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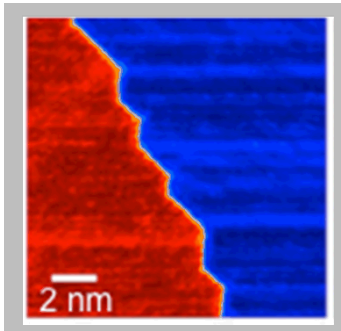

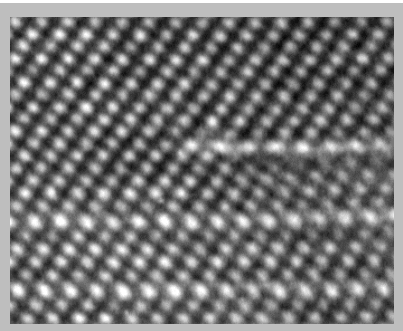
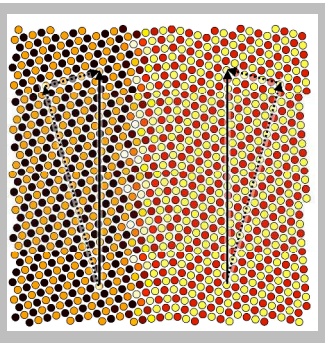
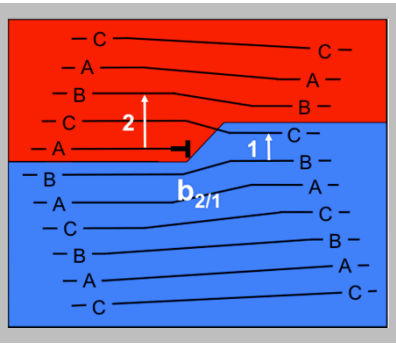

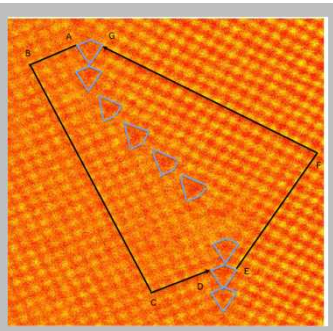

Atomic Scale Investigations of Interfacial Line Defects

Douglas L. Medlin

Sandia National Laboratories, Livermore, CA

dlmedli@sandia.gov

U.S. DEPARTMENT OF ENERGY

National Nuclear Security Administration

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Interfaces:
Central to materials properties and behavior

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-Barriers to slip.
- -Hardening.
- -Stress concentration

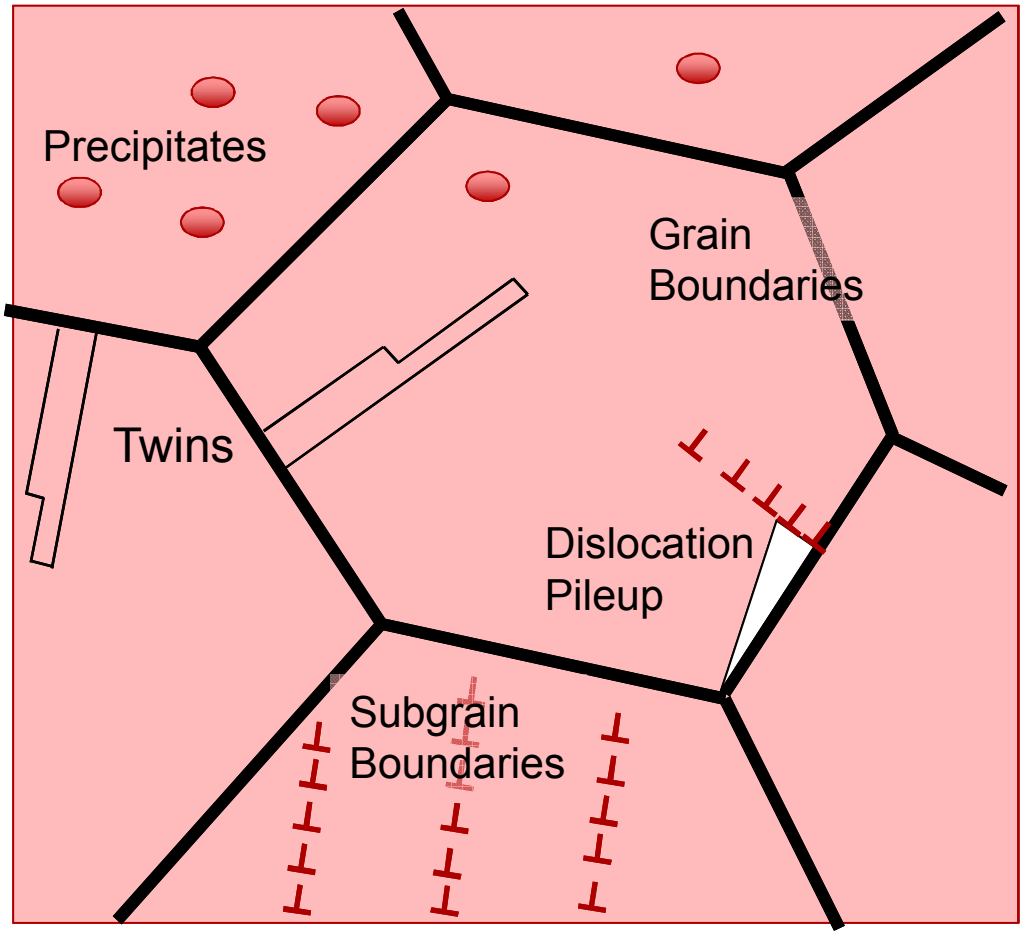
-Softening at high T.
- -e.g., gb sliding, creep

-Sinks for point defects, dislocations
- -e.g. recrystallization

-Heterogeneous nucleation sites

-Compositional segregation, diffusional pathways.

-Electronic and Thermal transport



Interfacial Line Defects: An important bridging concept

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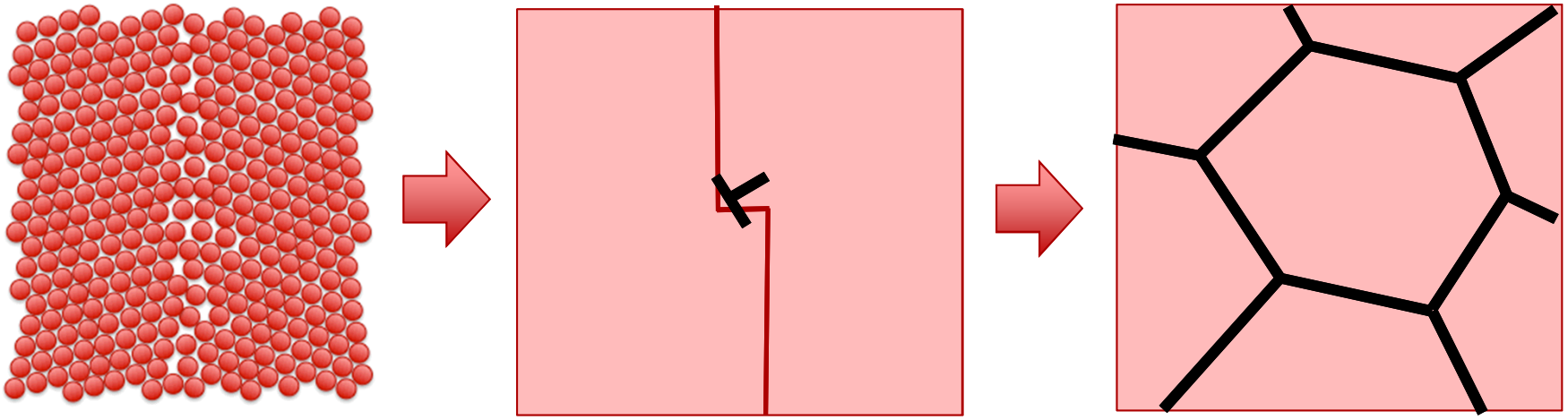


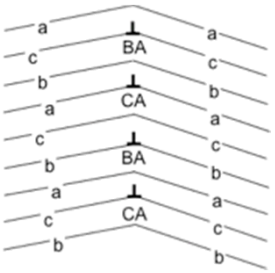
- Connection between details of atomic structure and larger-scale materials properties.
- Essential to extending from specific boundaries to more general boundaries
- Provide clues to essential physics and mechanisms controlling behavior and properties of interfaces.

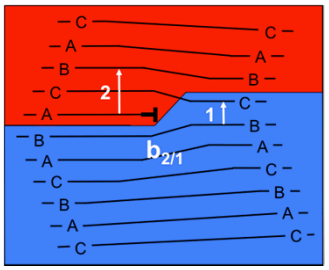
Outline

Background on Interfacial Line defects

-Overview of defect types

-Examples from low and high angle GBs.

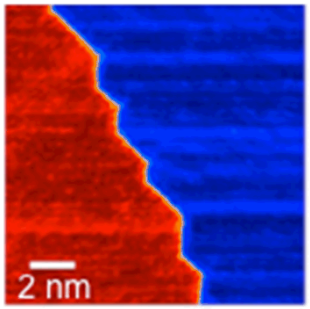


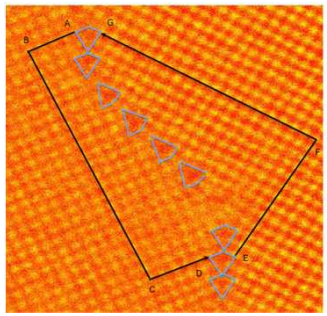


GB disconnections and facet junctions

-Asymmetric Σ=5 GB in BCC Fe

-Interplay of facet junctions and grain boundary disconnections

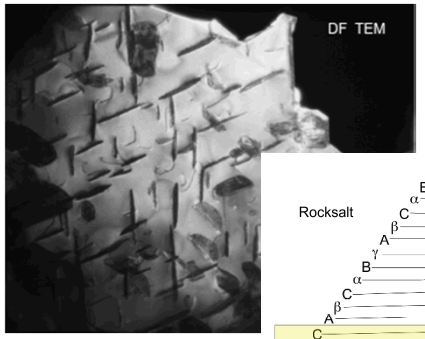


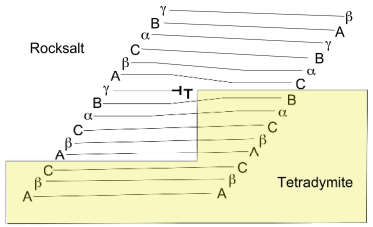


Disconnections at heterophase interfaces

-Telluride precipitates in thermoelectric alloy.

-Role of disconnections in transformation mechanism and interfacial strain relief.





Acknowledgements

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S.M. Foiles

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N.A. Heinz

T. Ikeda

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Line Defects:

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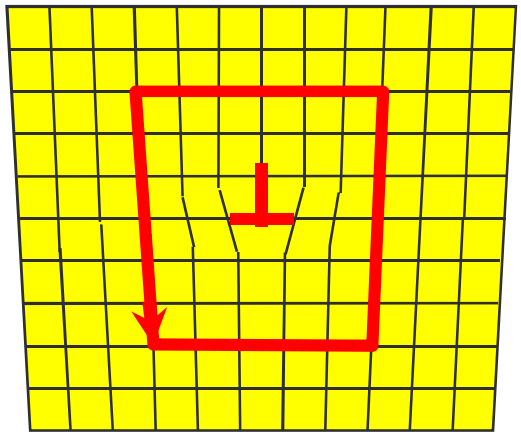
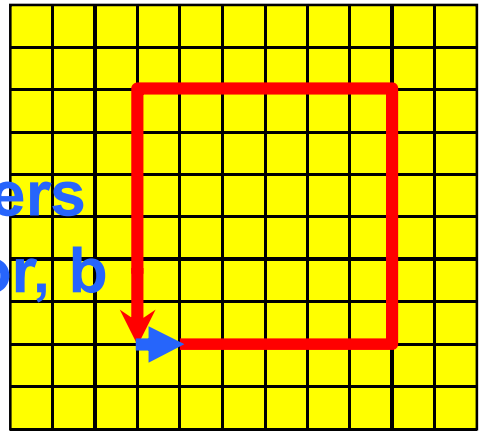
Edge Dislocation

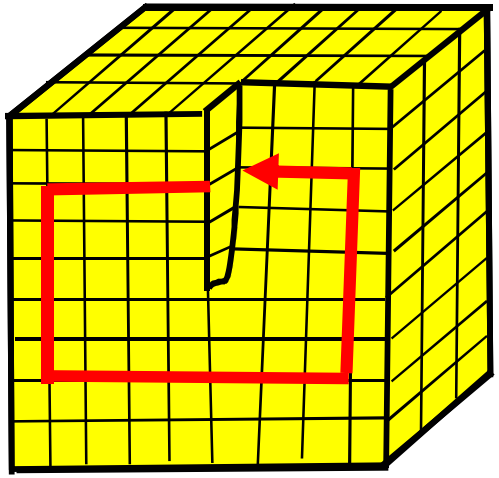


Reference Frame:
Perfect Crystal

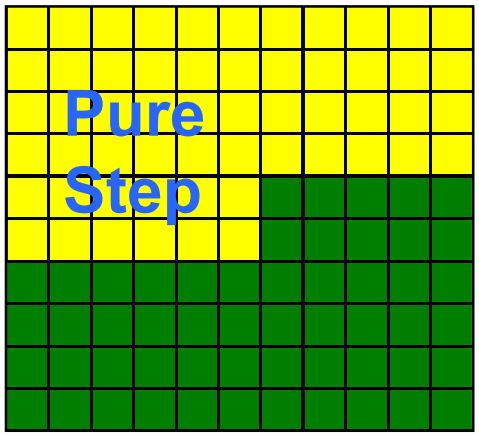


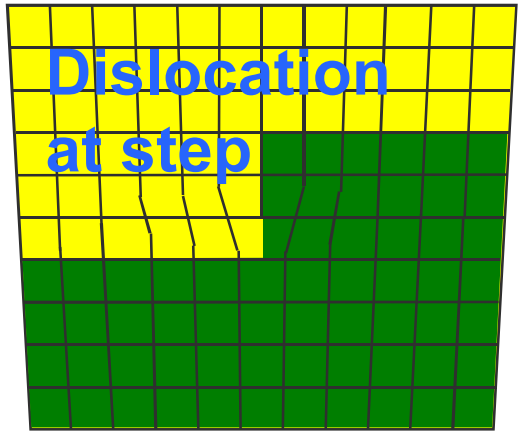
Burgers Vector, b

Screw Dislocation



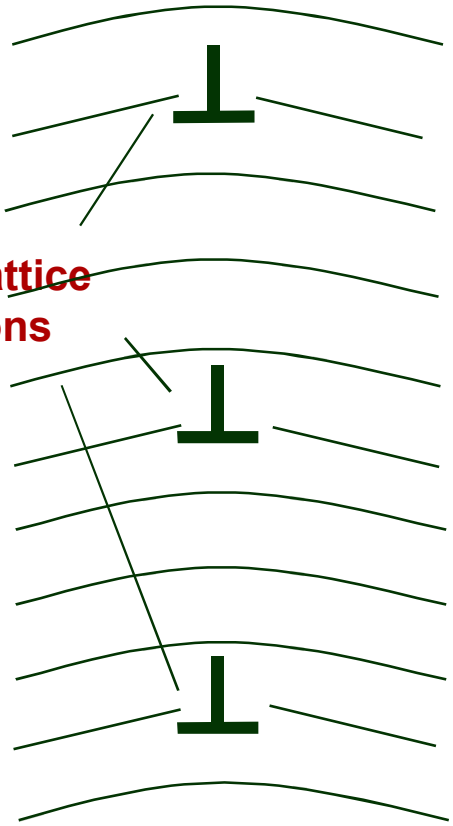
Interfacial Disconnection





Both topological and morphological characteristics are important

Low angle grain boundaries: Arrays of dislocations



Crystal Lattice Dislocations

Reference Frame:
Single Crystal

For symmetric tilt boundaries:

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

Misorientation

Burgers vector

Spacing

Low Angle Grain Boundaries in Various contexts

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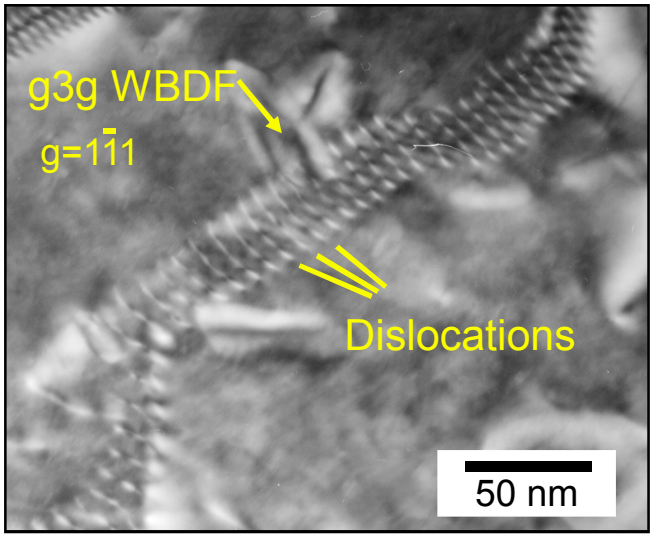
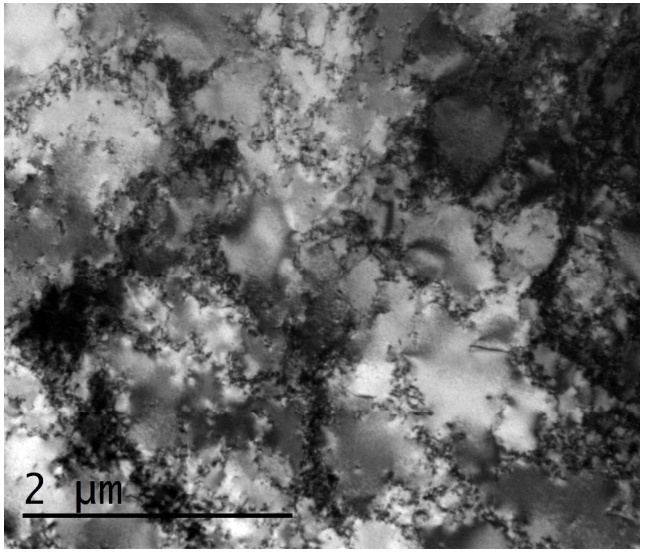
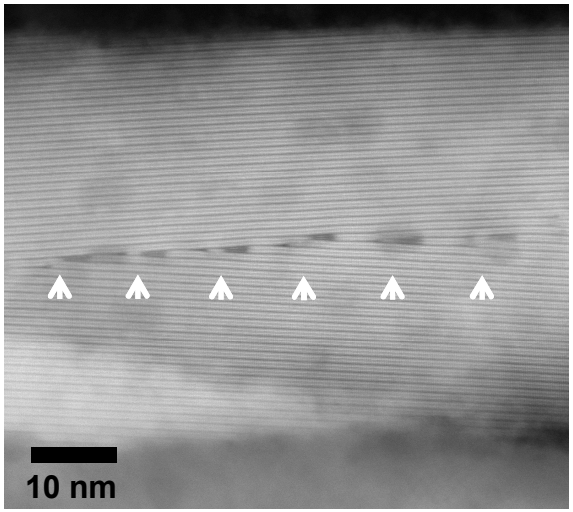
Low angle tilt boundary in Al thin film.

