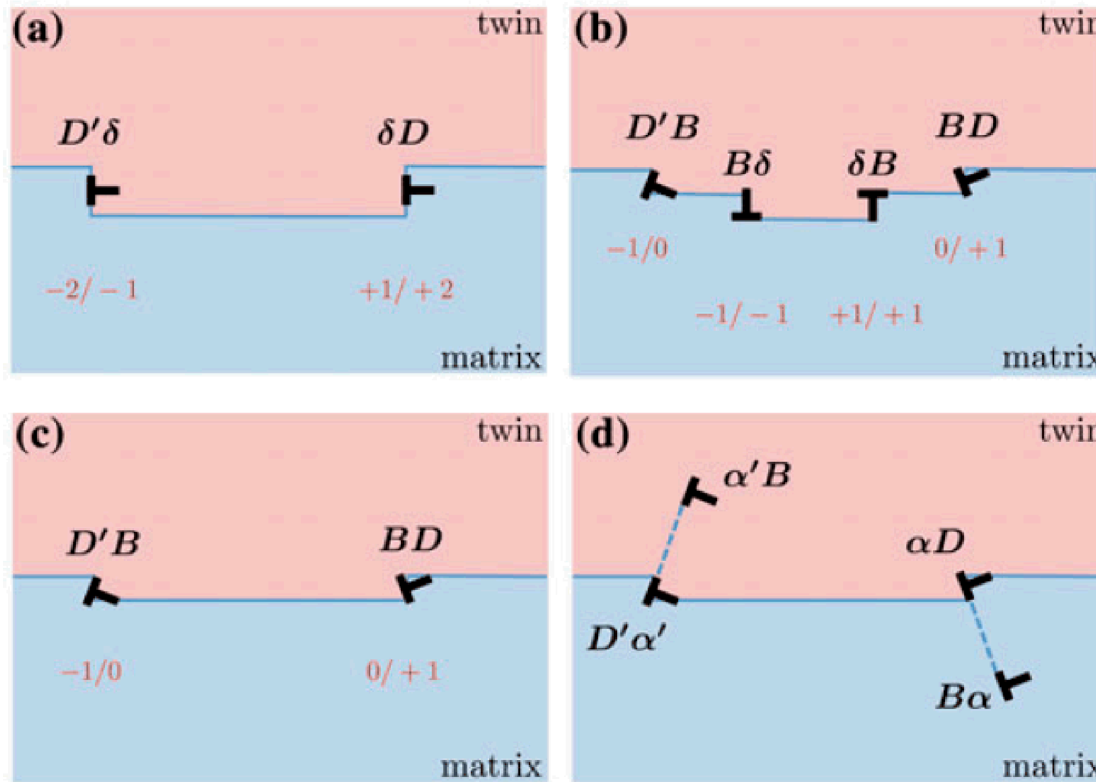
GB Free Energy vs Misorientation from Σ=3
Transition Mechanism:
(Nickel, EAM)
900 300 K 700 K

(1/3)<111> disconnections emit oppositely signed (1/6)<112> disconnections on twin terraces

Compact Core



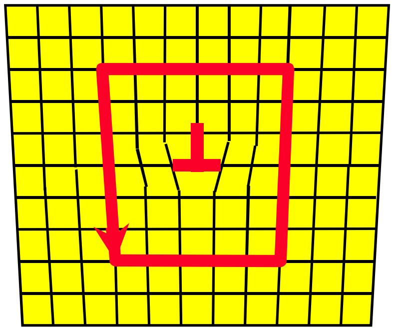
Dissociated

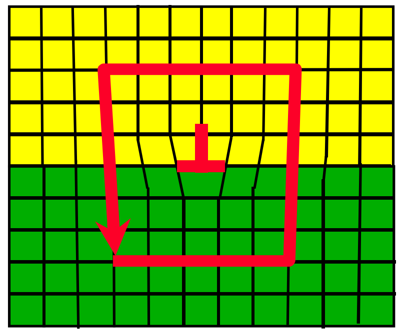


C.J. O'Brien, D.L. Medlin, S.M. Foiles, Philosophical Magazine (2016)

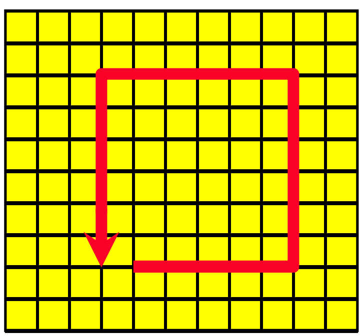
Misfit Dislocations: topological analysis in *coherent* reference frame

Bulk Lattice Dislocation. Heteroepitaxial Misfit Dislocation.

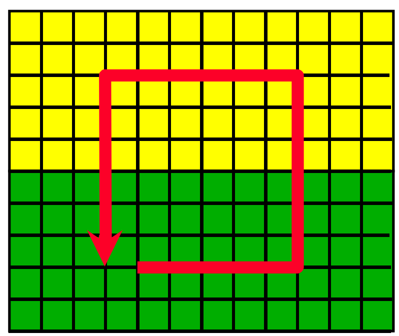




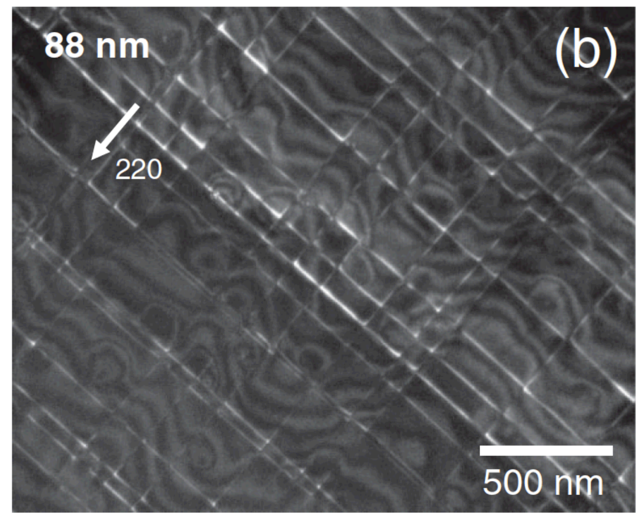
Reference Frame:
Perfect Crystal



Reference Frame:
Coherently Strained Interface



Example: Misfit dislocations $Si/Si_{0.8}Ge_{0.2}$ interface (Plan-view TEM)

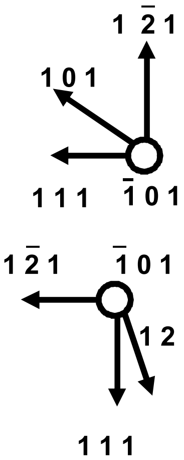


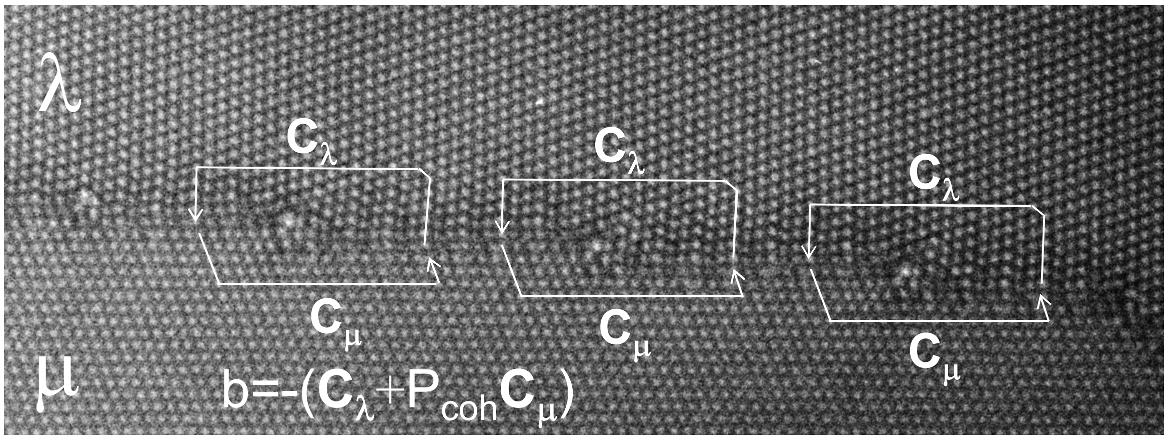
Cheaito, Duda, Beechem, Hattar,Ihlefeld, Medlin, Rodriguez, Campion, Piekos, Hopkins, Phys. Rev. Letts., **109**, 195901 (2012)

Equilibrium density of misfit dislocations cancels the long range coherency strain

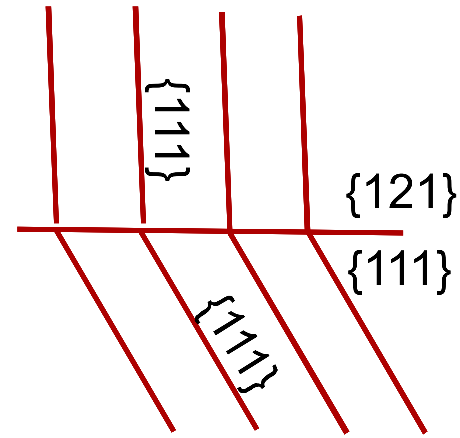
Accomodation of Grain Boundary Coherency Strain by Disconnections

90° Boundary in Gold





5.7% strain across terraces



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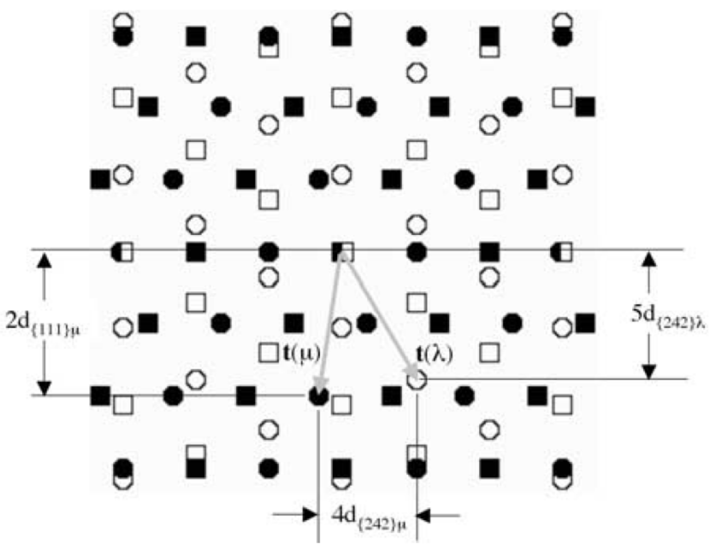

- P_{coh} describes 90° crystal rotation and strain to bring λ and μ into coherency.
- Defects efficiently accommodate the 5.7% misfit on the {111}/{112} facets.
- Nearest CSL is Σ=99

D.L. Medlin, D. Cohen, and R.C. Pond, Phil. Mag. Letts. (2003).