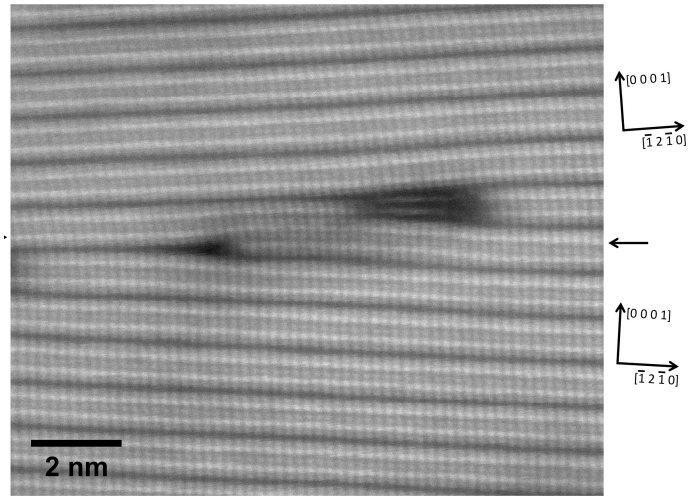


Dislocation Cells in Deformed Ni.



Low Angle GB in Bi_2Te_3 thermoelectric Nanowire

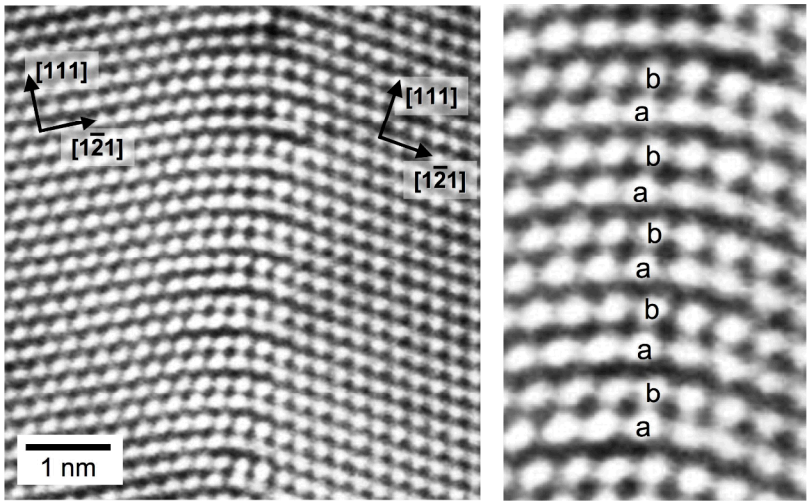




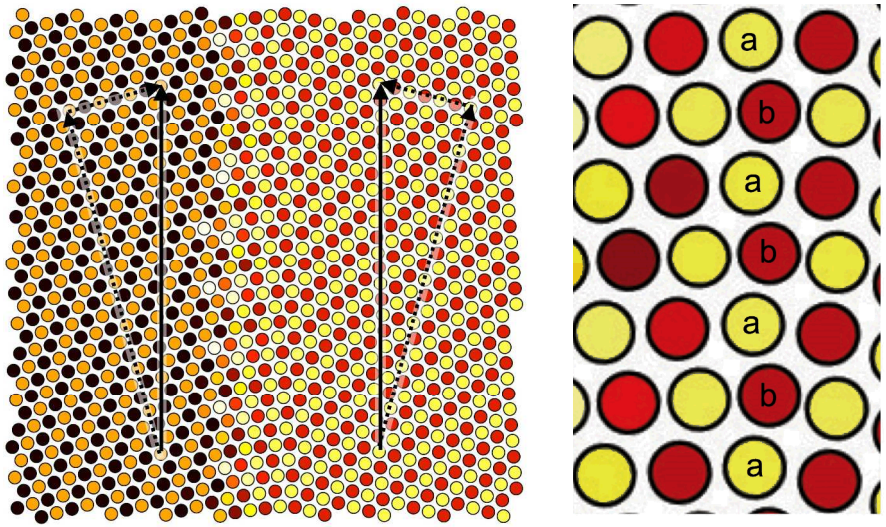
Limit for Low-Angle GBs: Dislocation Core Overlap

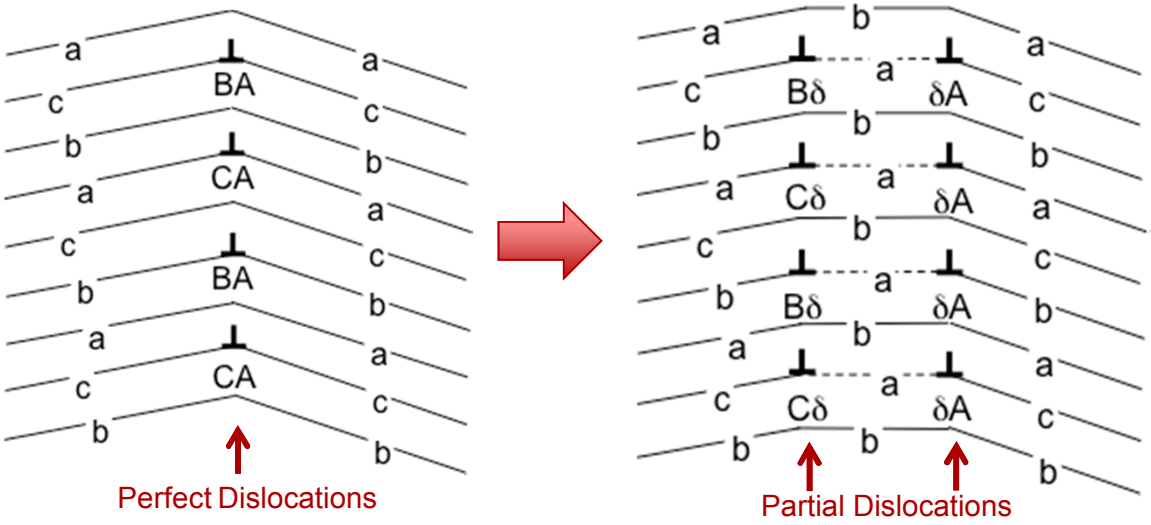
An extreme example: HCP Stacking at 29° boundary in Gold

HRTEM



EAM





Dissociation into partial dislocations.

Stacking fault every 2 planes gives HCP stacking

Medlin & Hamilton, J. Mat Sci 2009.

Dislocations in High Angle Boundaries

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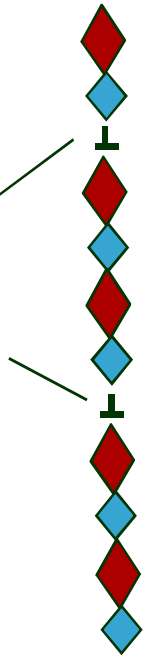
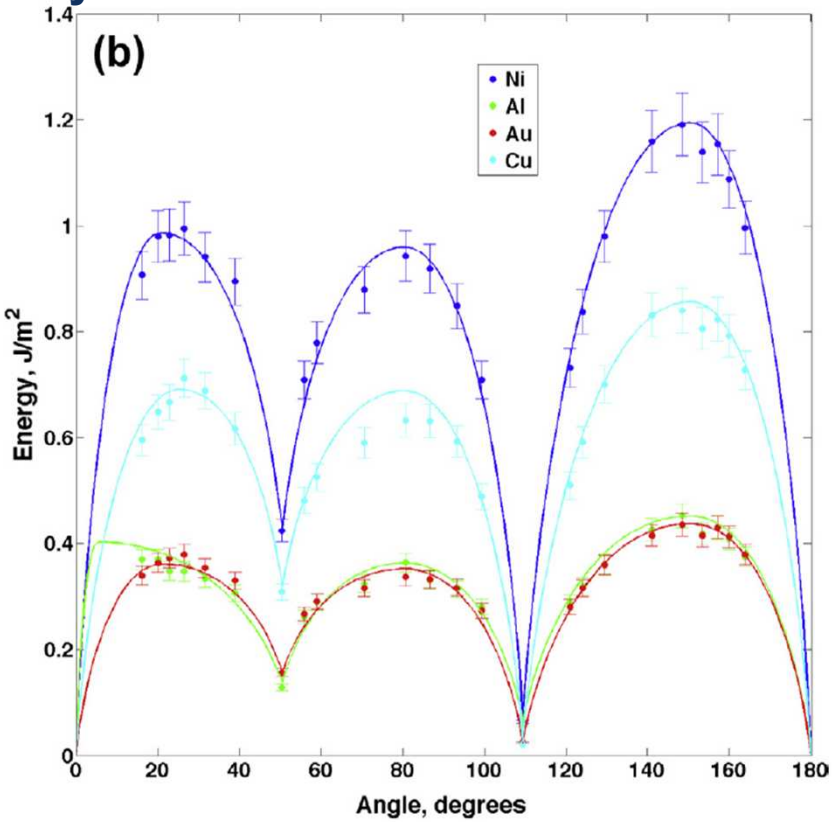
High Angle GB



Reference Frame:

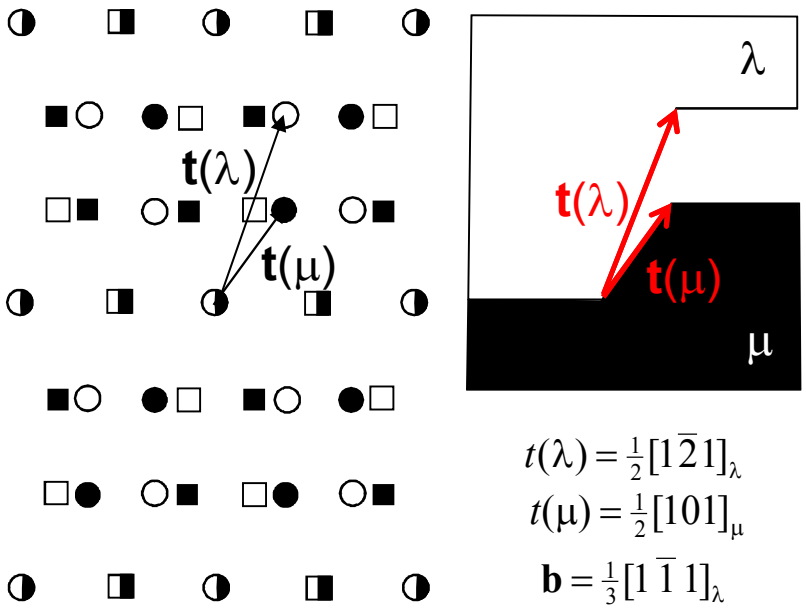
Energy Minima in misorientation/inclination space

Energy vs misorientation
Symmetric FCC <110> tilt boundaries



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

Interfacial Line defects: in general have both dislocation and step content



$$t(\lambda) = \tfrac{1}{2}[1\bar{2}1]_{\lambda}$$
$$t(\mu) = \tfrac{1}{2}[101]_{\mu}$$
$$\mathbf{b} = \tfrac{1}{3}[1\,\bar{1}\,1]_{\lambda}$$

Crystal lattice translation vectors

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

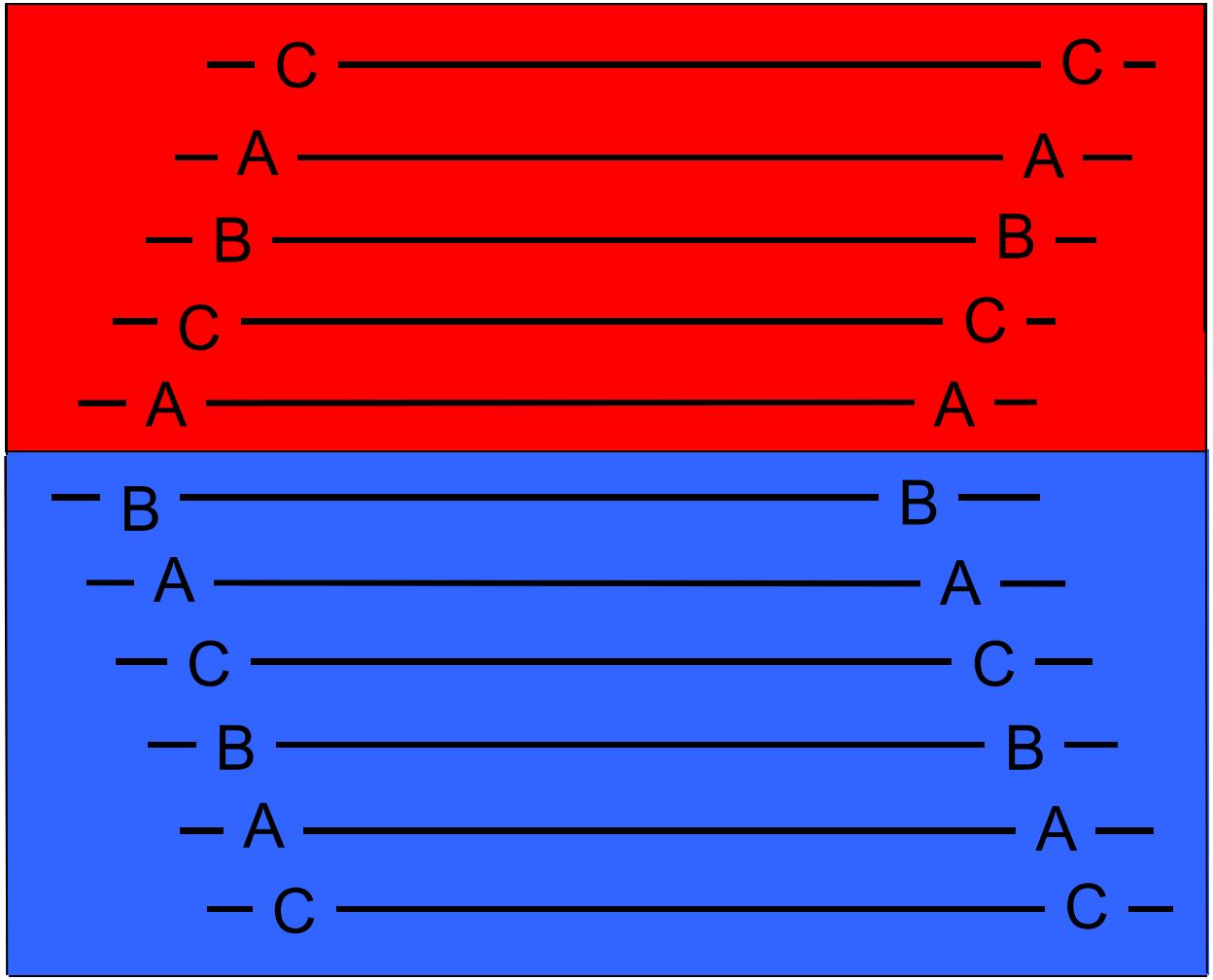
Burgers vectors of the set of "admissible" defects