Disconnections in Phase Transformations

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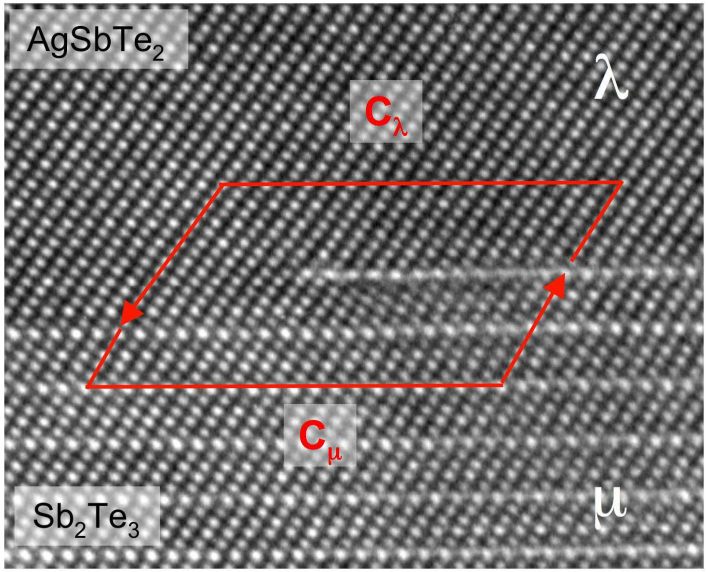
Example: Sb_2Te_3 precipitate in $AgSbTe_2$ thermoelectric

Burgers vector:



Upper crystal circuit

Lower crystal circuit

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

-Coordinate Transformation from Tetradymite to Rock-salt.

-Coherently strained reference frame

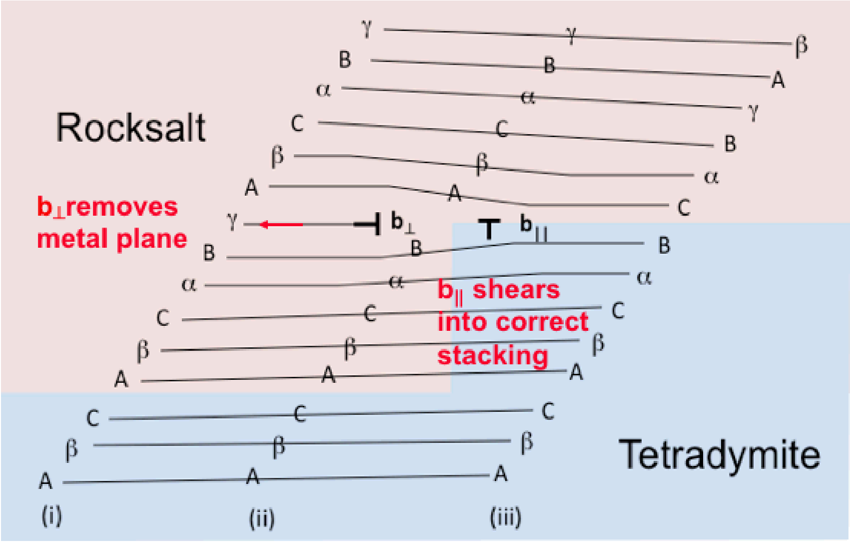
Resolve b into components normal and parallel to interface

$$\mathbf{b}_n = (a_{cub} - c_{hex}/3\sqrt{3})[111]$$

- ***mismatch of step heights.***
- ***$|b_n|=0.3747Å$***

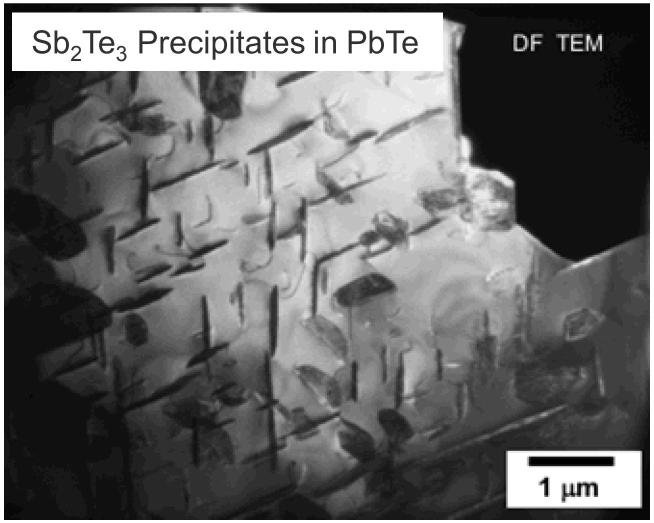
$$\mathbf{b}_{||} = \frac{a_{cub}}{6}[\bar{1}2\bar{1}]$$

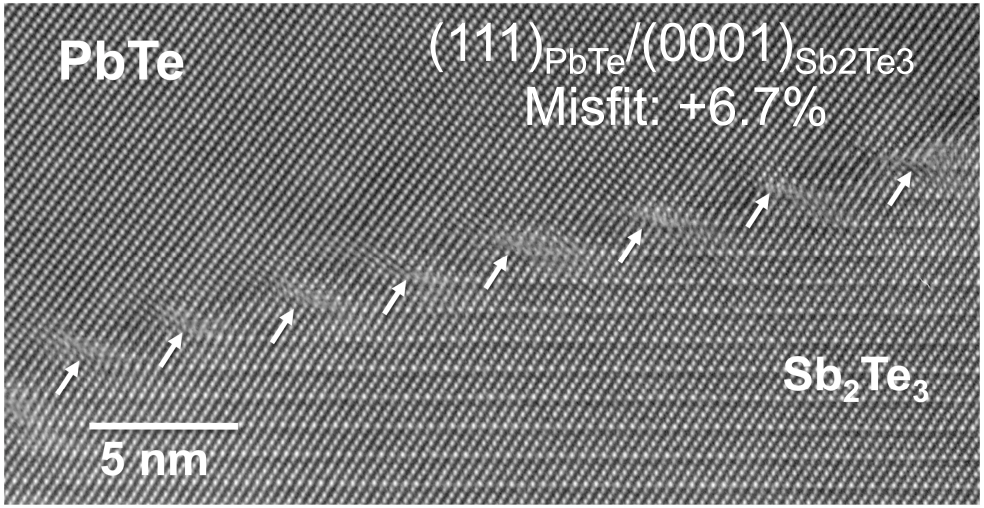
- ***Analogous to Shockley partial Dislocation***
- ***$|b_{||}|=2.48Å$***

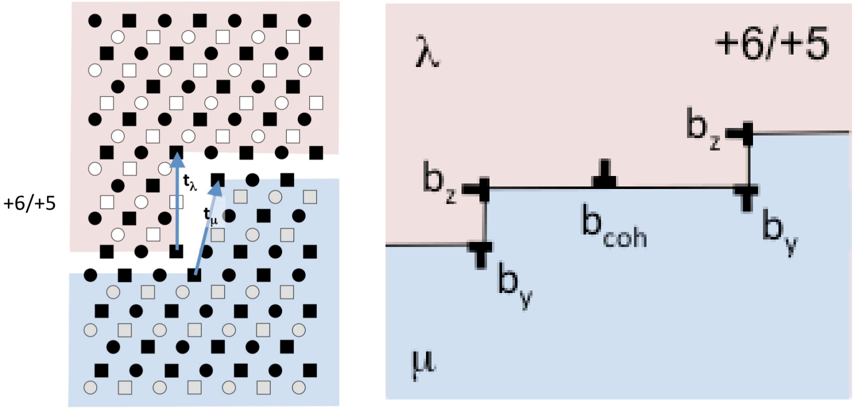


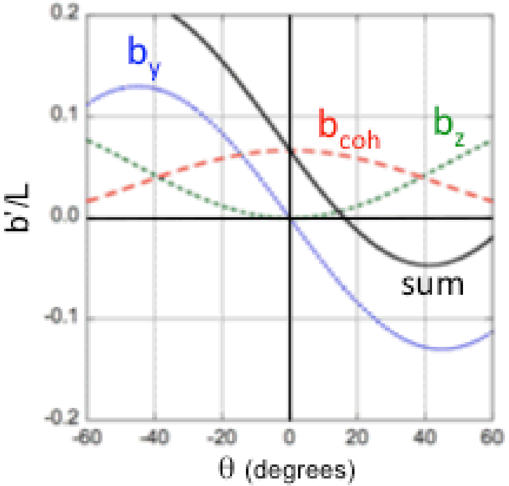
Medlin and Sugar, Scripta Materialia, 2010.

A system with larger misfit: $PbTe/Sb_2Te_3$







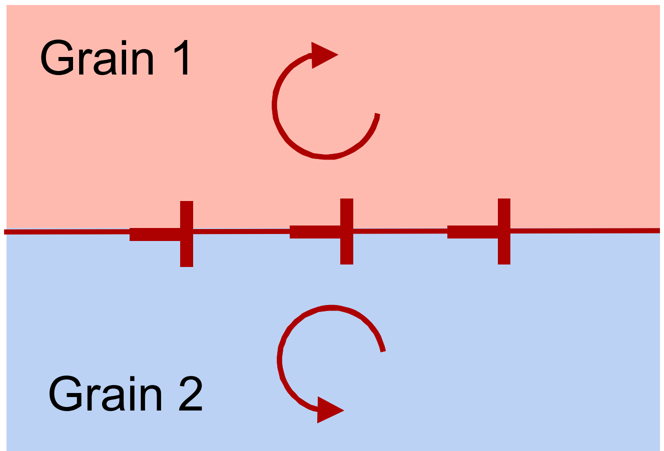


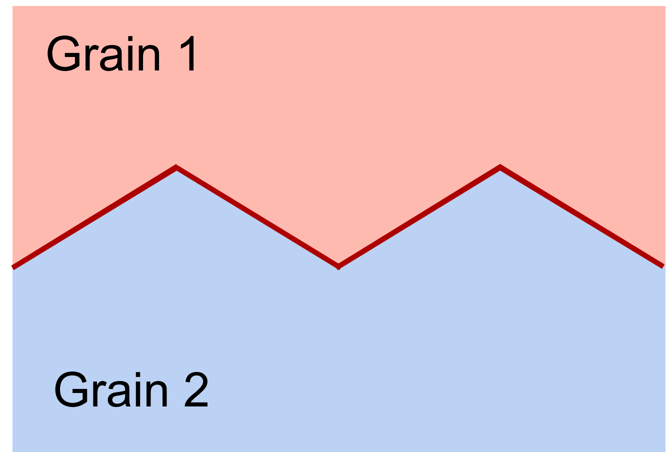
<u>Habit plane inclination:</u>

Measured: 14.8°
Predicted: 16.2°

Defect spacing accommodates the (111)/(0001) coherency strain.

Facet Junctions and Grain Boundary Dislocations: Accommodating deviations from low energy interfaces





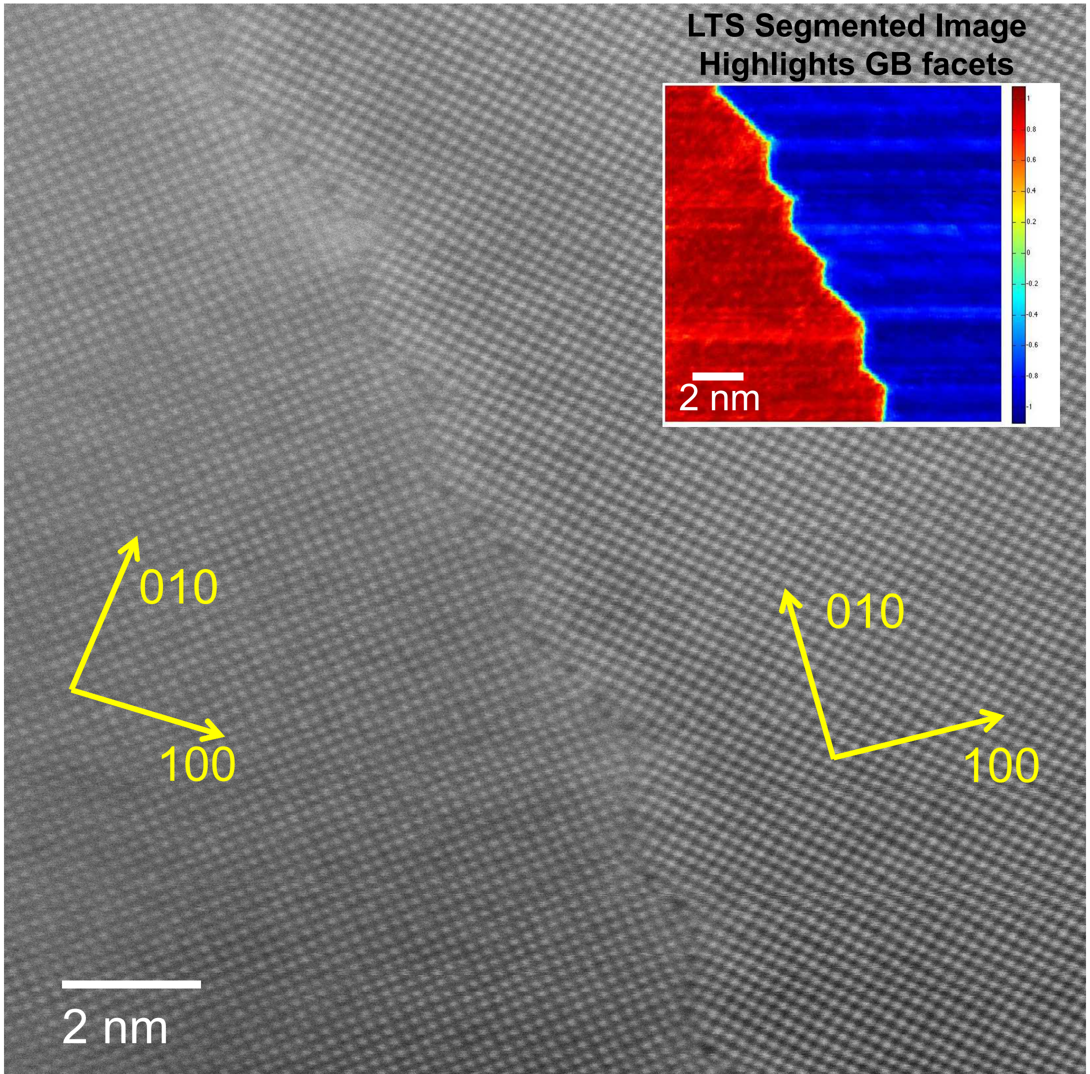
- **Misorientation:**
  - **-Accomodate deviation with grain boundary dislocations**

- **Inclination:**
  - **-Reduce energy by faceting on lower energy planes**
  - **-Facet junctions.**

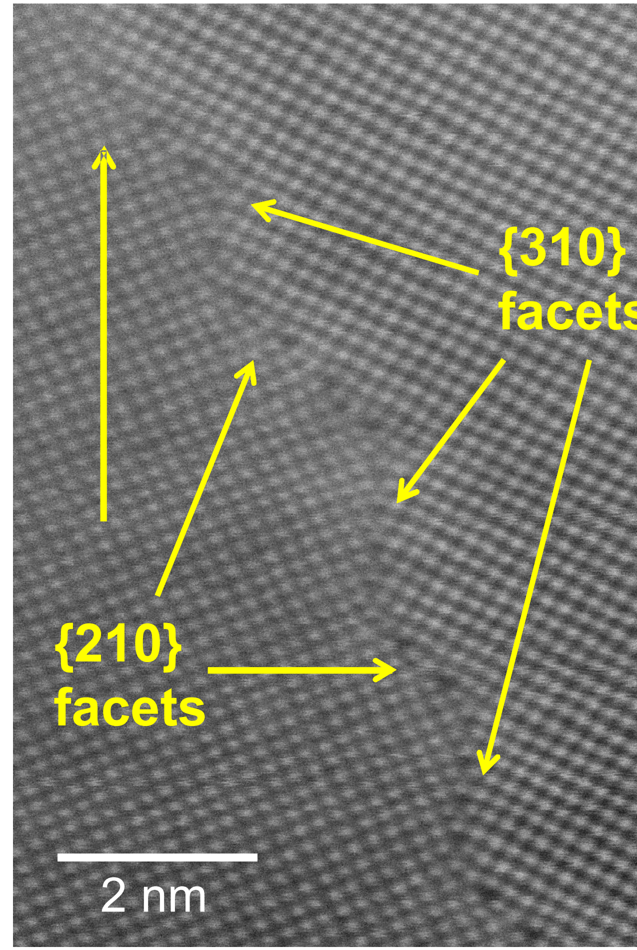
Interaction of grain boundary dislocation and facet junctions?

HRSTEM shows nanoscale faceting at Grain boundary

HAADF-STEM Σ=5 <001> Boundary in Fe



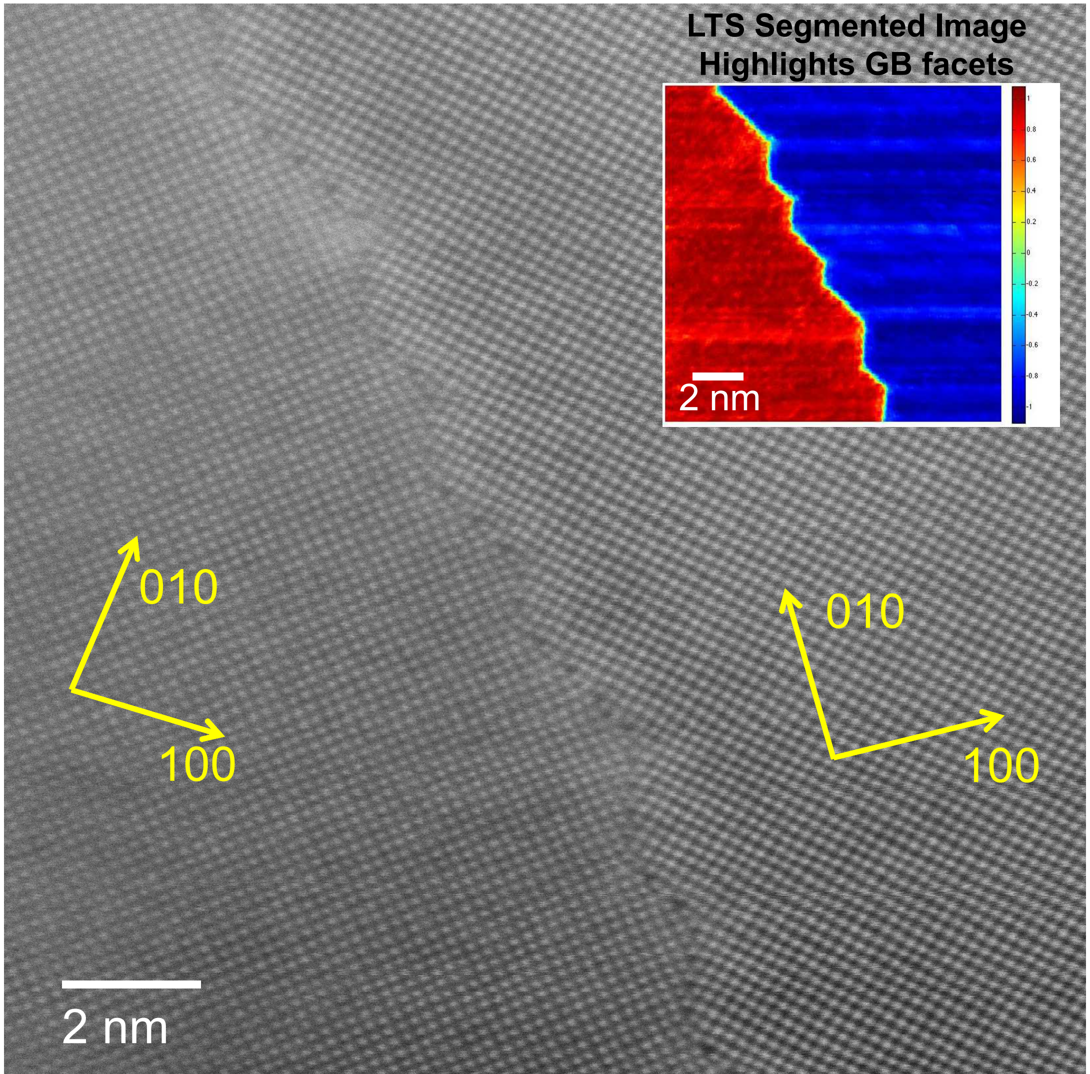
Boundary is faceted on
{210} and {310} type inclinations



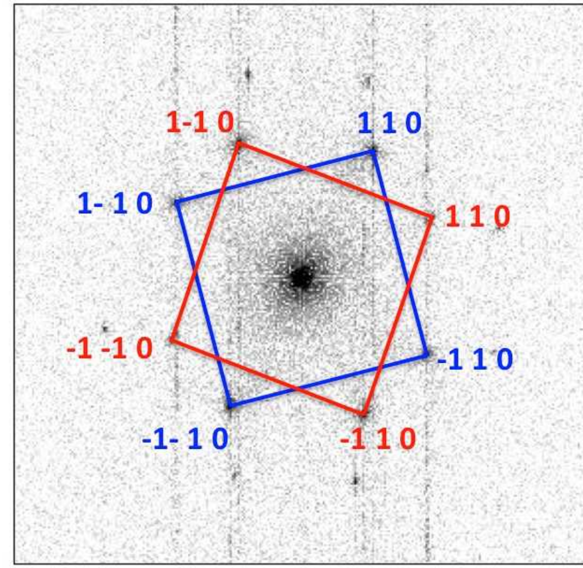
Pulsed Laser Deposited Fe on Rocksalt (NaCl).
36 nm thickness. Specimen released and annealed on Mo grid 675°C, 2 hours, under vacuum