Matrix converts from μ to λ crystal coordinates

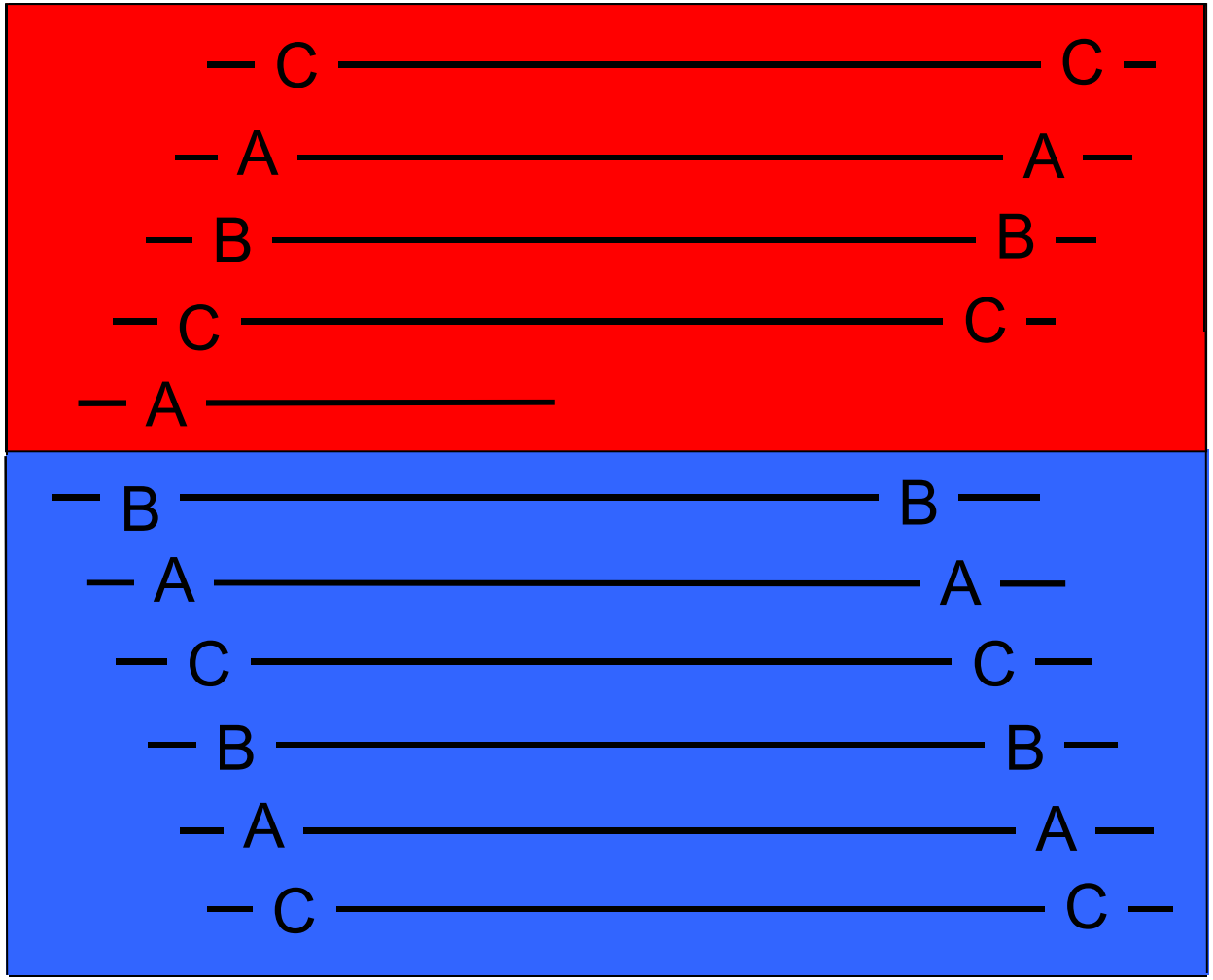
"disconnection" = both step and dislocation content

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

Example: (1/3)<111> twin disconnections



Example: (1/3)<111> twin disconnections



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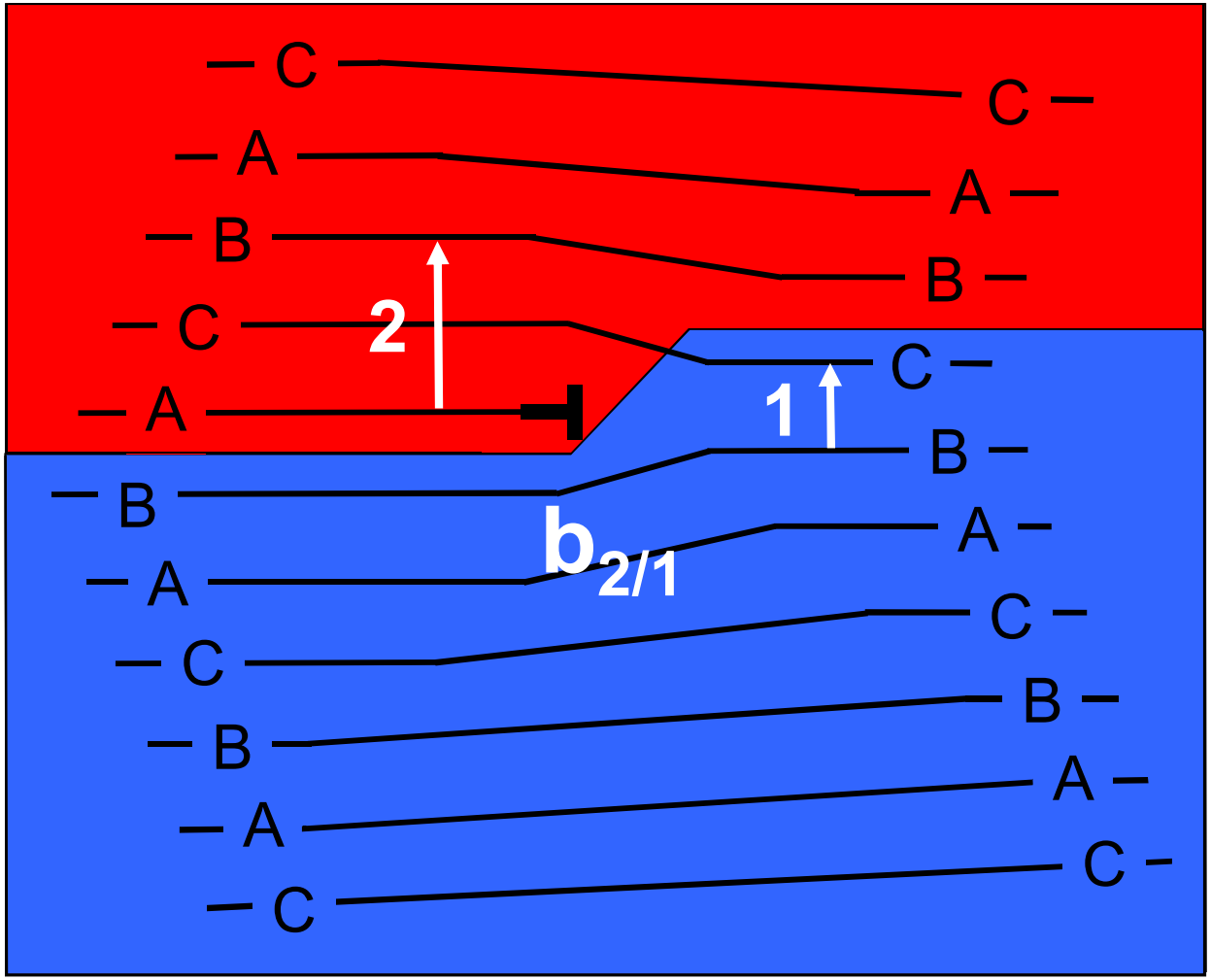
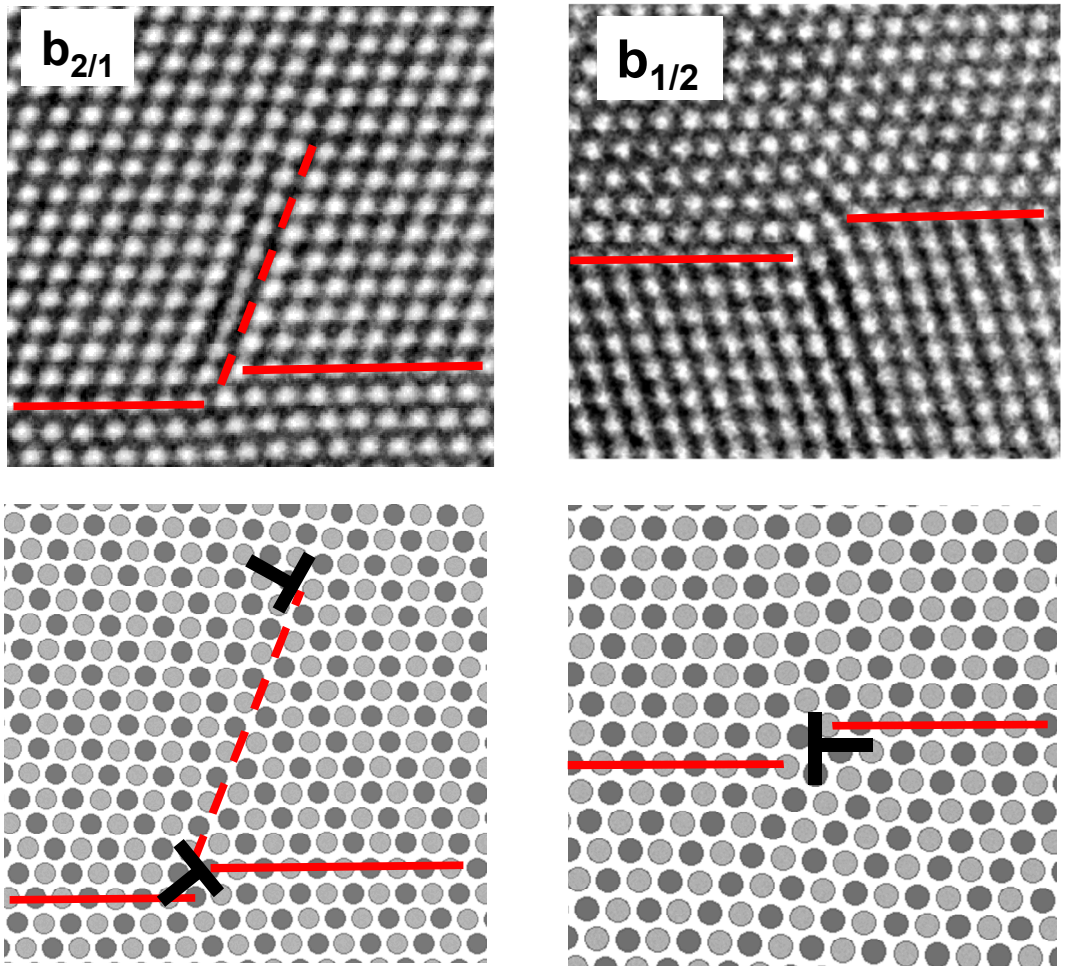


Example:
(1/3) <111> Disconnection at twin in Au



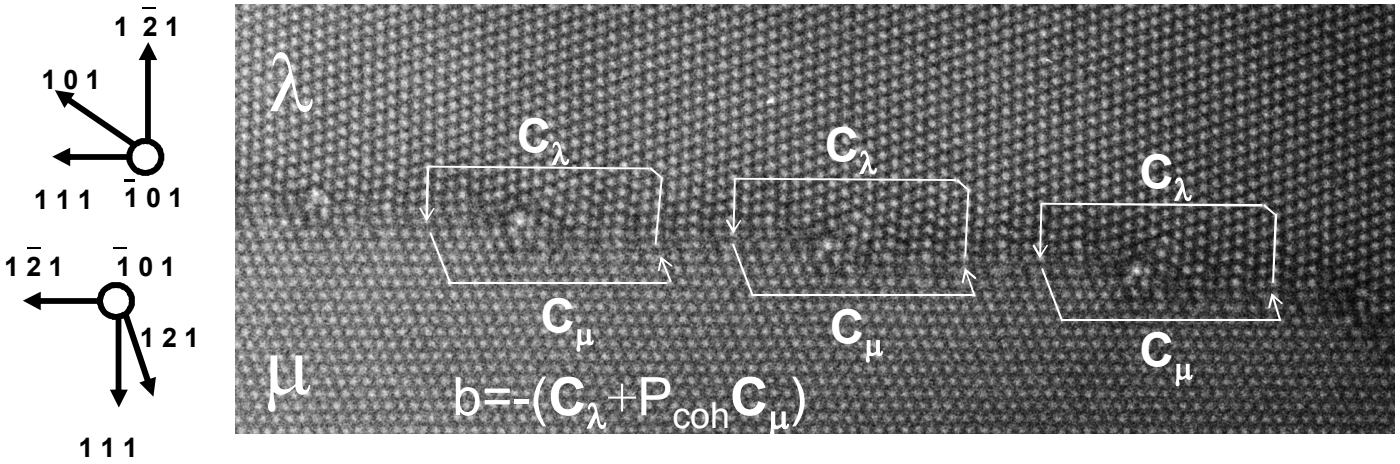
← Opposite Burgers Vectors →

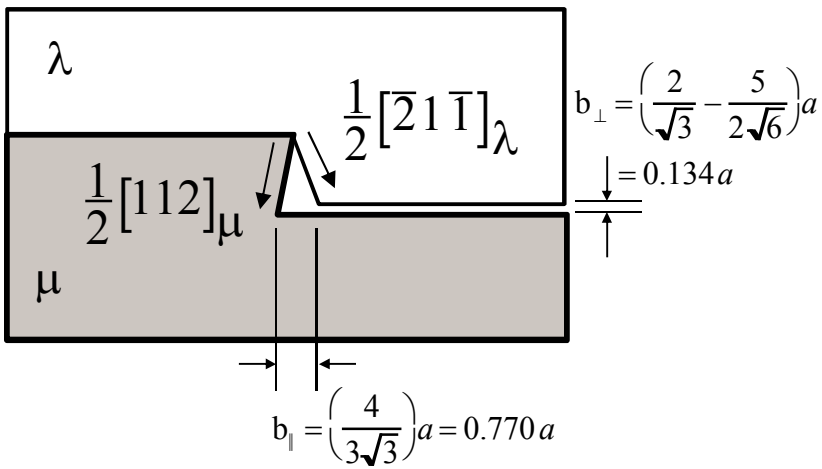
- Interface breaks symmetry of dislocation.
- $b_{2/1}$ reduces strain energy by dissociating into Shockley and stair rod dislocations.
- $b_{1/2}$ disconnection cannot dissociate without creating unfavorable "AA" stacking.

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

Example: Accomodation of Grain Boundary Misfit by Disconnections

90° Boundary in Gold





- Coherent reference frame, P_{coh}, describes the 90° rotation of coordinates and strain to bring λ and μ into coherency.
- Defects efficiently accommodate the 5.7% misfit parallel to the {111}/{112} facets.
- Nearest CSL is Σ=99

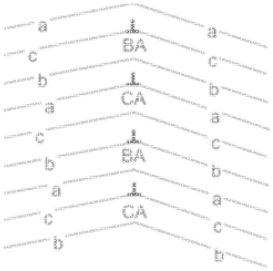
D.L. Medlin, D. Cohen, and R.C. Pond, Phil. Mag. Letts., 2003.

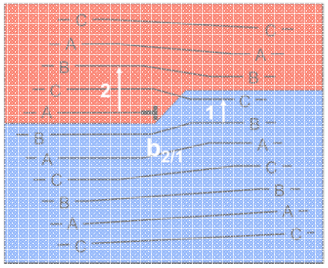
Outline

Background on Interfacial Line defects

-Overview of defect types

-Examples from low and high angle GBs.

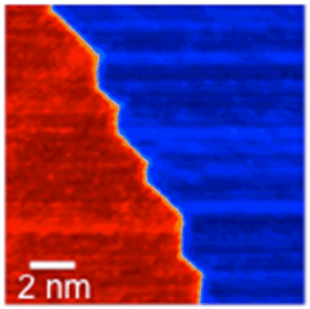


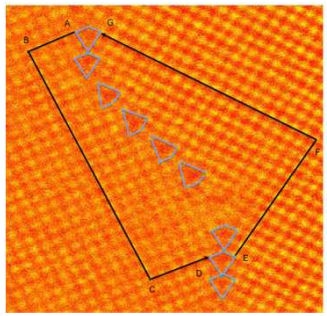


GB disconnections and facet junctions

-Asymmetric Σ=5 GB in BCC Fe

-Interplay of facet junctions and grain boundary disconnections

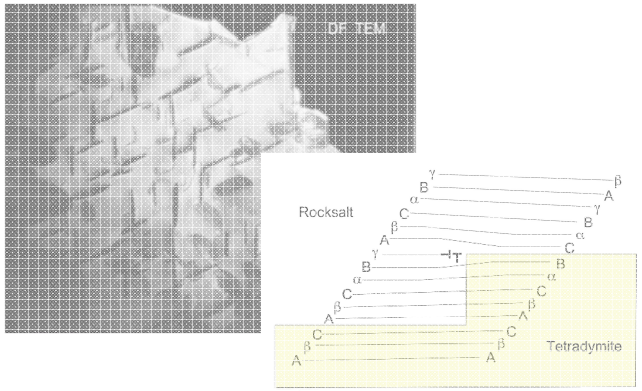




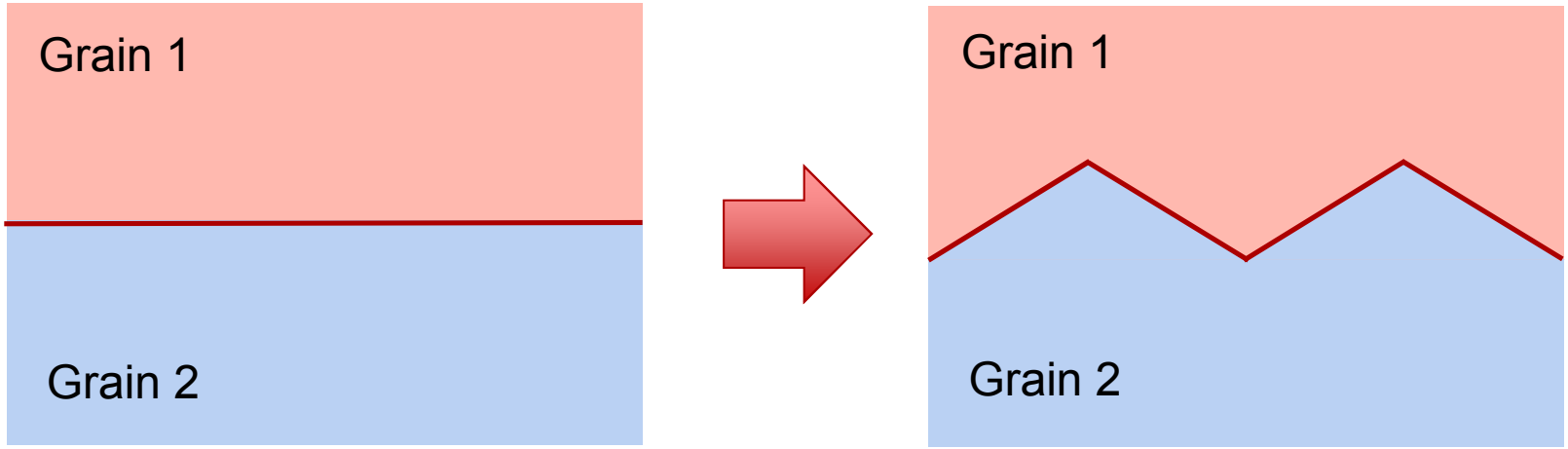
Disconnections at heterophase interfaces

-Telluride precipitates in thermoelectric alloy.

-Role of disconnections in transformation mechanism and interfacial strain relief.



Grain Boundary Faceting



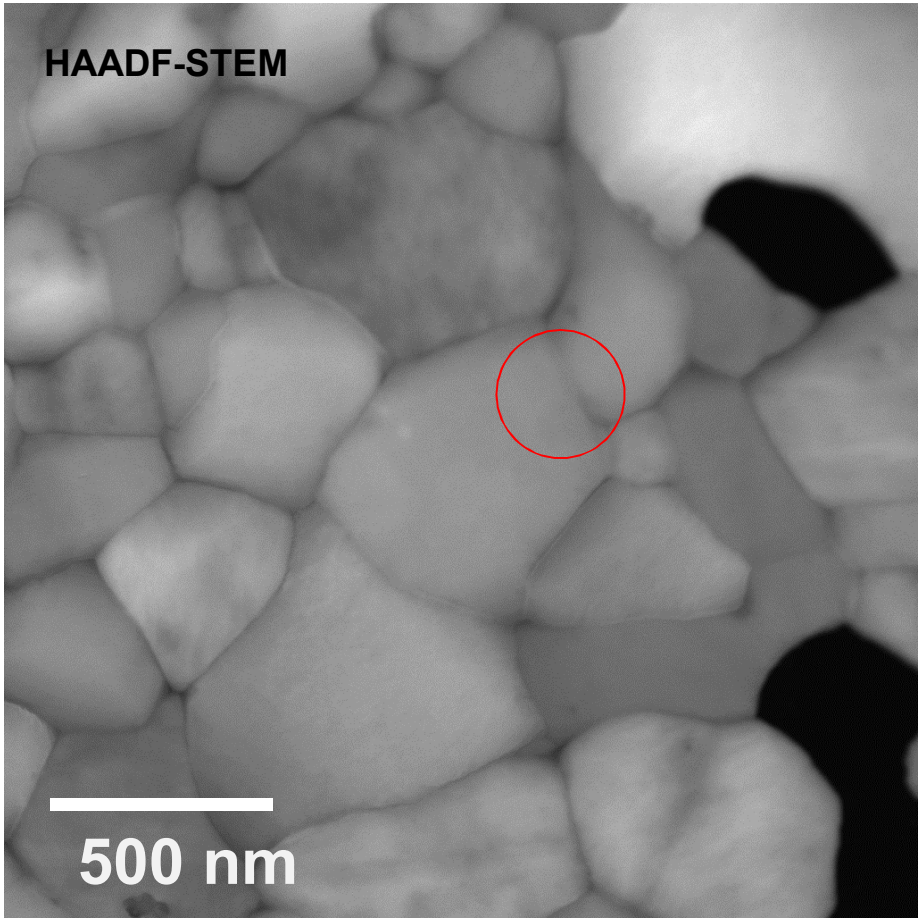
- **Reduce interface energy by faceting on lower energy inclinations.**

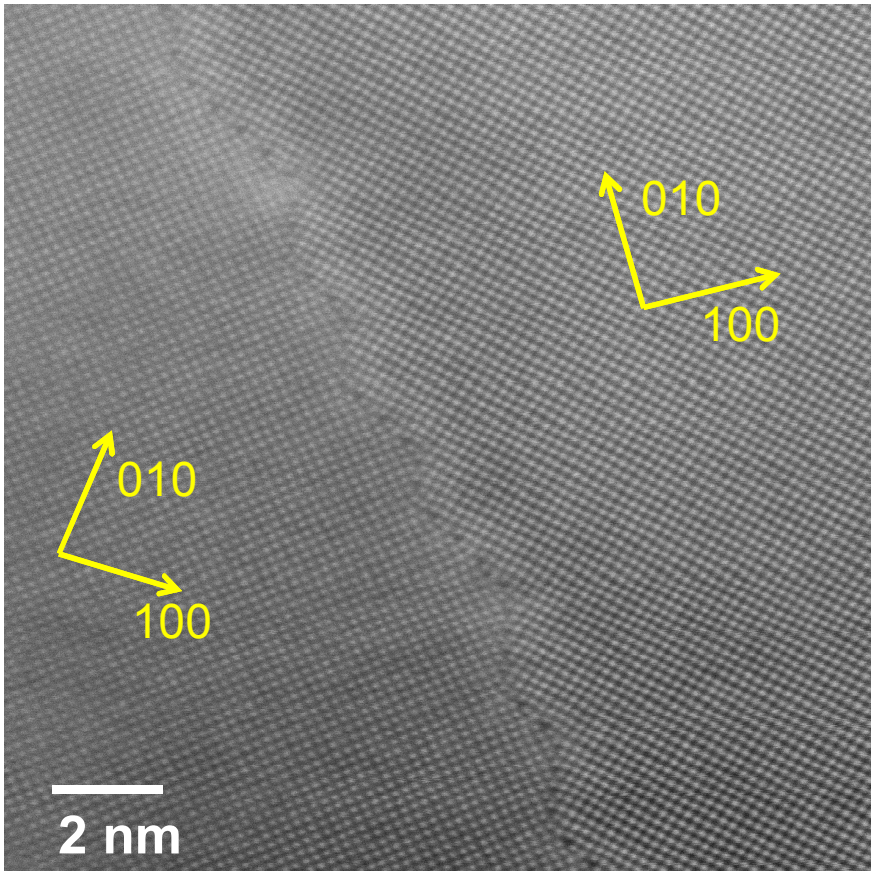
- **How do grain boundary dislocations affect the structure of the junctions and the length-scale of the faceting?**

- **Explore in a faceted Σ=5 boundary in BCC Fe.**

D.L. Medlin, K. Hattar, F. Abdeljawad, J.A. Zimmerman, S.M. Foiles
in preparation for Acta Materialia

Observations: Polycrystalline BCC Fe film

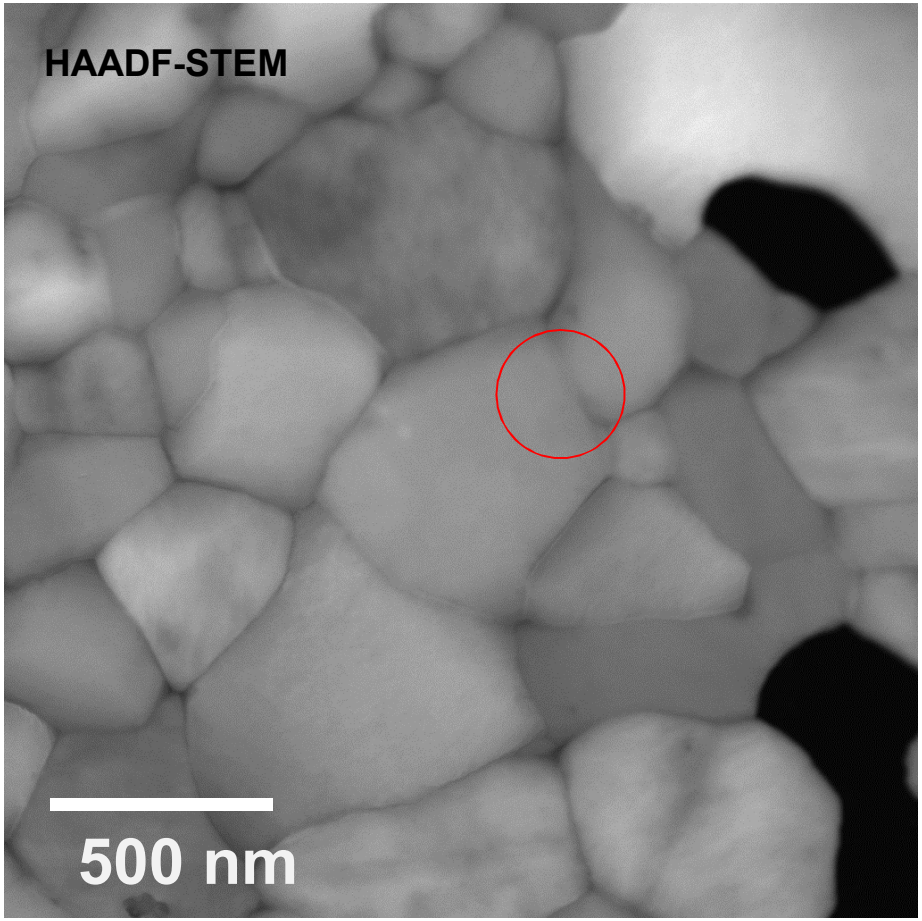


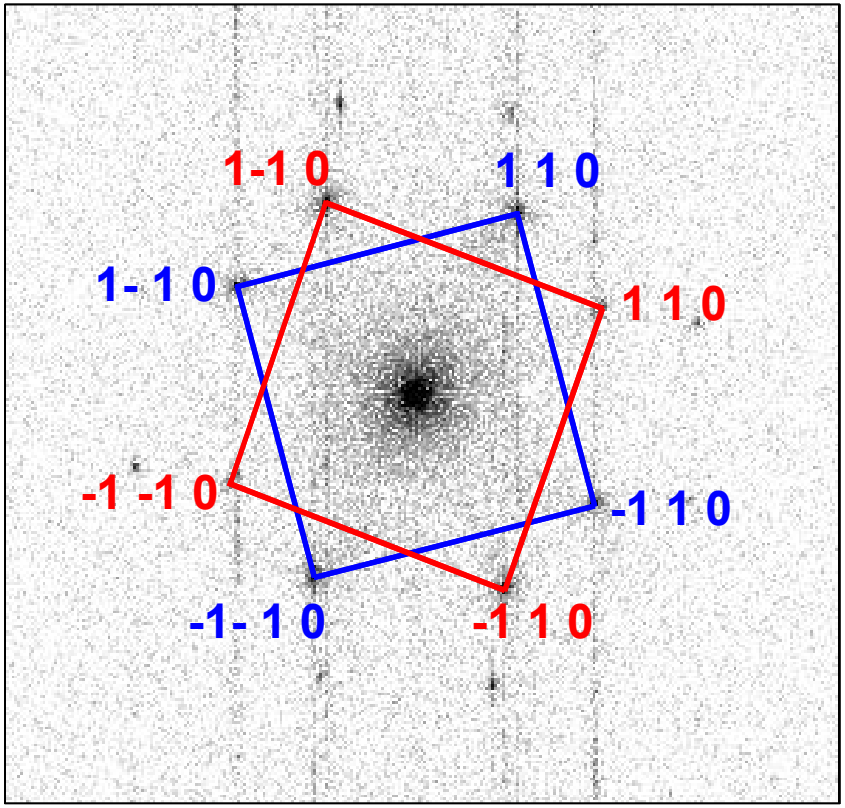


Pulsed Laser Deposited Fe on Rocksalt (NaCl). 36 nm thickness.
Specimen released and annealed on Mo grid 675°C, 2 hours.
under vacuum

HAADF-STEM
FEI-200 keV probe corrected Titan

Observations: Polycrystalline BCC Fe film

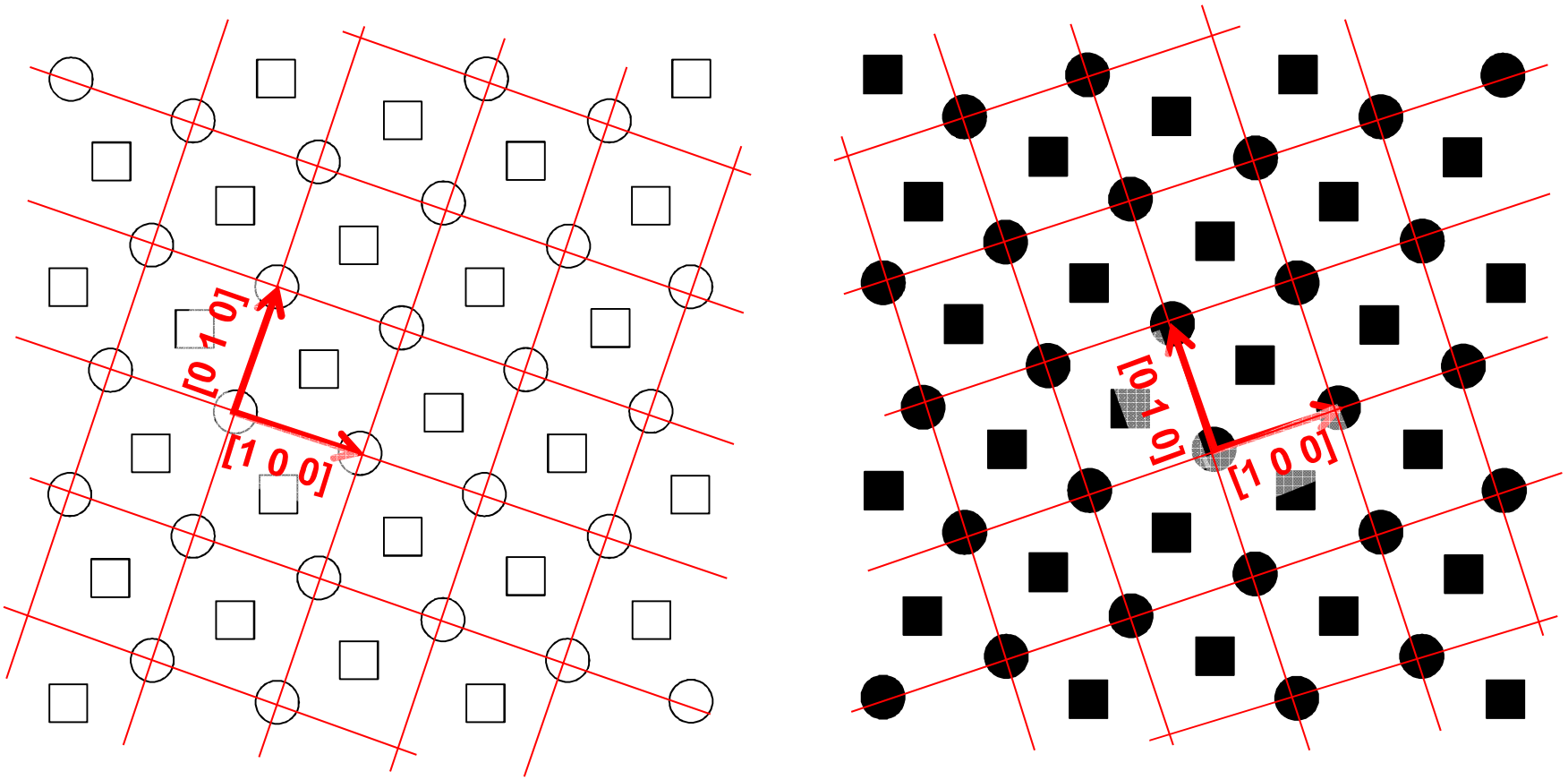




Pulsed Laser Deposited Fe on Rocksalt (NaCl). 36 nm thickness.
Specimen released and annealed on Mo grid 675°C, 2 hours.
under vacuum