HRSTEM shows nanoscale faceting at Grain boundary

HAADF-STEM Σ=5 <001> Boundary in Fe



Boundary Geometry



Inclination from {310}:
ϕ = 26.3° ± 1°

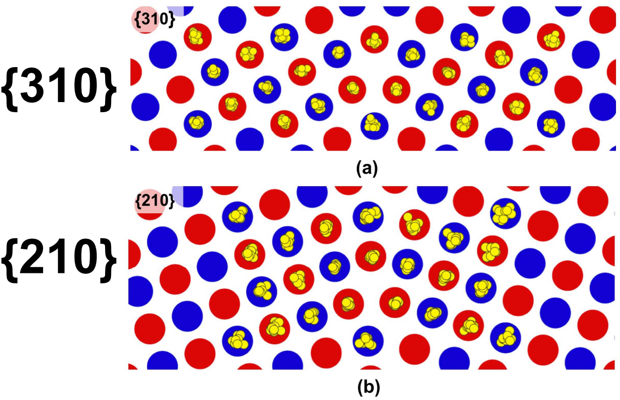
Misorientation:
θ=34.49 ± 0.75°

$\Delta\theta$ = -2.38 ± 0.75°
from exact Σ=5

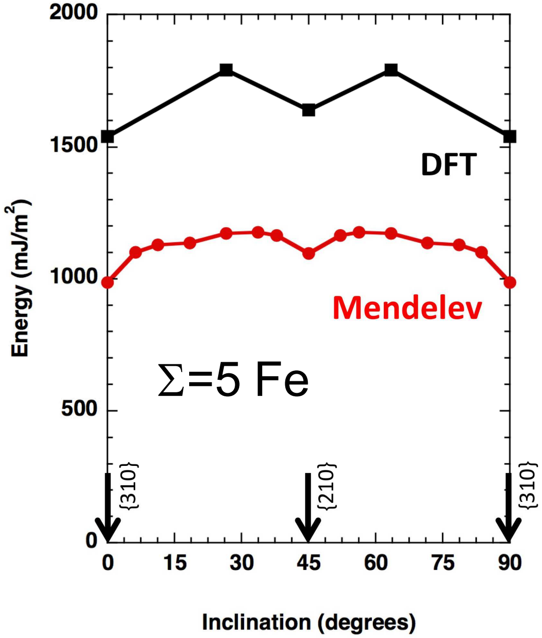
Medlin, Hattar, Zimmerman, Abdeljawad, Foiles, Acta Materialia (2017)

Energetics predict growth of {210} and {310} facets

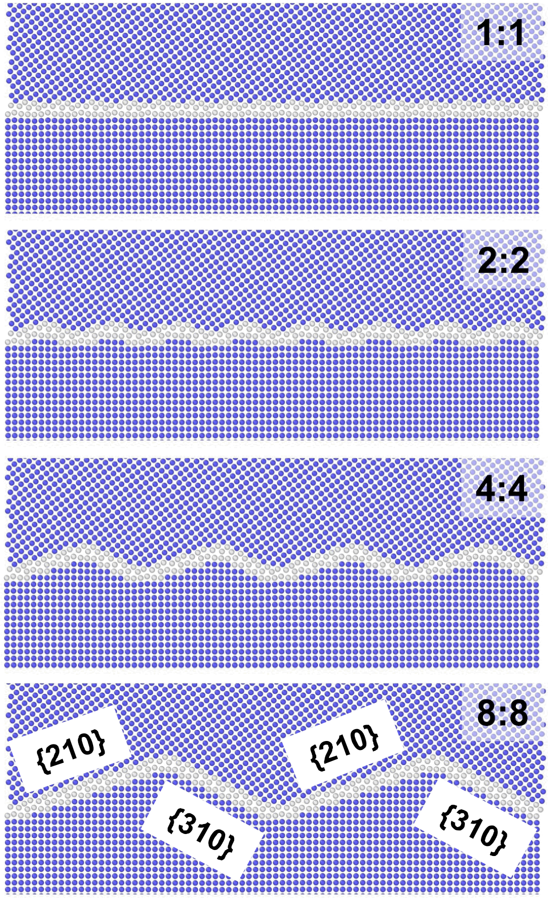
Atomistic Simulation
(HAADF-STEM peak positions overlaid)

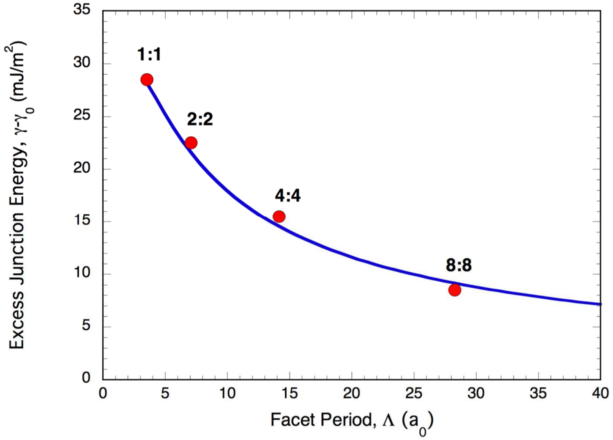


Energy vs Boundary Inclination



Reduction of Energy with Facet Coarsening



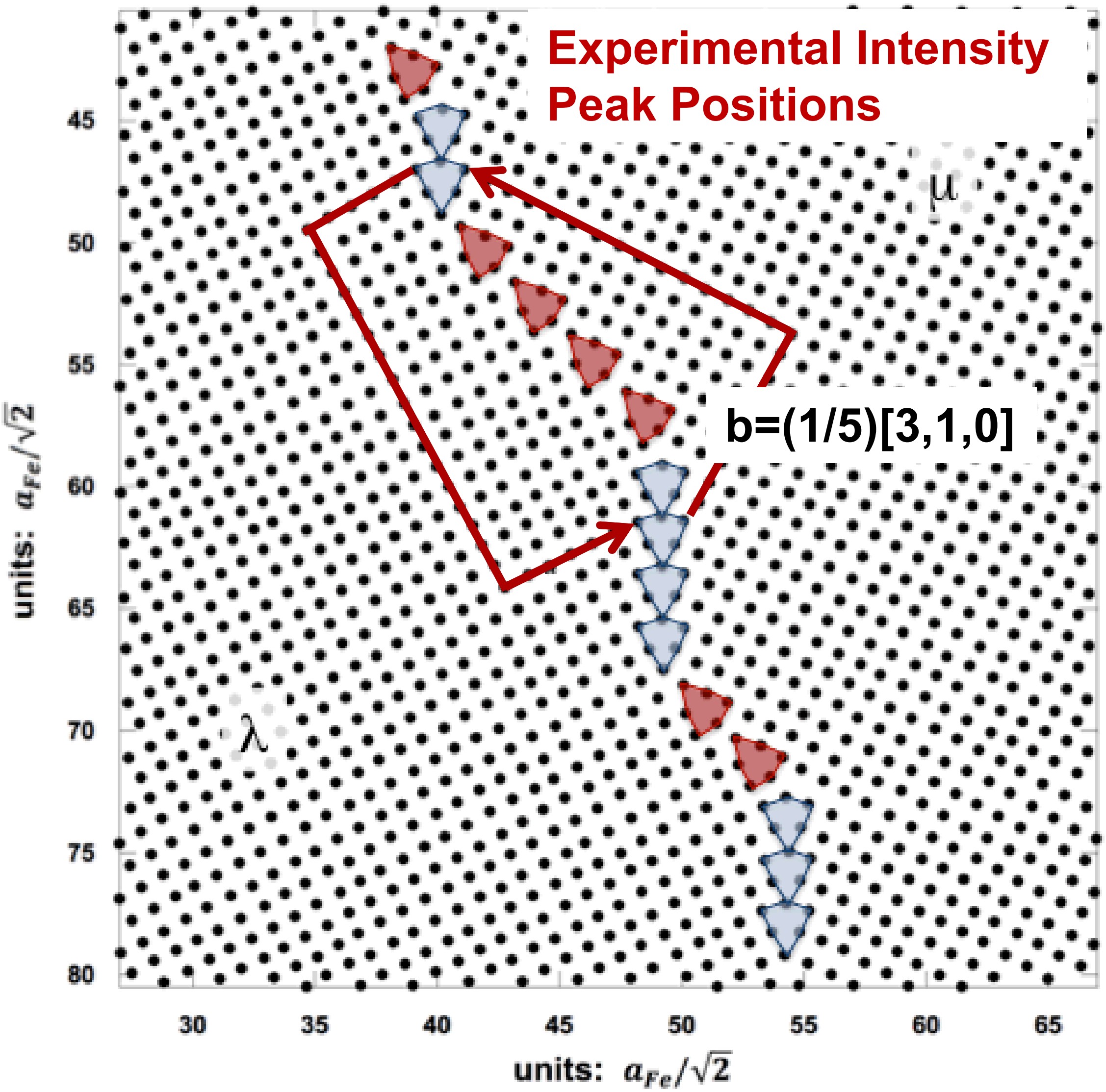


$$(\gamma - \gamma_0) = (C_1/\Lambda)\ln\Lambda + C_2/\Lambda$$

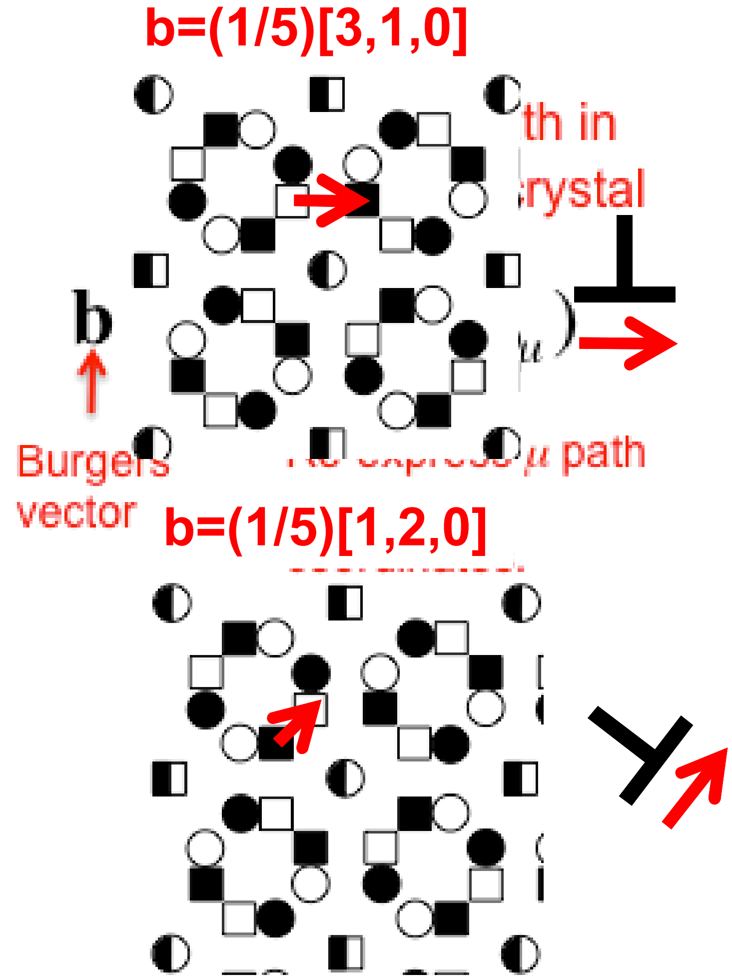
Stable facets only for $C_1 < 0$

fit: C_1=+76.55 mJ/m^2
C_2=+2.94 mJ/m^2

Circuit Mapping: Grain Boundary Disconnections at all Facet Junction Pairs



Two types of defect observed:



Defect spacing accounts for misorientation and boundary inclination

Observed SGBD Density Accommodates Deviation from Exact Σ=5 Misorientation

Dislocation Content Required is function of both Misorientation *and* Inclination

Frank-Bilby Equation:

b-vector density → $\mathbf{B}=(\mathbf{I}-\mathbf{P}^{-1})\mathbf{v}$ ← Interface vector, defining inclination

Matrix defining misorientation from reference

Predicted Burgers Vector Density:

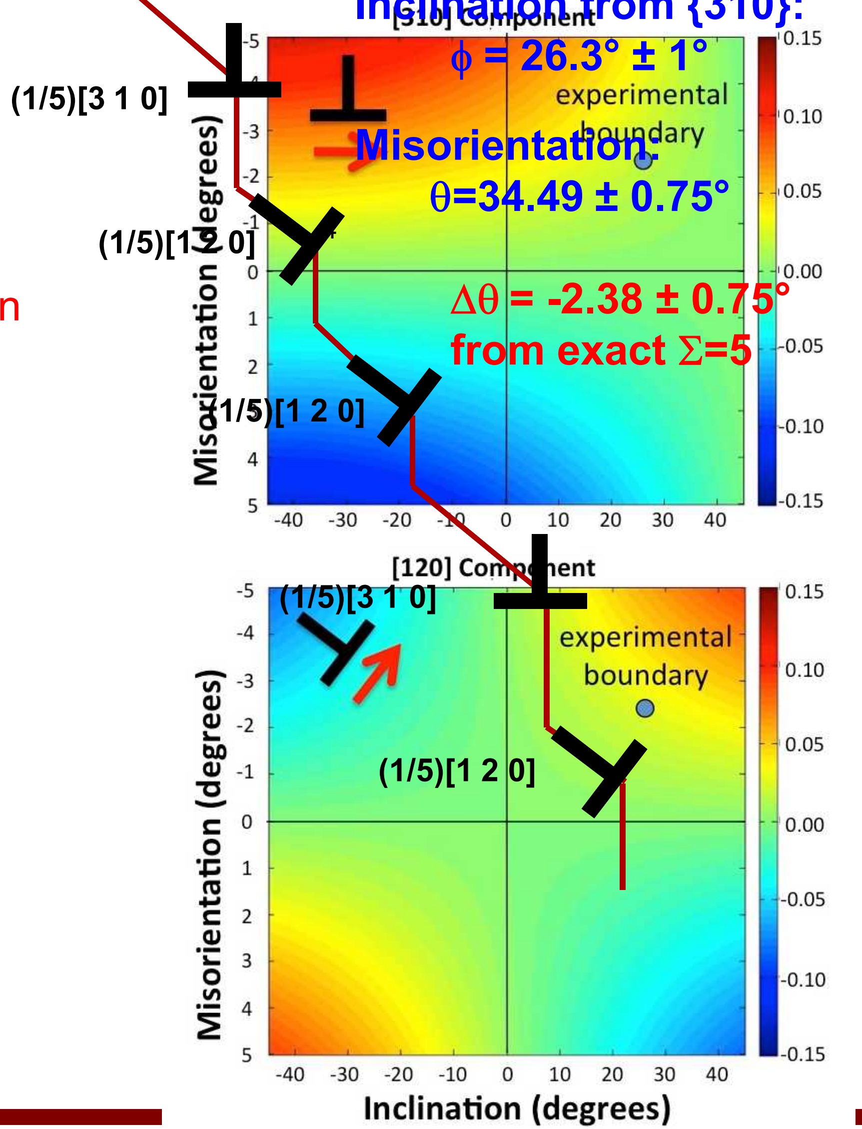
B=[0.029 ± 0.010, 0.030 ± 0.010, 0]

Observed Burgers Vector Density:

B=[0.030 ± 0.002, 0.027 ± 0.002, 0]
(b per unit length of boundary)

Coupling of SGBDs and junctions dictates the facet length scale

Burgers Vector Density from Frank-Bilby Equation



Conclusions

Rich set of phenomena associated with interfacial line defects

-Strain accomodation.
-Interfacial motion
-Phase transformation.
-Interfacial properties.

Interfacial defect crystallography provides a framework for evaluating and interpreting complex interfacial structures.

-Determining interfacial mechanisms.
-Informing and guiding modeling.

Collaborators

Sandia National Laboratories

J. Hamilton
E.A. Marquis (now Univ. Michigan)
D. Cohen
J.D. Sugar
S.M. Foiles

J. Zimmerman
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University of Exeter

R.C. Pond

California Institute of Technology

J. Snyder (now Northwestern University)
N. Heinz
T. Ikeda (now Ibaraki University)

Acknowledgement

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EXTRA

Grain Boundaries: Lattice Dislocation Description limited by overlap of defect cores

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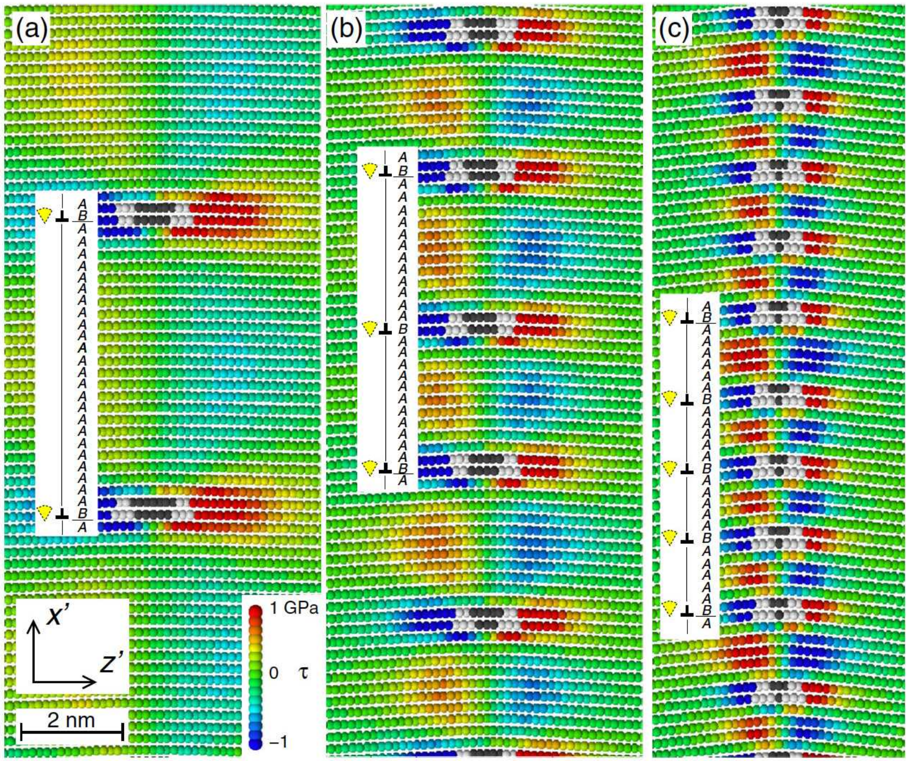
Example: Atomistic simulations LAGB in Al

θ=2.81° θ=5.61° θ=11.91°

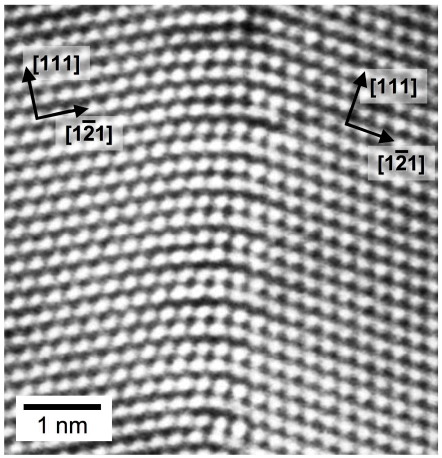


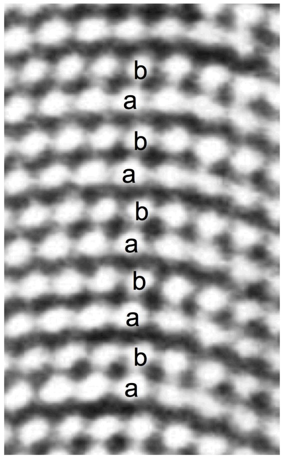
T. Shimokawa, PRB (2010)

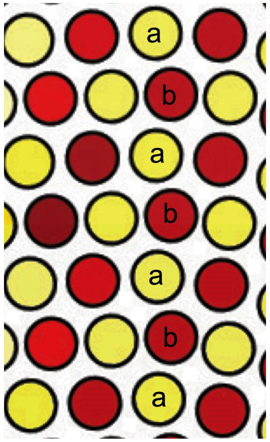
Low Angle Grain Boundary cut-off typically between 5° and 15°

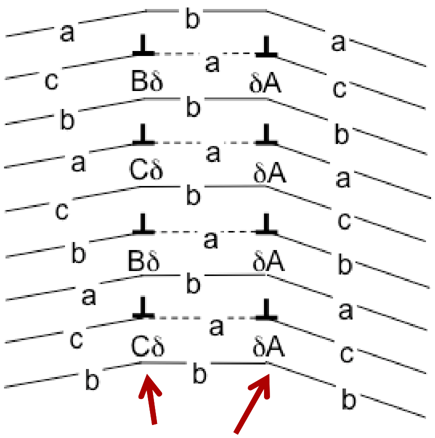
Example: HCP Stacking at Au GB

θ=29°: Dislocations separated by 1 atomic plane







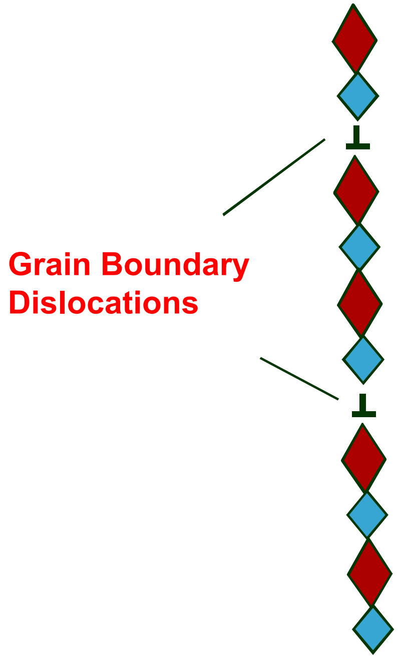


Medlin & Hamilton, J. Mat Sci 2009.