Measured misorientation: 34.49° ± 0.7°
Very close to Σ=5: $\theta_{\Sigma=5}$=36.87°
$\Delta\theta$= -2.38°

BCC Σ=5 [001]: Interfacial Crystallography



36.87° Rotation about [001]

BCC Σ=5 [001]: Interfacial Crystallography

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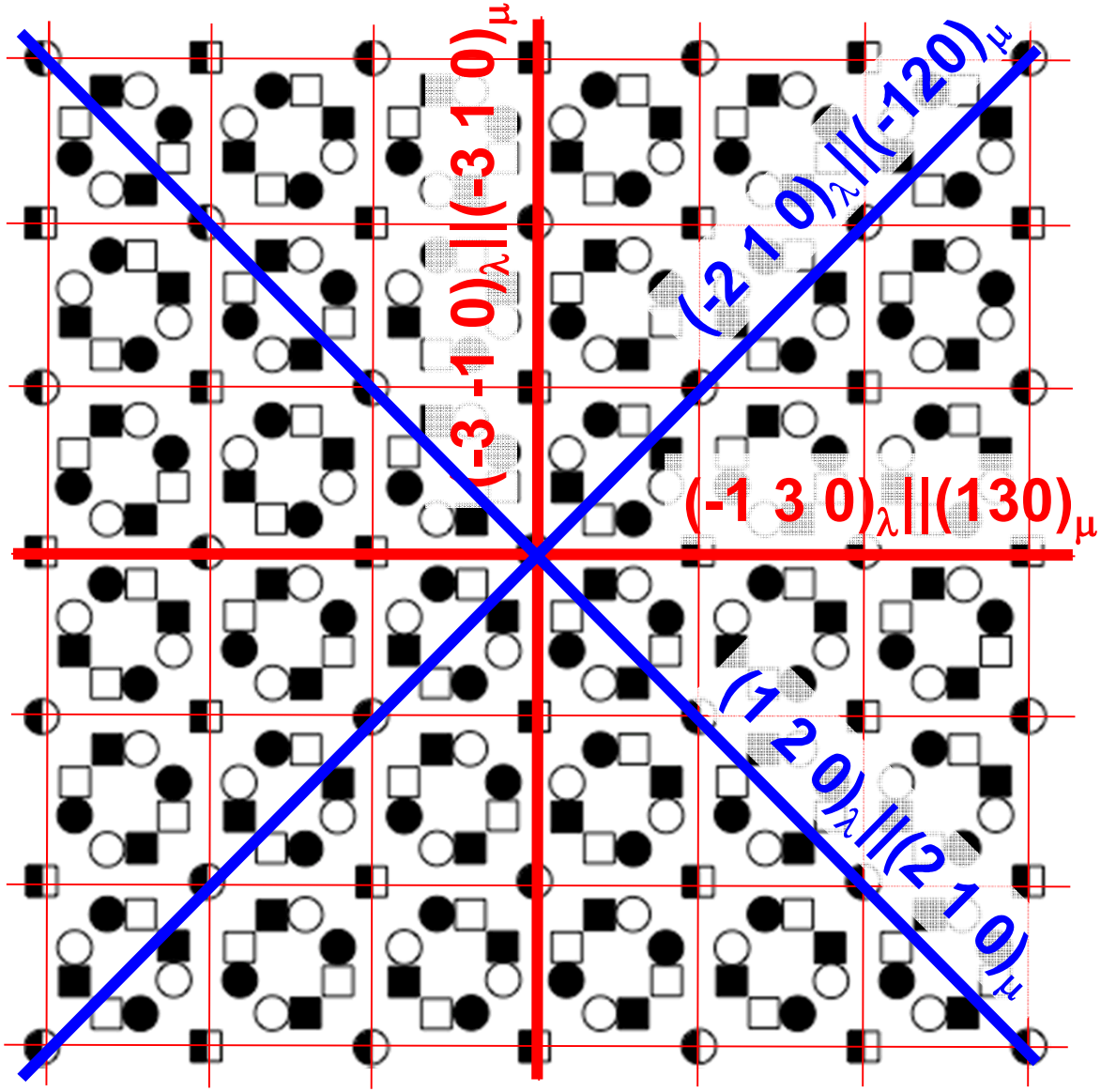
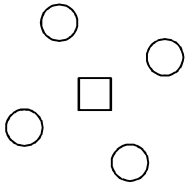
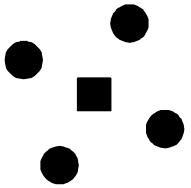
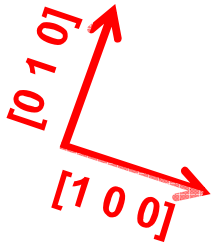
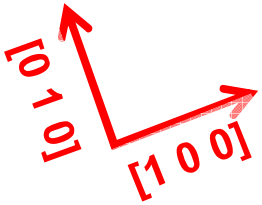
Dichromatic Pattern











HRSTEM shows nanoscale faceting at Grain boundary

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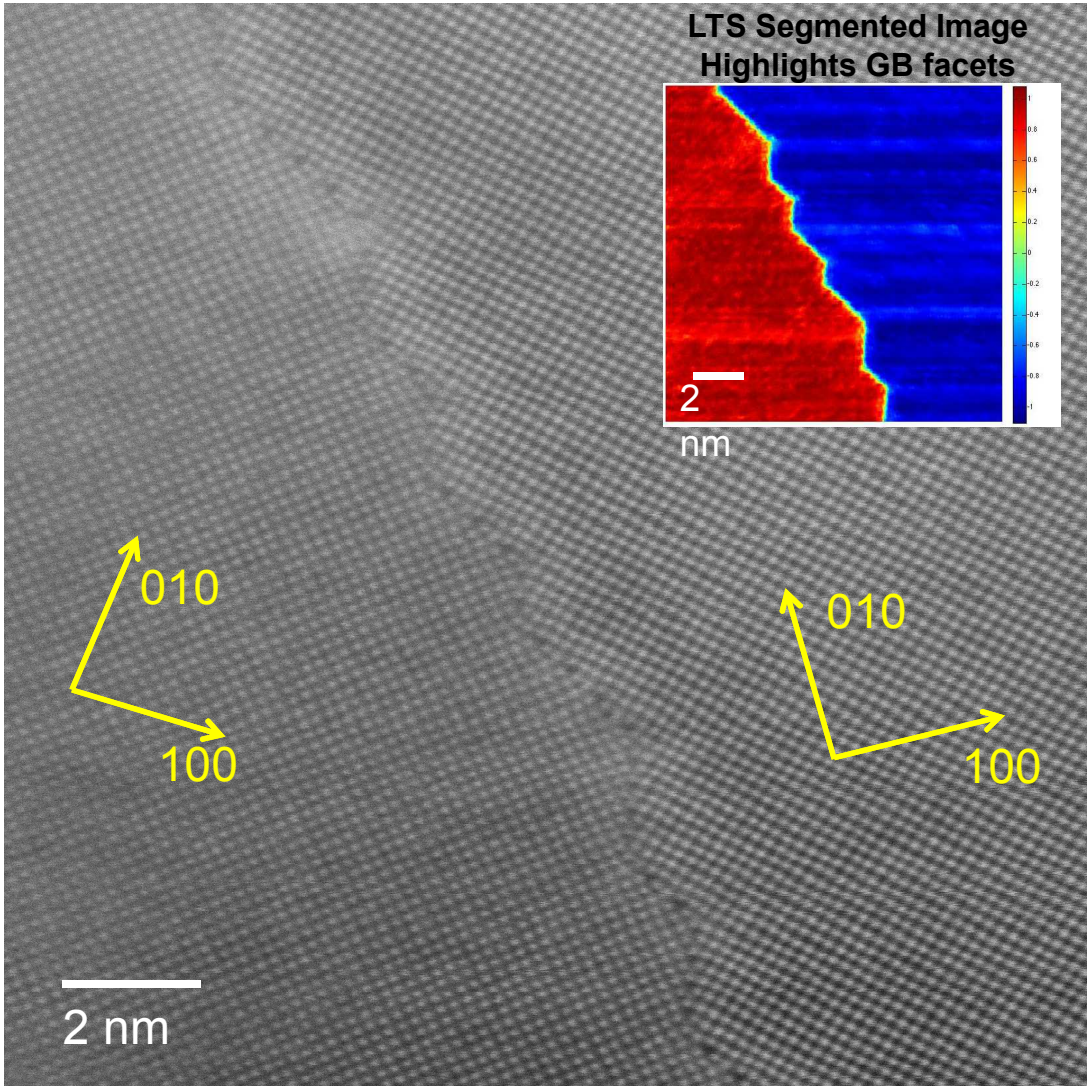
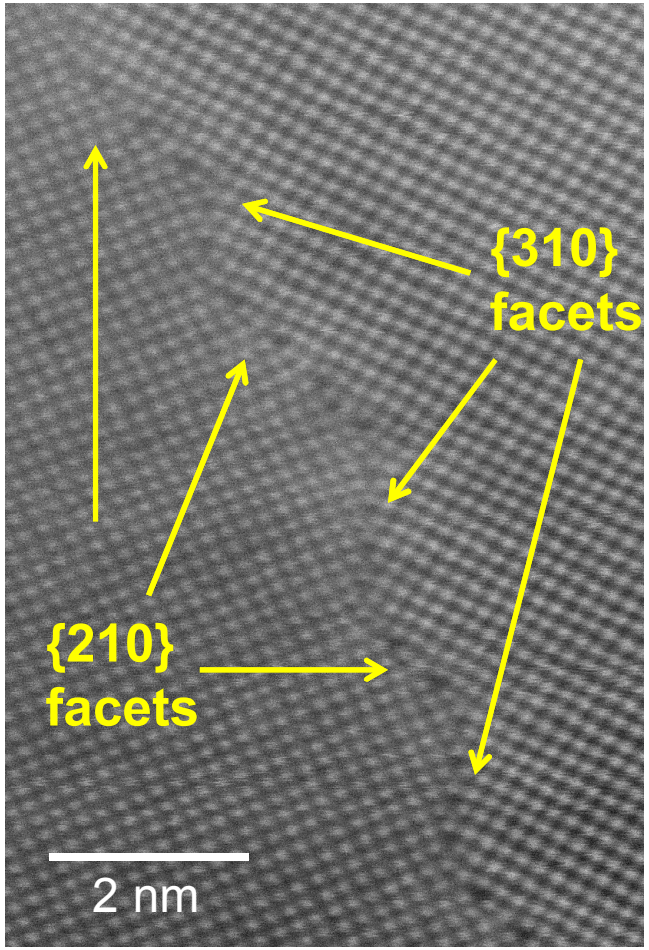
HAADF-STEM Σ=5 <001> Boundary in Fe



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



Inclination from {310}: ≈25°

Variation in Structure and Energy with inclination: MD shows 310 and 210 faceting

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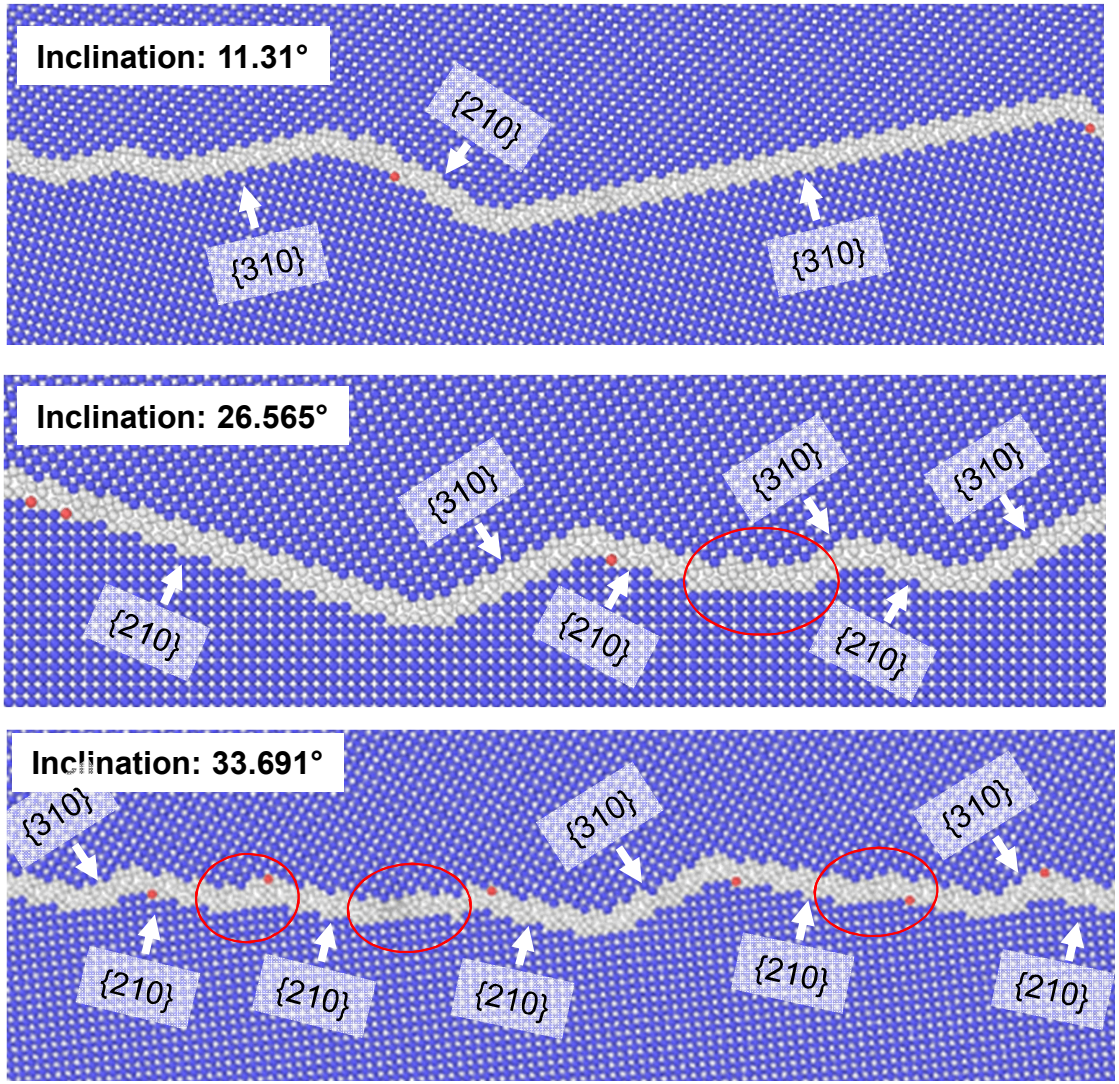
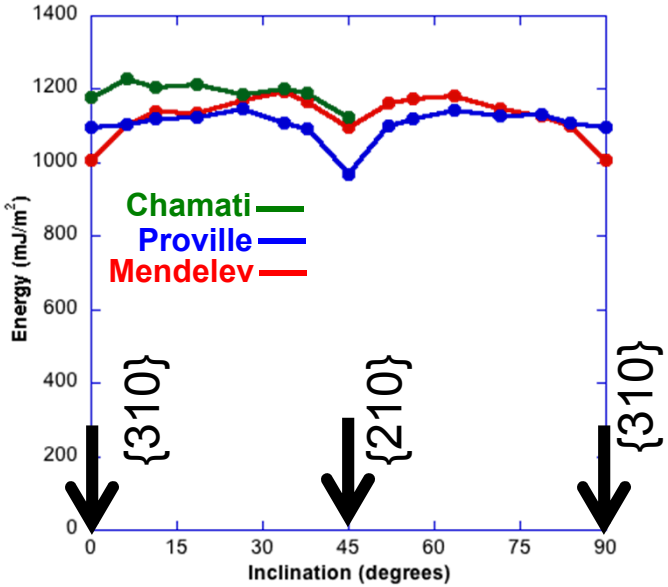


Mendelev Potential

GB Energy vs. Inclination



Atomistics show dissociation into coexisting {310} and {210} facets.

Additional faceting on {710}/{110} planes:

-1:1 ratio of {310} and {210} units

-Not fully coarsened into lower energy {210}, {310} facets.

Atoms shaded by CNA

Quantifying the GB Images: Peak Location

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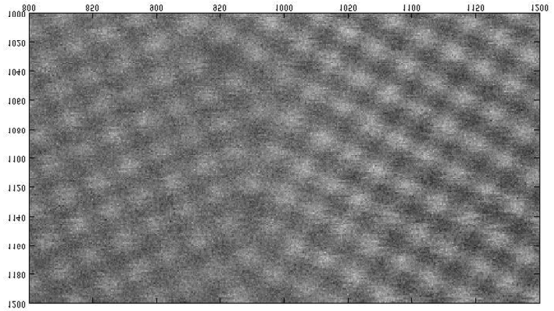
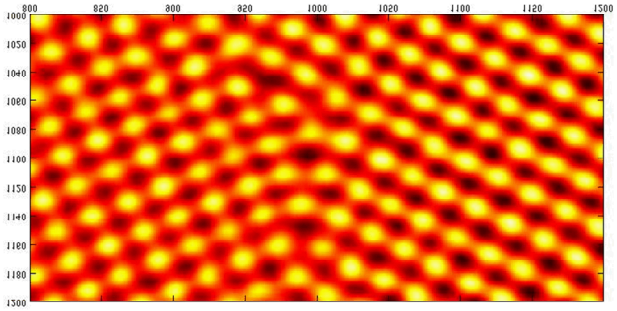
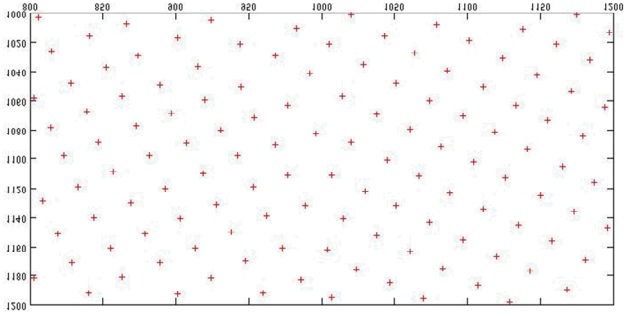
Raw HAADF STEM Image

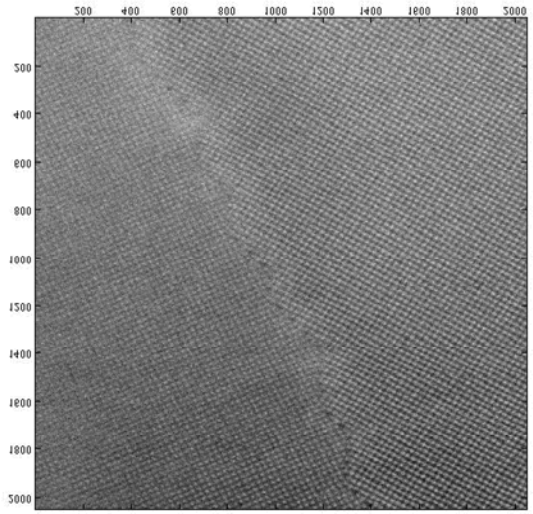


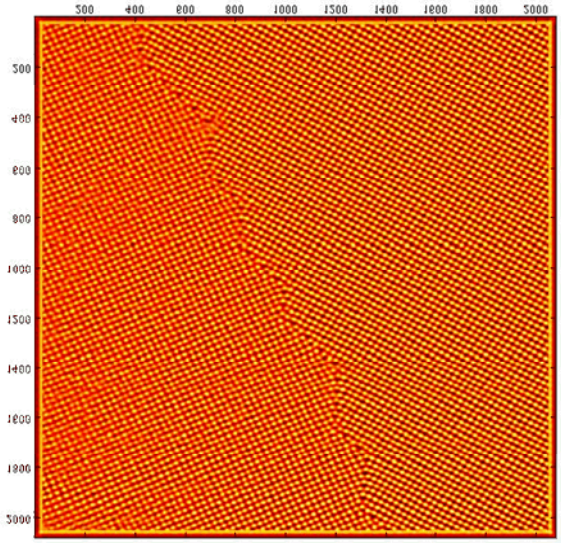
Correlation Image-Guassian

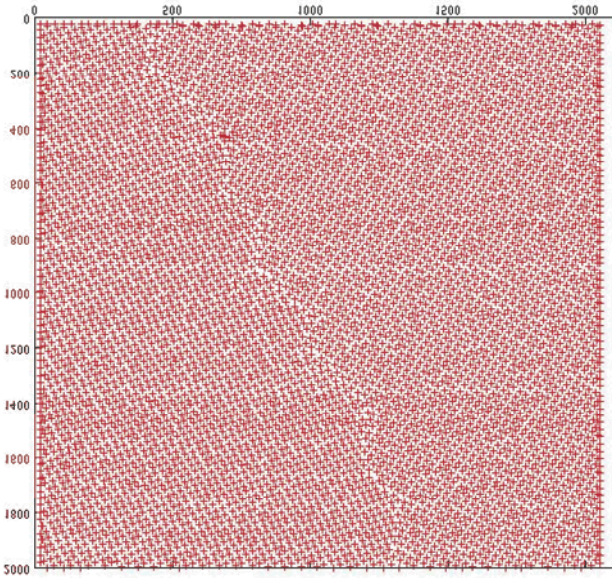


Peak Positions

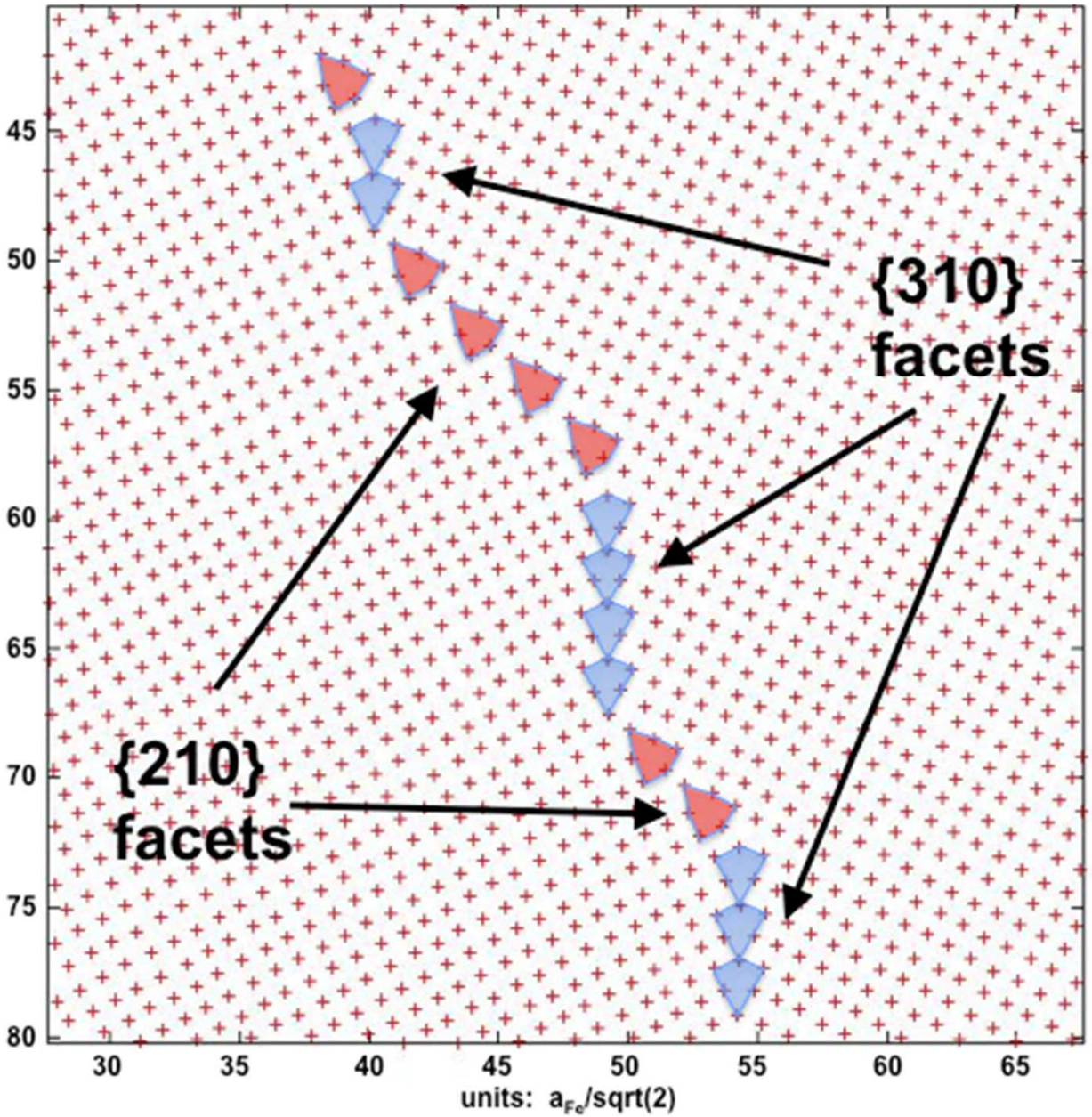








Shear distortion due to specimen drift during image acquisition.
Corrected by affine transformation to peak position array.



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Intensity peak positions from HAADF-STEM of Fe Σ=5 grain boundary

How do the {310} and {210} structural units compare with atomistic predictions?

Σ=5 {310} Structures with different Potentials

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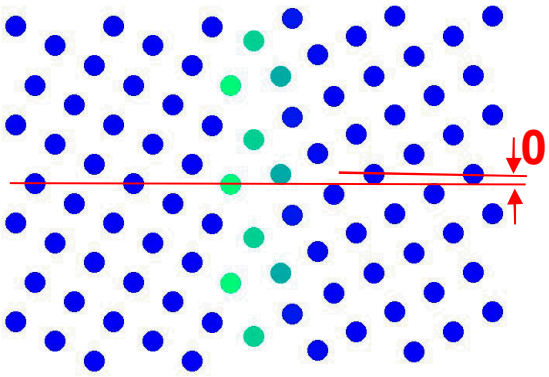
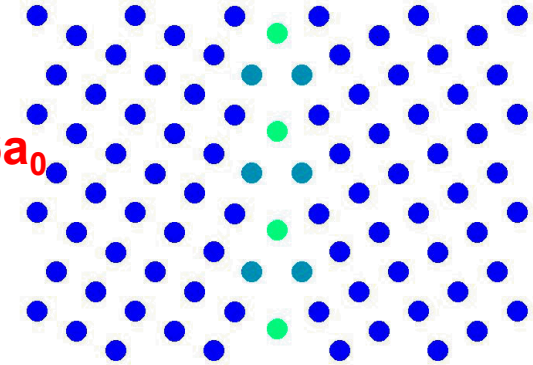
Asymmetric



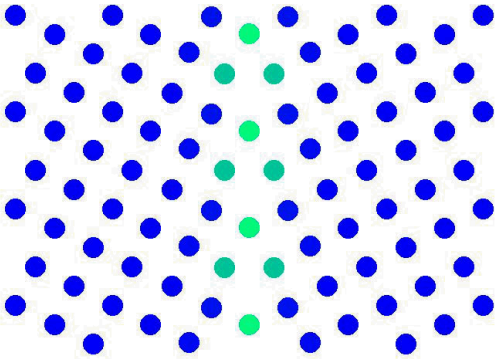
Potential: Chamati, 2006

Symmetric



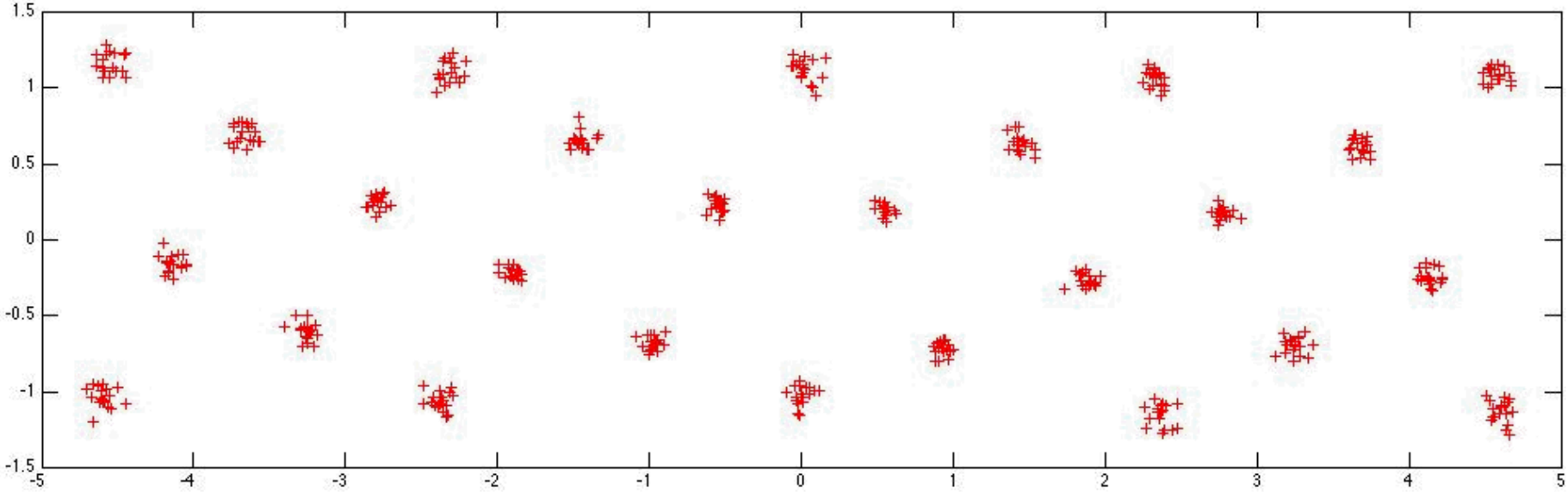
Potential: Mendelev, 2003

Symmetric



Potential: Proville, 2012

Experimental Peak Positions (HAADF STEM) $\Delta y = -0.015 \pm 0.036\ a_0$



Σ=5 {210} Structures with different Potentials

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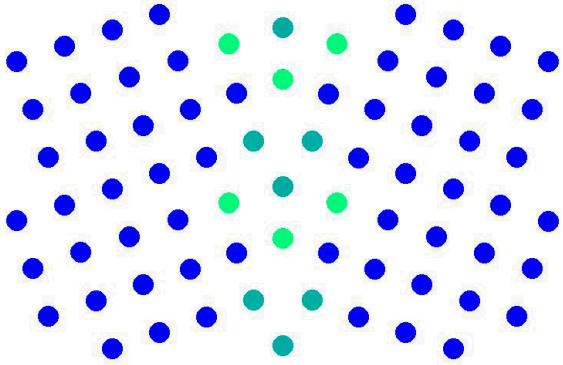
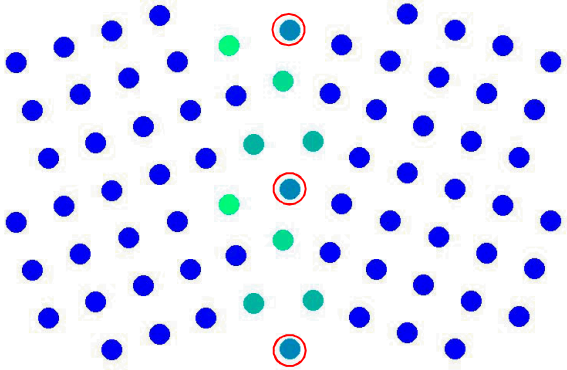
Symmetric



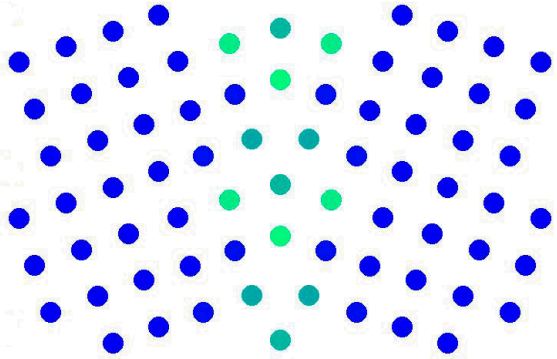
Potential: Chamati, 2006

Asymmetric



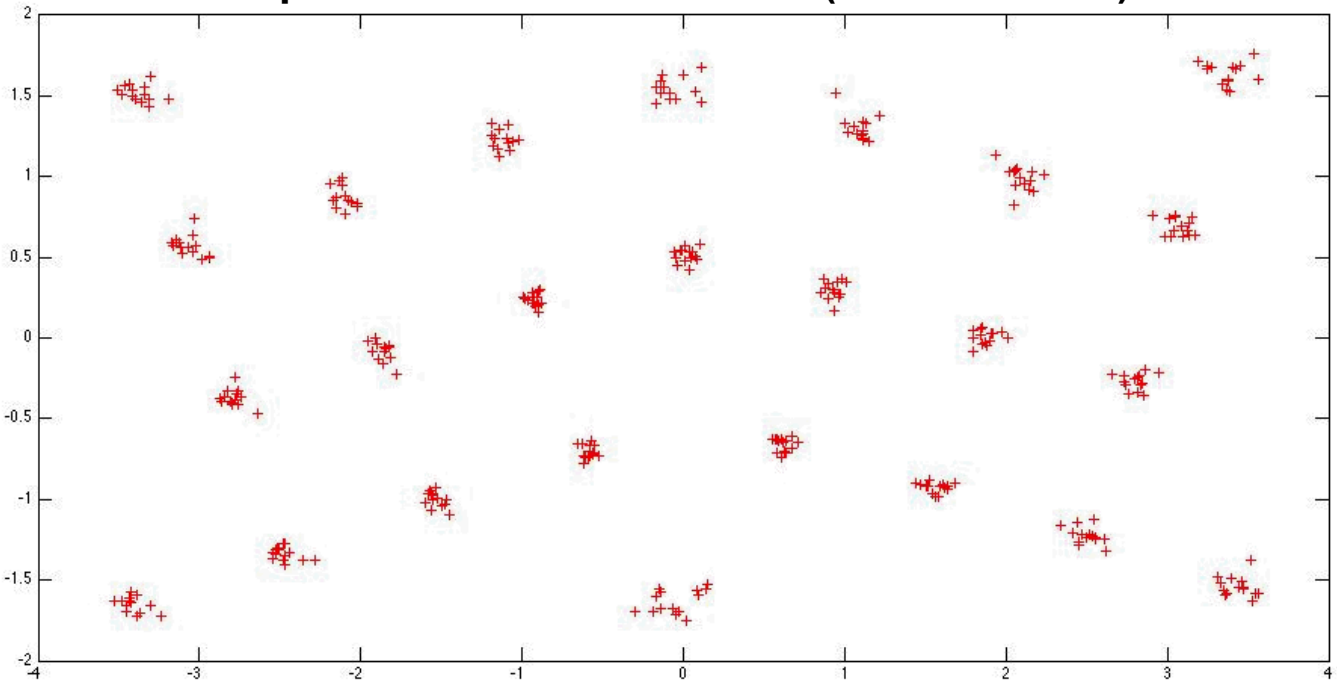
Potential: Mendelev, 2003

Symmetric



Potential: Proville, 2012

Experimental Peak Positions (HAADF STEM)



$\Delta y = 0.035 \pm 0.015\ a_0$

Are Grain Boundary Dislocations Present?