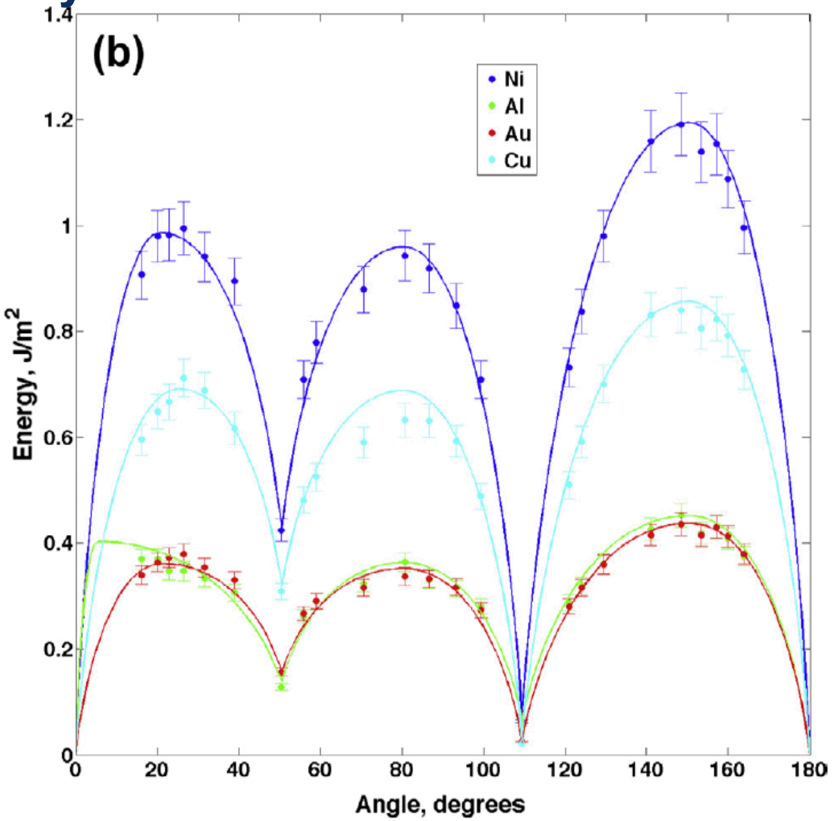
Dissociated dislocations give stacking faults every other plane

Dislocations in High Angle Boundaries

High Angle GB



Energy vs misorientation
Symmetric FCC <110> tilt boundaries



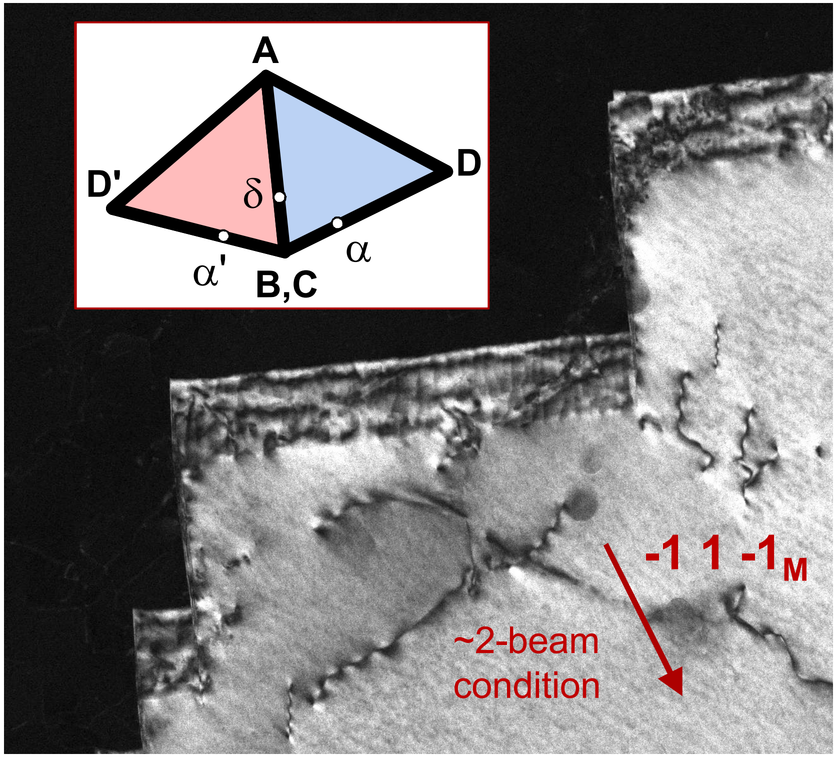
Reference Frame:

Typically choose energy minimum in misorientation/inclination space.

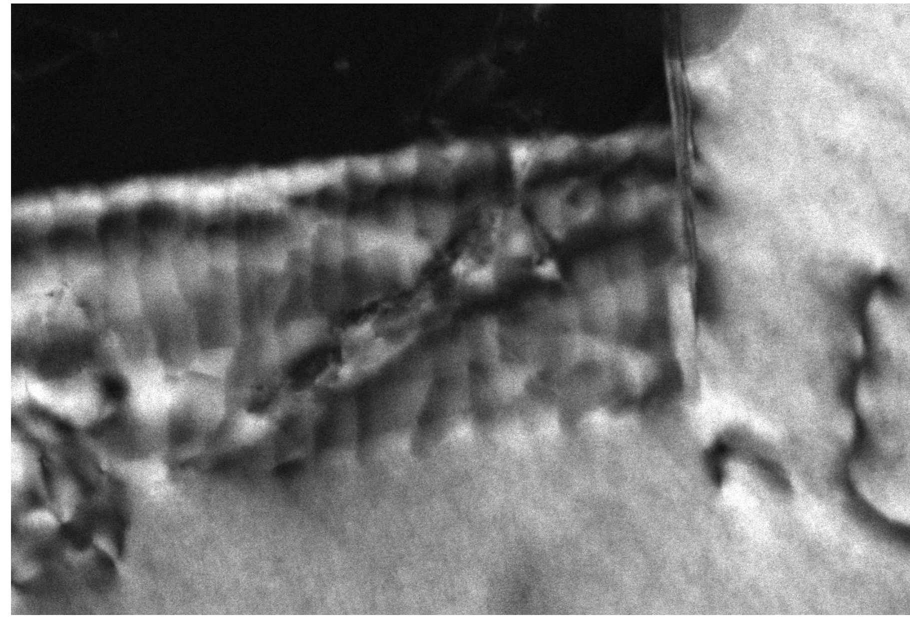
Often a low CSL boundary, but not always!

V.V. Bulatov, B.W. Reed, M. Kumar, Acta Mat 2014

Example: GB dislocation network at Σ=3 boundary facets in Nickel (Diffraction Contrast STEM)



200 nm



100 nm

Average dislocation spacing: ~15 ± 2 nm

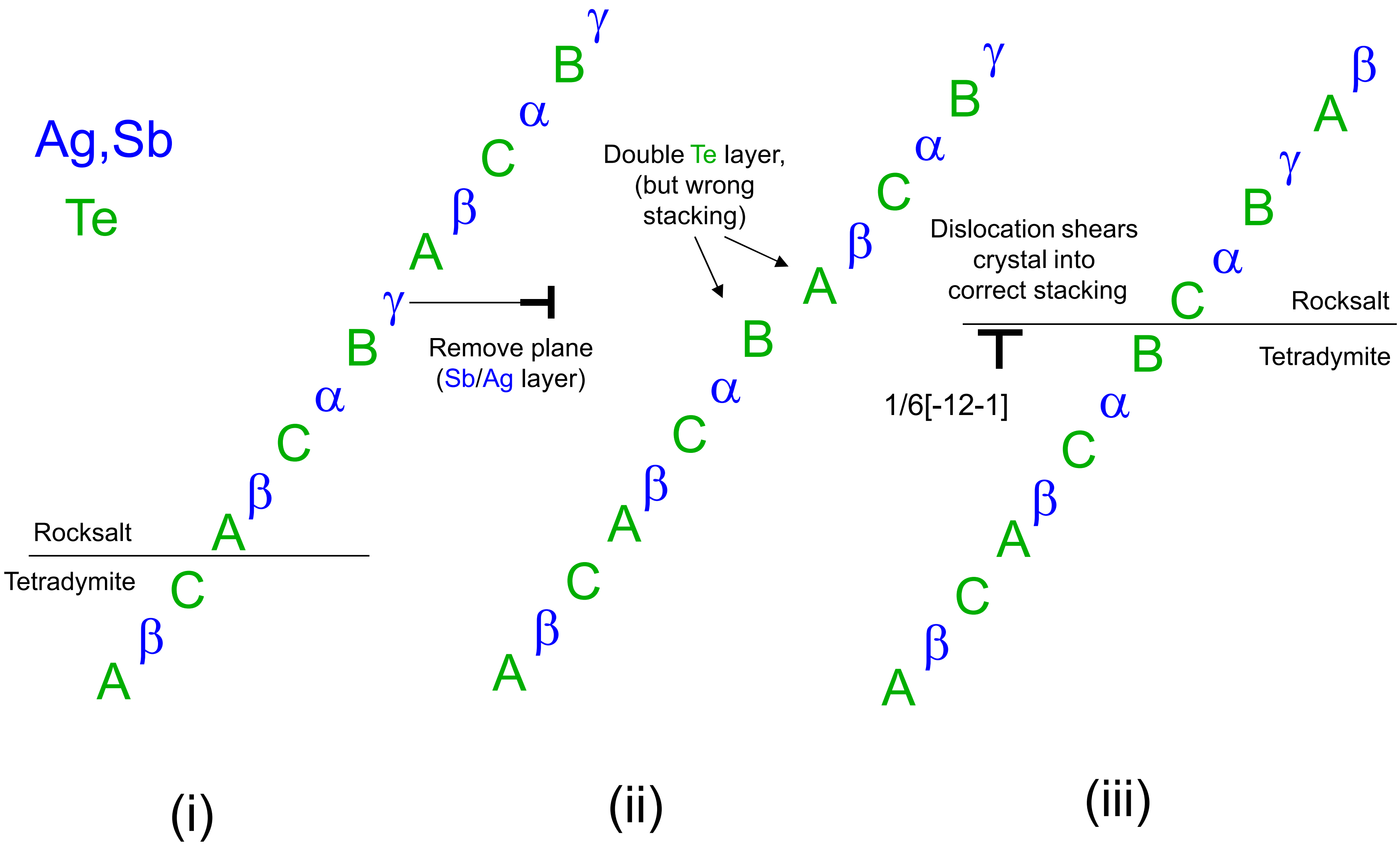
Measured misorientation from exact Σ=3: 0.41°

$$d \approx |b|/(2\sin(\theta/2))$$

$$|b|\ (a/6) < 112 > = 0.14\ nm$$

Dislocation spacing to accommodate misorientation: ~20 nm

Schematic of Transformation Sequence



Medlin and Sugar, Scripta Materialia, 2010.