Boundary is misoriented from exact Σ=5 (Δθ=-2.38°)

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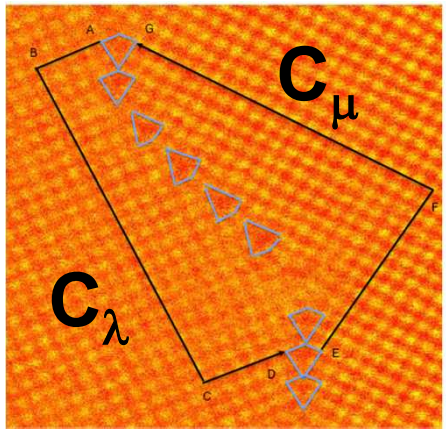
Determine defect content by Circuit Mapping over all facet junctions



Path in μ crystal

Path in λ crystal

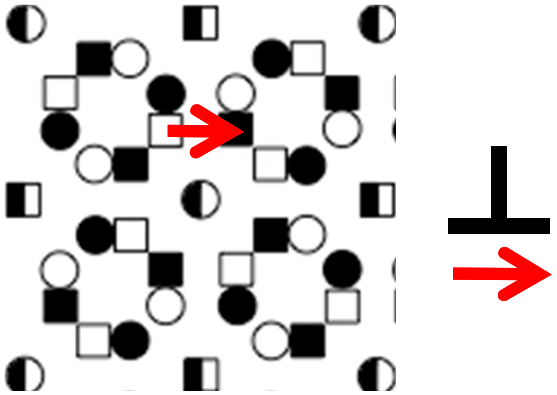
$$\mathbf{b} = -(C_\lambda + \mathbf{P}C_\mu)$$

Burgers vector

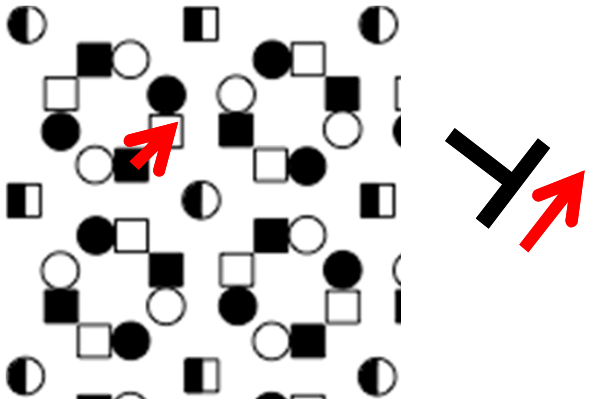
Re-express μ path in λ crystal coordinates.

Two types of defect observed:

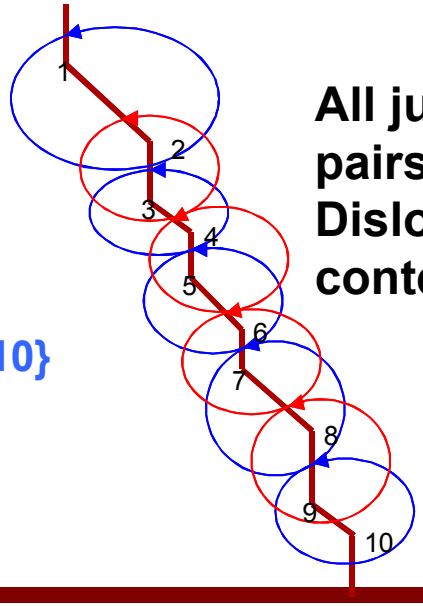
b=(1/5)[3,1,0]



b=(1/5)[1,2,0]

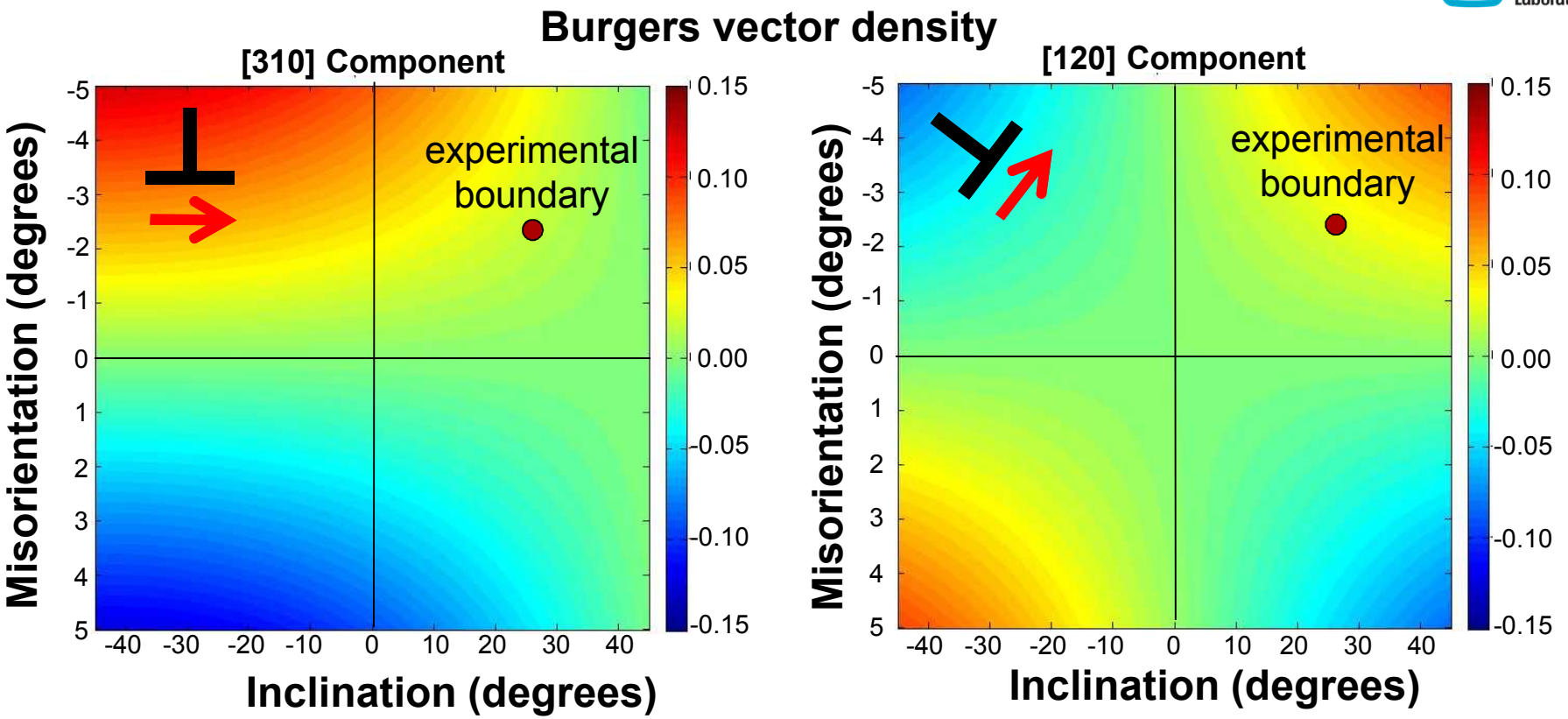


-Circuits must cross at equivalent GB sites
-Every circuit then includes 2 junctions.
-Alternate between circuits on {210} and {310} inclinations



All junction pairs exhibited Dislocation content

Defect content tied to misorientation and inclination



- **Burgers vector density related to misorientation and inclination through Frank-Bilby Equation: $B=(I-P^{-1})\,v$**

Experimental	Frank-Bilby equation (θ=-2.38°±0.8°, ϕ=25.9±1.0°)
<310> component: 0.0323	<310> component: 0.0180 ±0.006
<120> component: 0.0152	<120> component: 0.027 ± 0.010

- **For inclinations away from {310}, b_{120} component required to accommodate interfacial coherency strains.**

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

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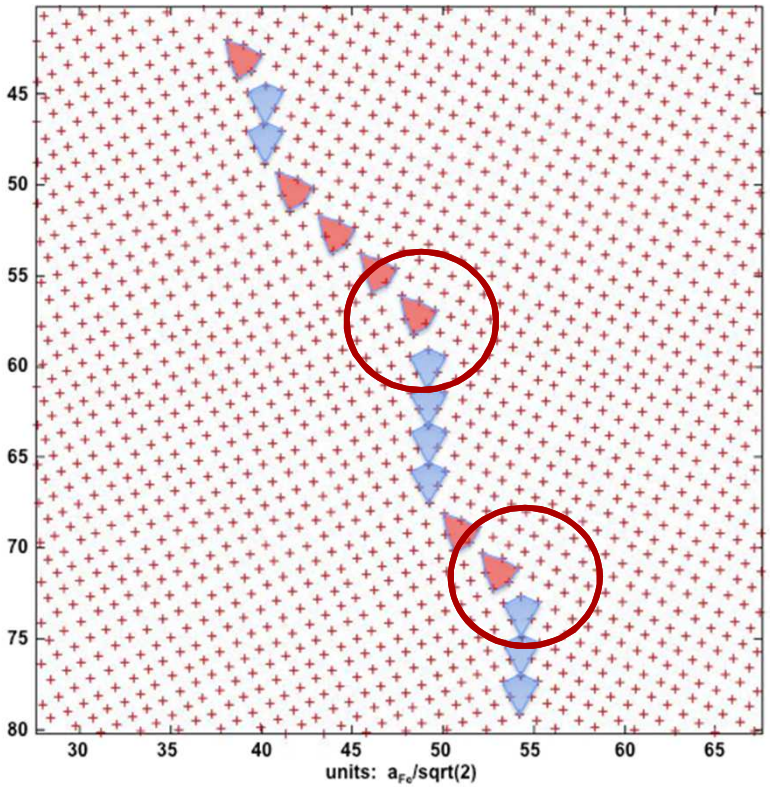
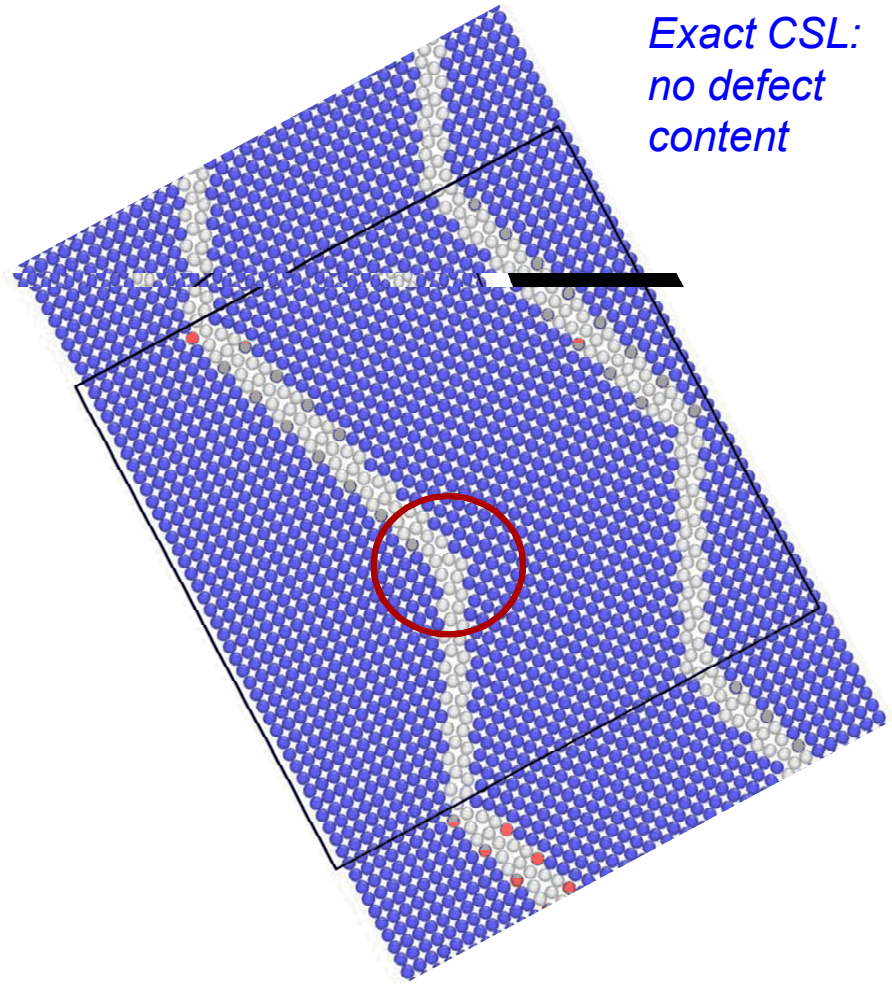
Experimental Junctions
b=(1/5)(120) and (1/5)(310)



Relaxed Periodic Atomistic Structure

Exact CSL: no defect content



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

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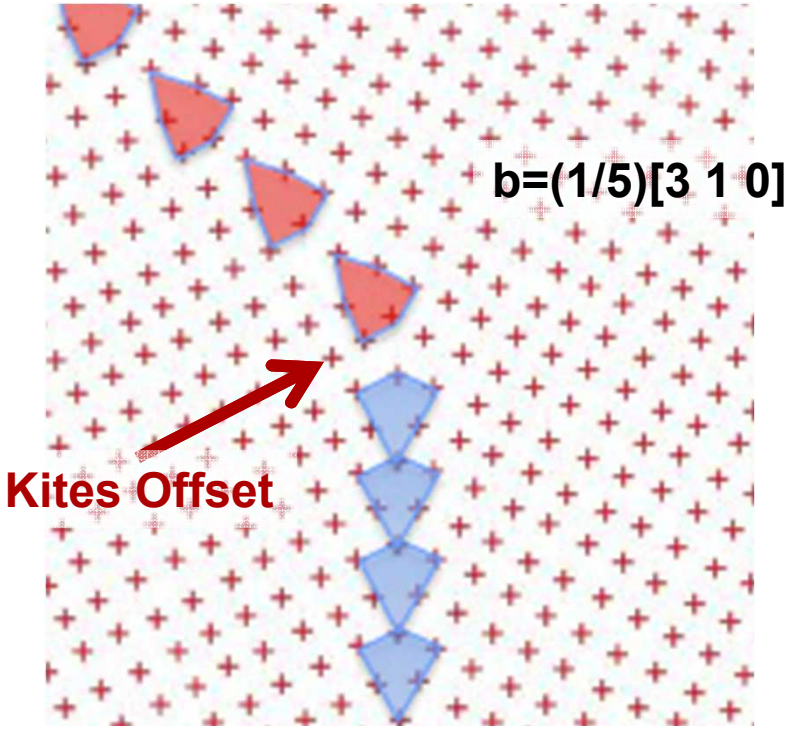
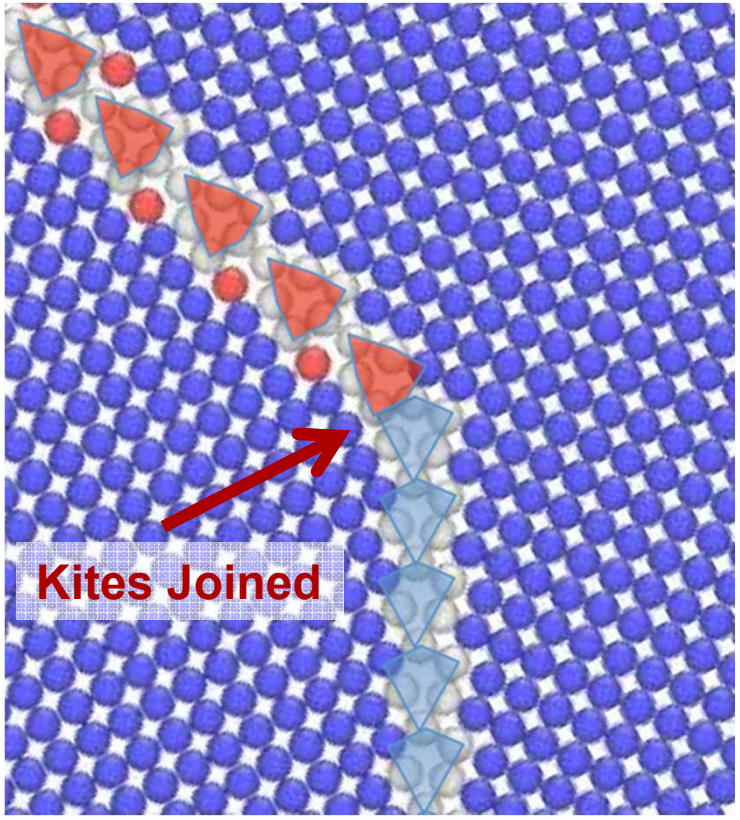
Experimental Junctions
b=(1/5)(120) and (1/5)(310)