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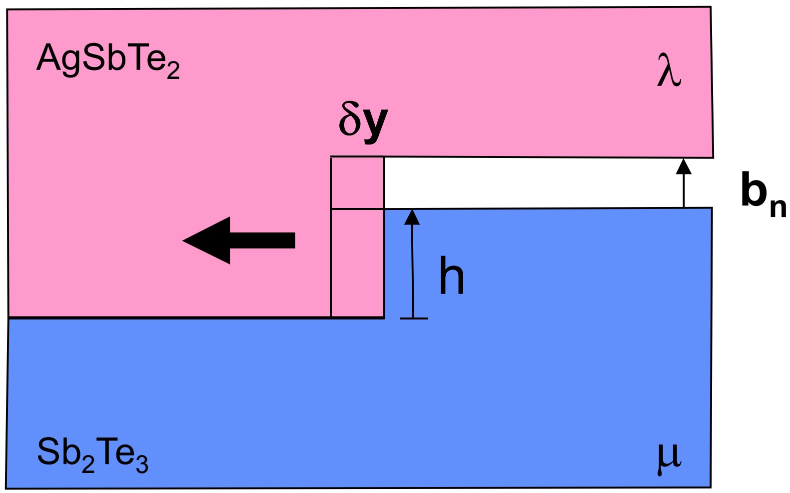
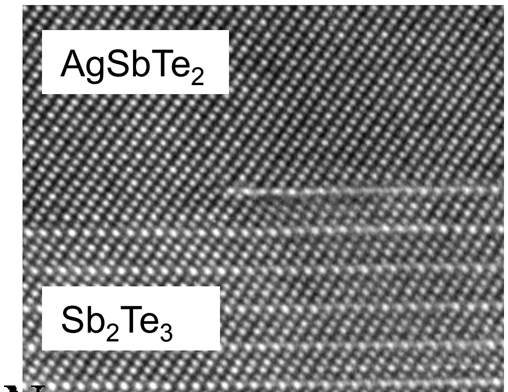
Defect properties give local mass flux required for transformation

Partition flux for defect motion into step and dislocation components





$$\frac{\Delta N_i}{L\delta y} = \underbrace{(\chi_i^{\lambda} - \chi_i^{\mu})h}_{\text{step}} + \underbrace{\chi_i^{\lambda} b_n}_{\text{dislocation}}$$

Hirth & Pond, Acta Mat 1996

Species	Step flux (atoms/Å^2)	Dislocation flux (atom/Å^2)	Total flux (atom/Å^2)
Ag	$\frac{2}{3}\frac{c_{hex}}{a_{cub}^3}$ +0.09043	$\frac{2}{a_{cub}^3}\left(\sqrt{3}a_{cub} - c_{hex}/3\right)$ +0.00334	$\frac{2\sqrt{3}}{a_{cub}^2}$ +0.09377
Sb	$\frac{2}{3}\frac{c_{hex}}{a_{cub}^3} - \frac{8\sqrt{3}}{3a_{cub}^2}$ -0.03459	$\frac{2}{a_{cub}^3}\left(\sqrt{3}a_{cub} - c_{hex}/3\right)$ +0.00334	$-\frac{2\sqrt{3}}{3a_{cub}^2}$ -0.03126
Te	$-\frac{4}{a_{cub}^3}\left(\sqrt{3}a_{cub} - c_{hex}/3\right)$ -0.00668	$+\frac{4}{a_{cub}^3}\left(\sqrt{3}a_{cub} - c_{hex}/3\right)$ +0.00668	0

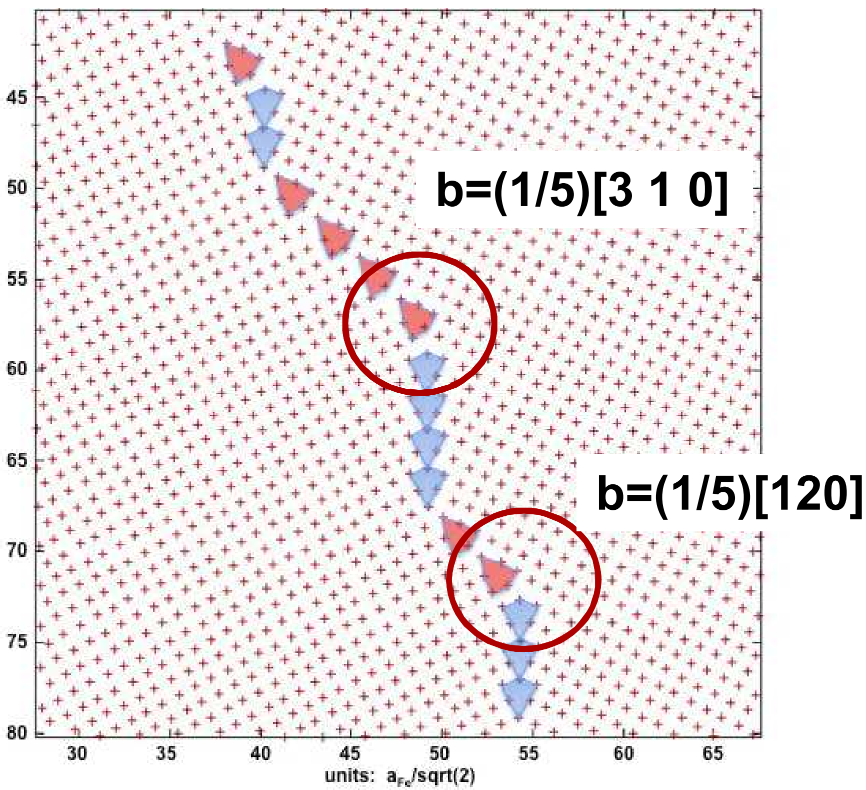
Reject Ag and Incorporate Sb in ratio of 3:1

Tellurium:
Step and Dislocation fluxes cancel.
No long-range Te transport required.

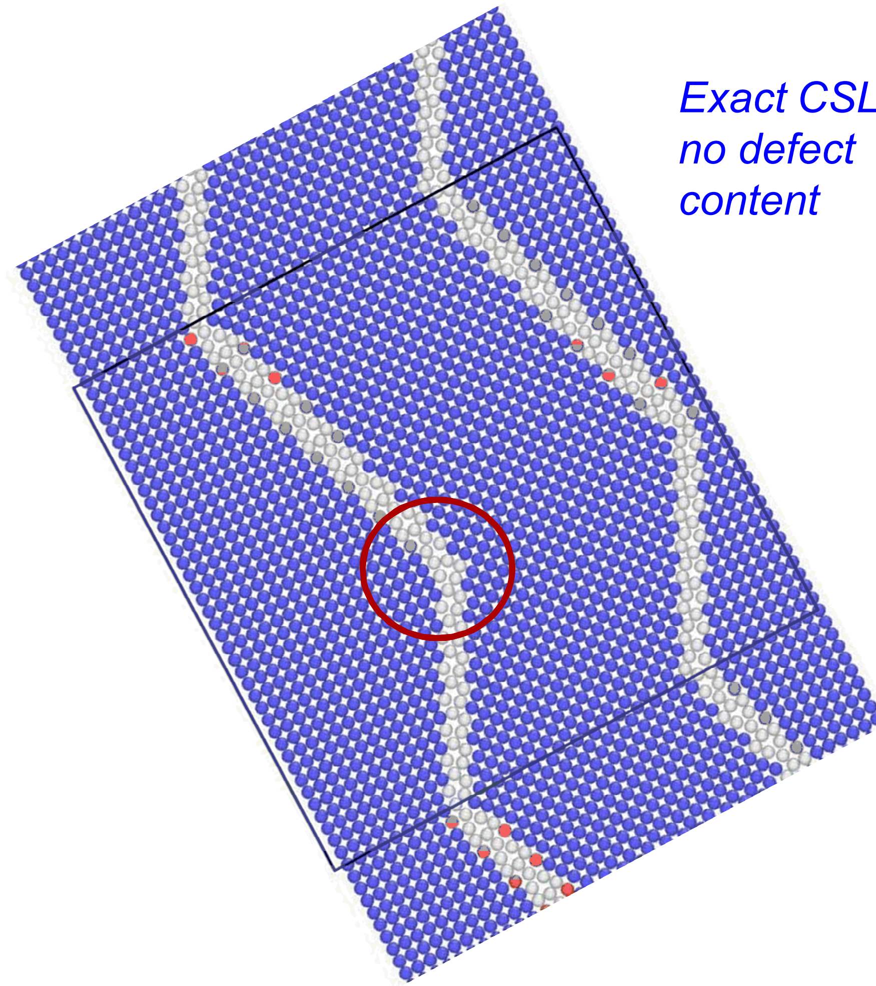
Sandia National Laboratories

How are the grain boundary dislocations manifested in the junction structure?

Experimental Junctions
b=(1/5)(120) and (1/5)(310)



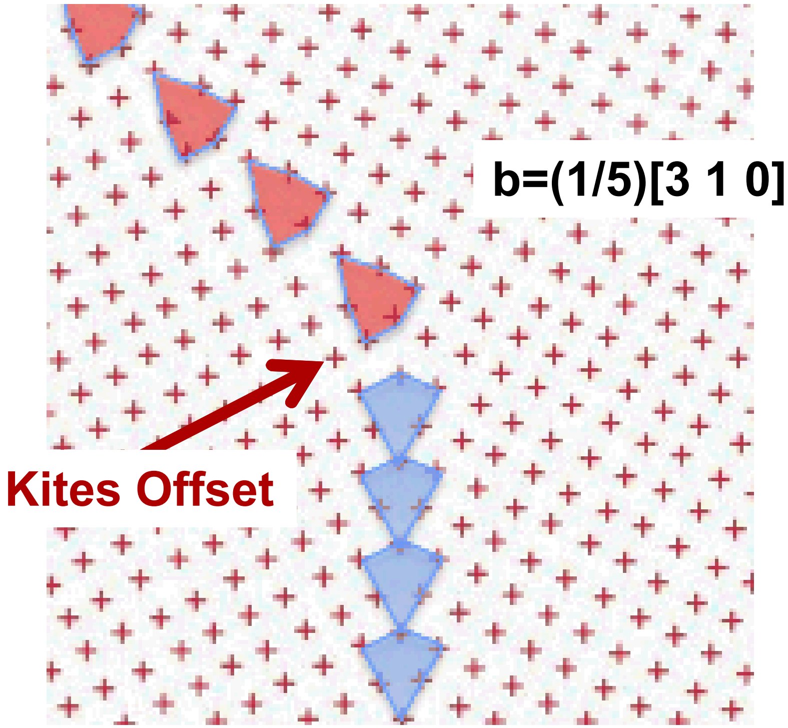
Relaxed Periodic Atomistic Structure



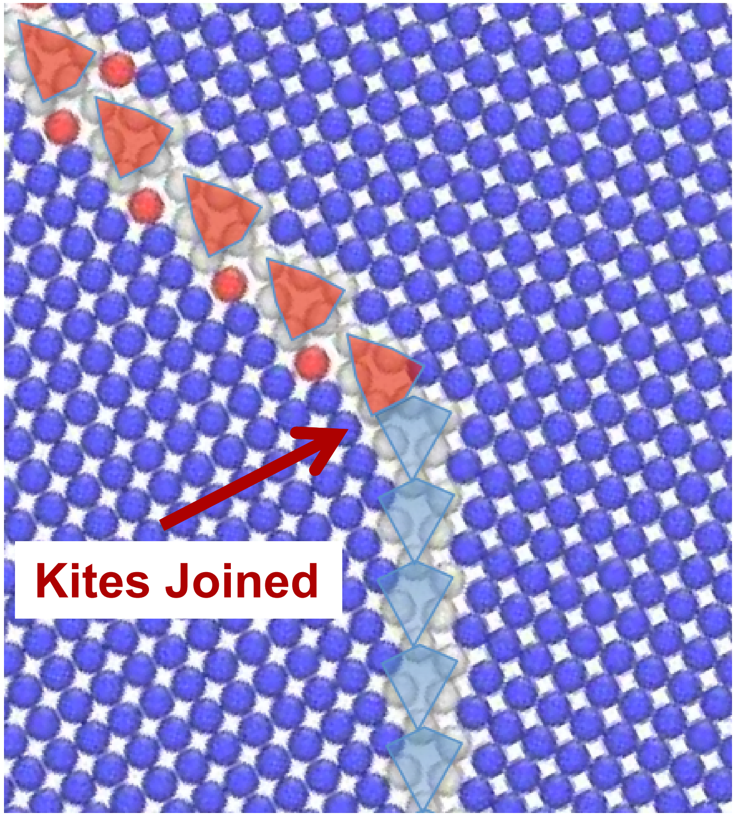
Exact CSL:
no defect
content

How are the grain boundary dislocations manifested in the junction structure?

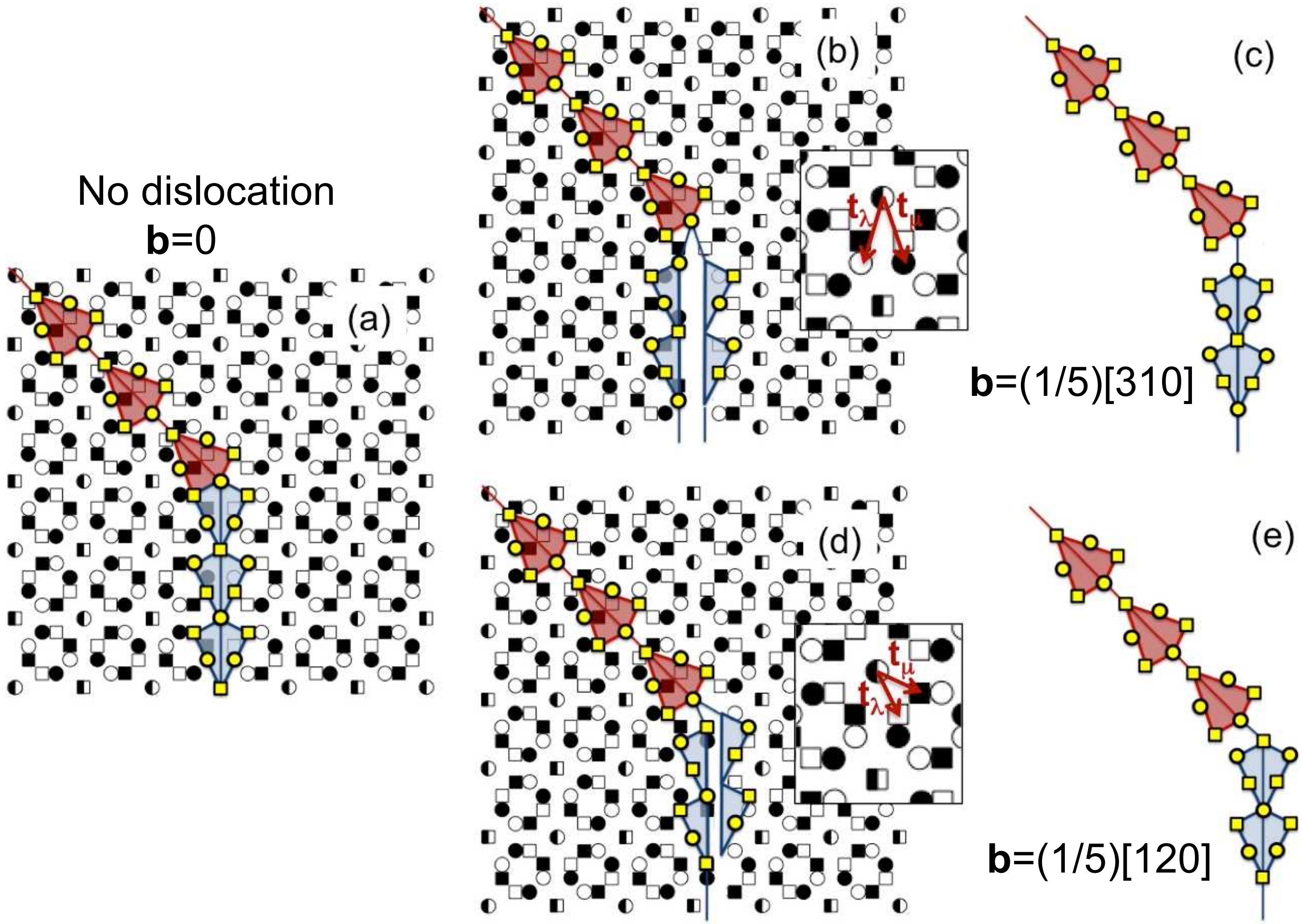
Experimental Junctions
b=(1/5)(120) and (1/5)(310)



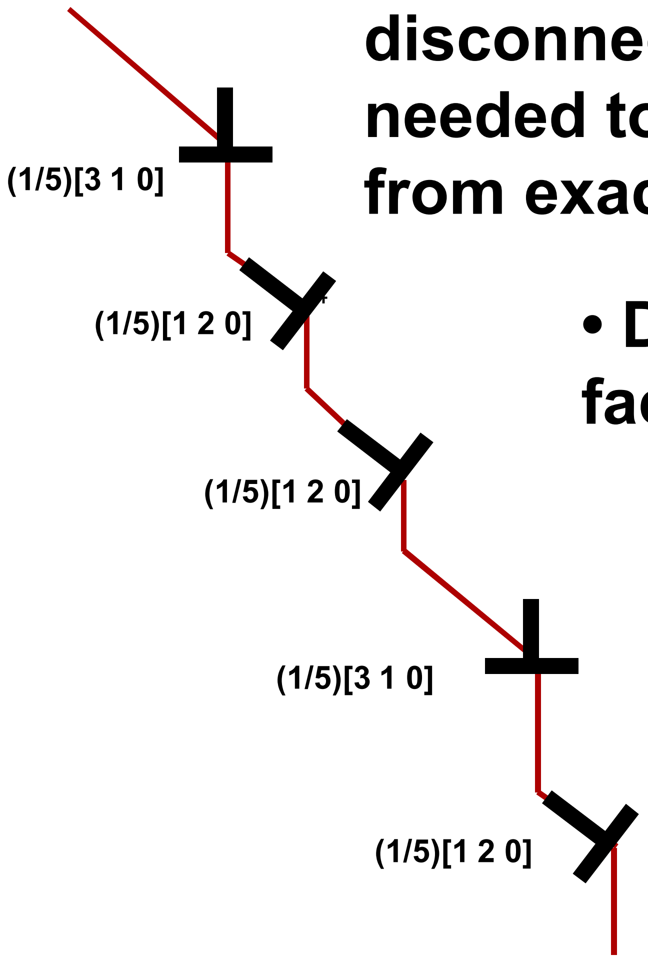
Relaxed Periodic Atomistic Structure



Geometric construction links junction core structure to defect content



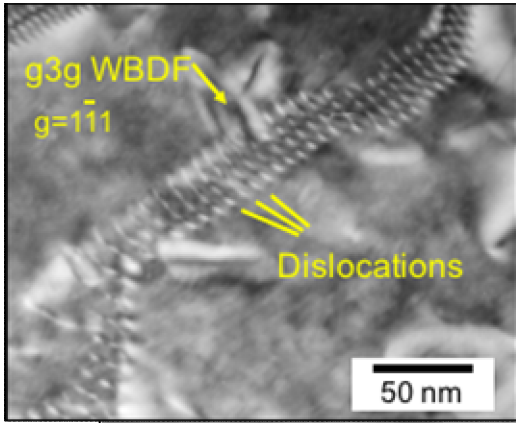
Impact on facet length scale



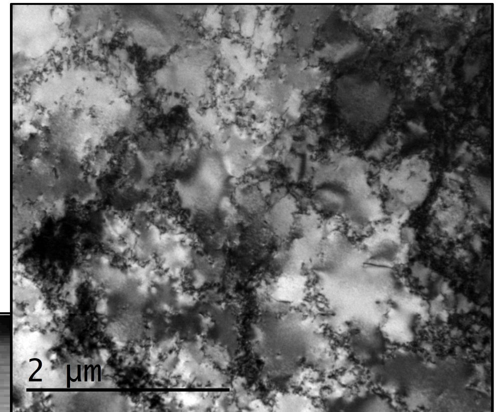
- Distribution of grain boundary disconnections consistent with that needed to accommodate misorientation from exact Σ=5 misorientation.
- Disconnection cores located at facet junctions.
- Suggests that facet length scale here is tied to misorientation/inclination via dislocation content.

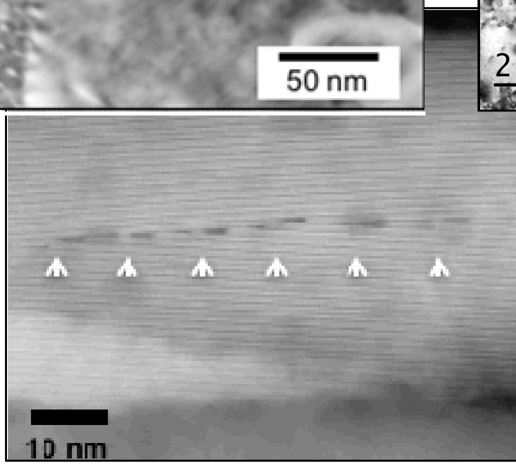
Low angle boundaries: Arrays of dislocations

Low angle GB in Al thin film



Dislocation Cells in Ni





Low Angle grain boundary in Bi_2Te_3 Nanowire

Reference Frame:
Single Crystal

Dislocation density depends on misorientation and inclination (Frank-Bilby Equation)

$$\mathbf{B}=(\mathbf{I}-\mathbf{P}^{-1})\mathbf{v}$$

b-vector density → B

Matrix defining misorientation → P

Interface vector, defining inclination → v

Symmetric tilt boundaries:

$$\theta=2\sin^{-1}(b/2D)$$

Misorientation → θ

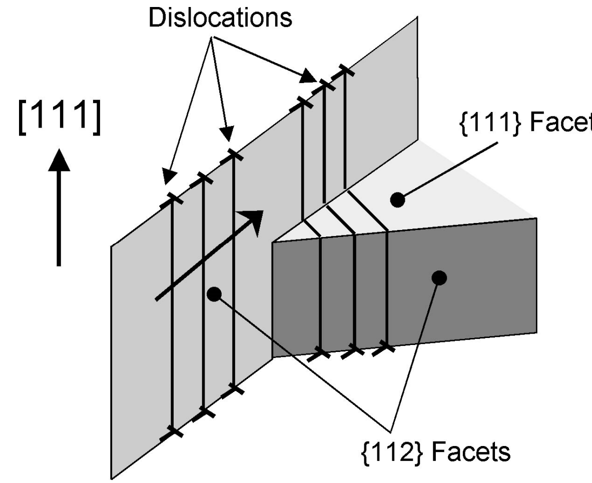
Burgers vector → b

Spacing → D

Coupling of GBD's with facet junctions

T=550° Δt=400 sec
Movie is repeated

20 nm



-(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

50 nm T=490°C 185 minutes

Understanding dislocation/junction interactions important to relating grain evolution to local plastic strain.

G. Lucadamo and D.L. Medlin, Acta Materialia 50 (2002)
D.L. Medlin and G. Lucadamo, MRS Symp 252 (2001)