Relaxed Periodic Atomistic Structure



Geometric origin of the junction structure

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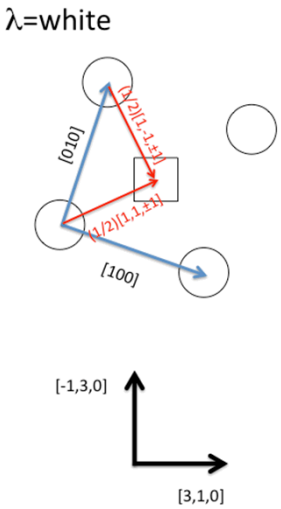
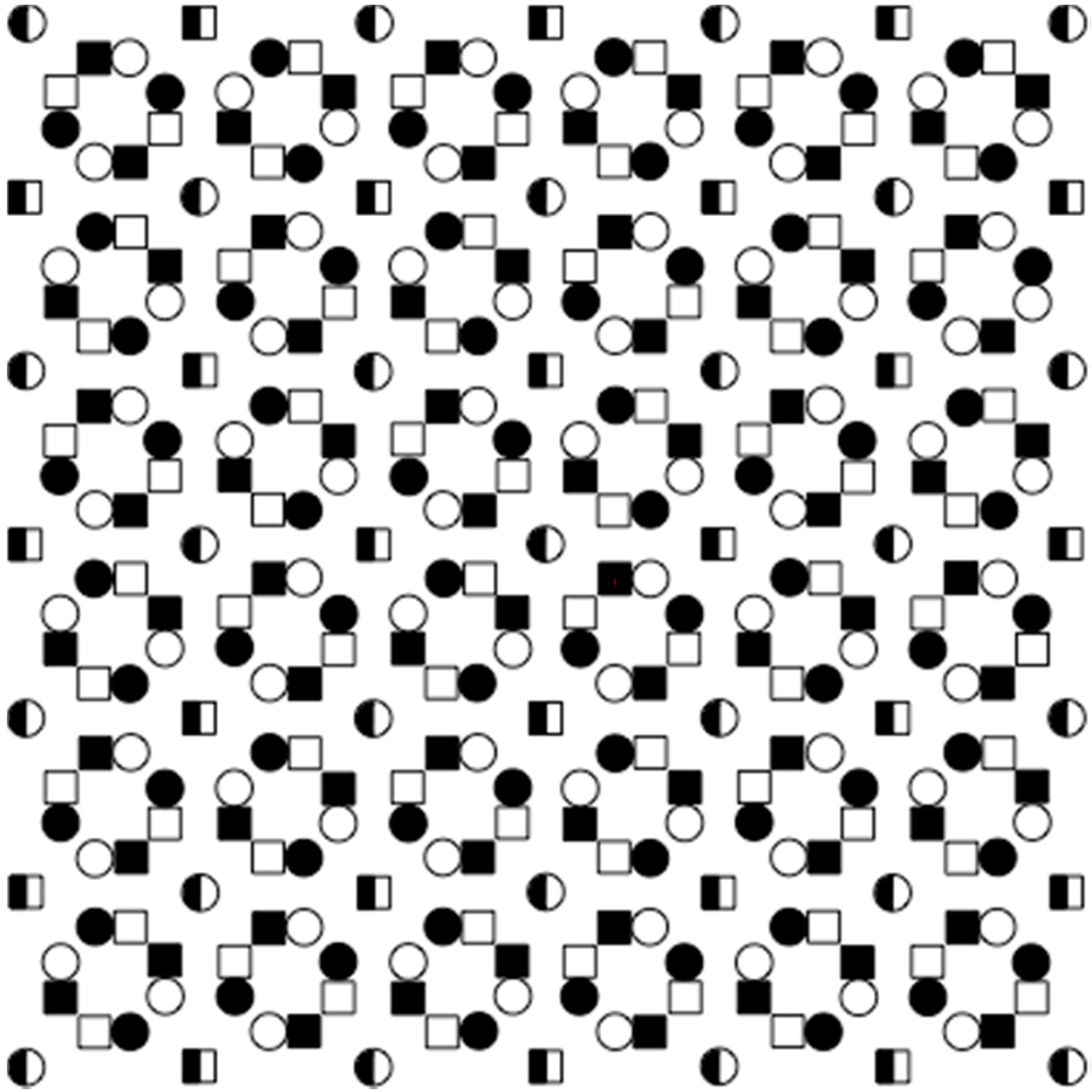
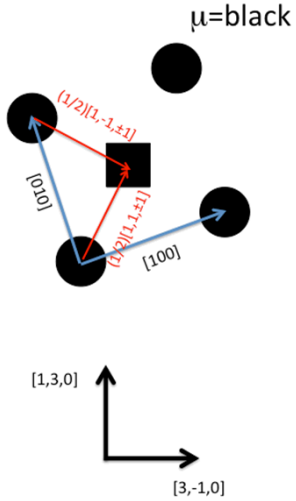
Σ=5 Dichromatic Pattern







Geometric origin of the junction structure

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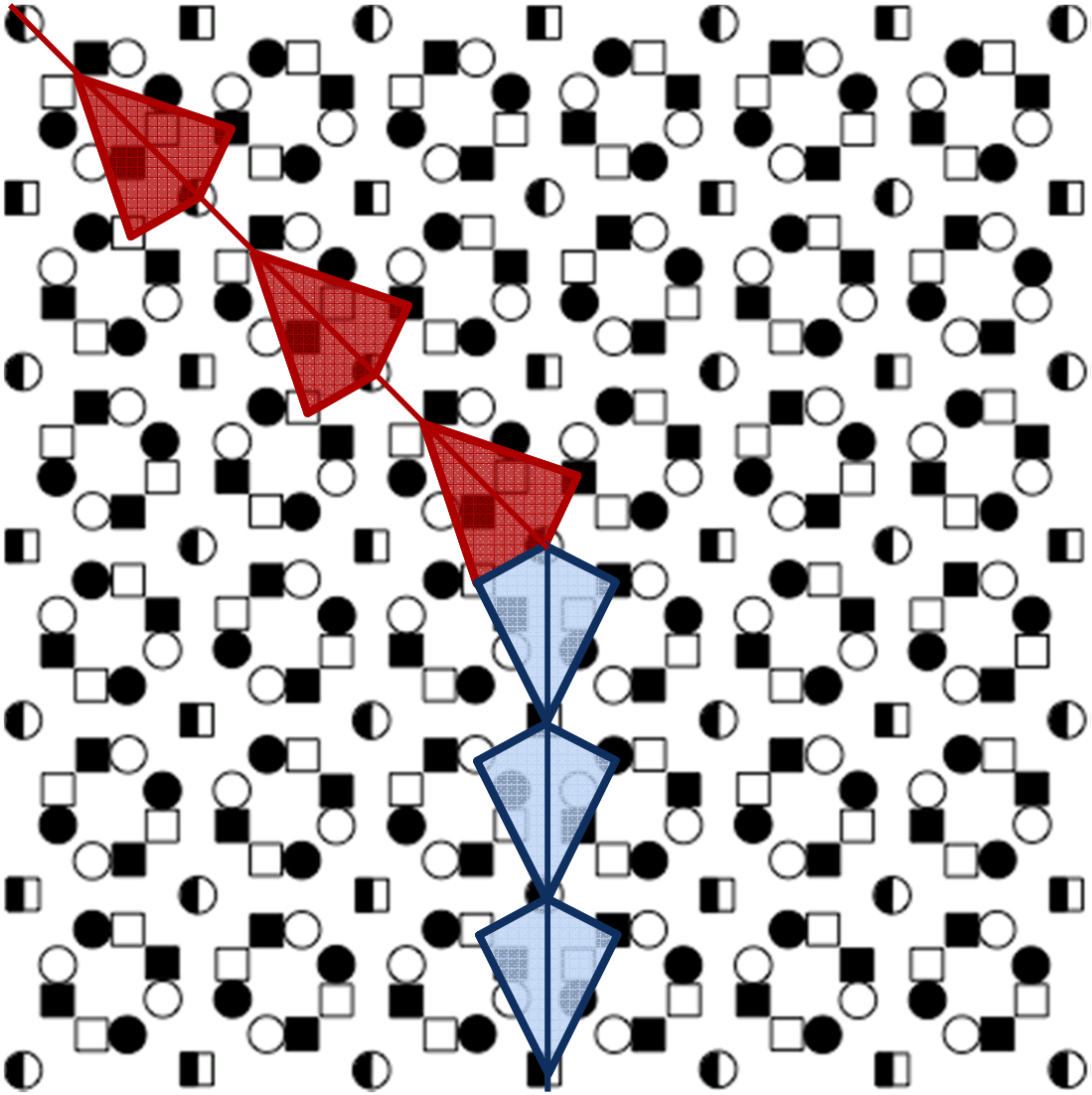

Geometric origin of the junction structure

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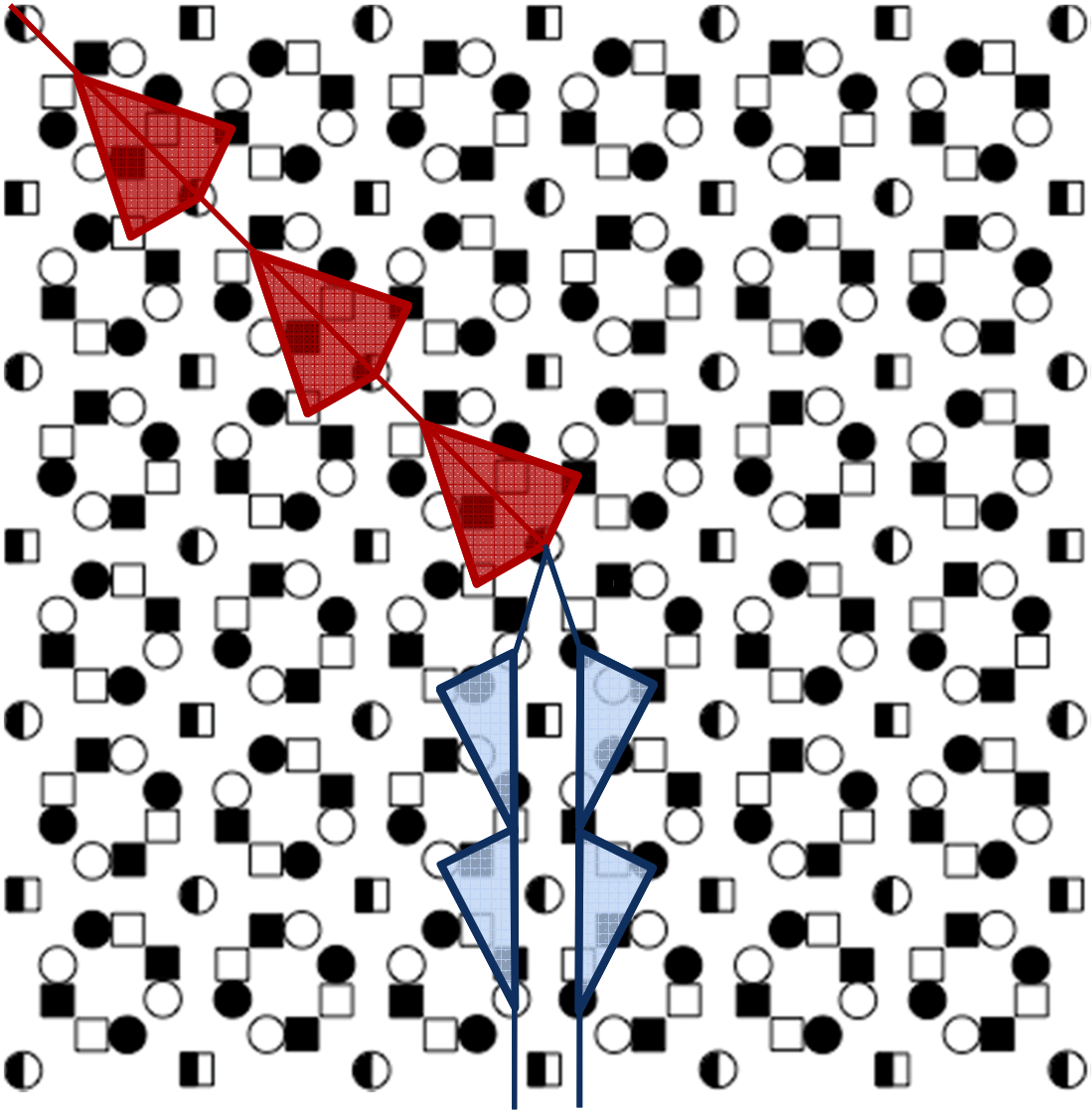
Remove material from half-plane of width (1/5)[310]



Geometric origin of the junction structure

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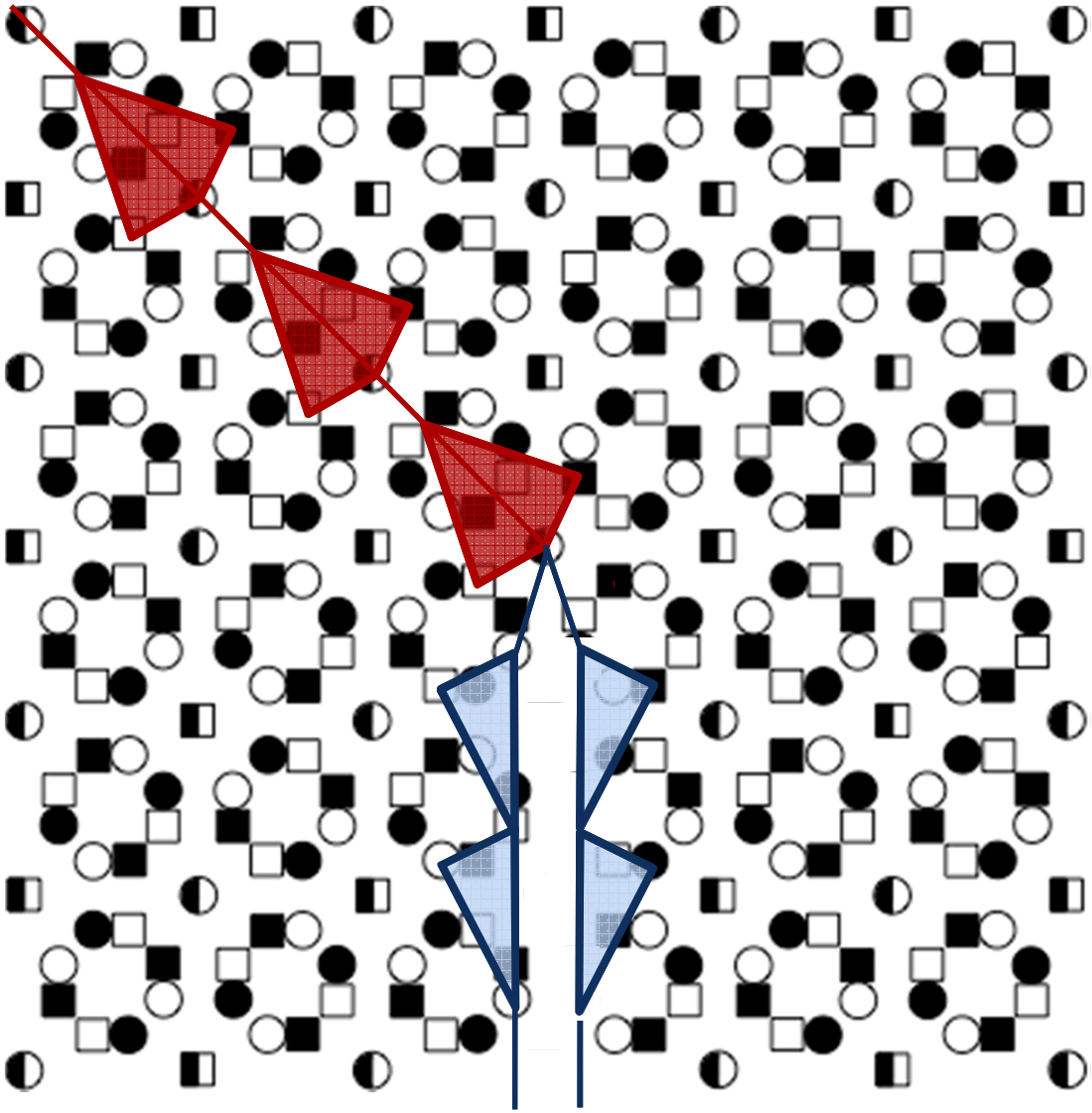
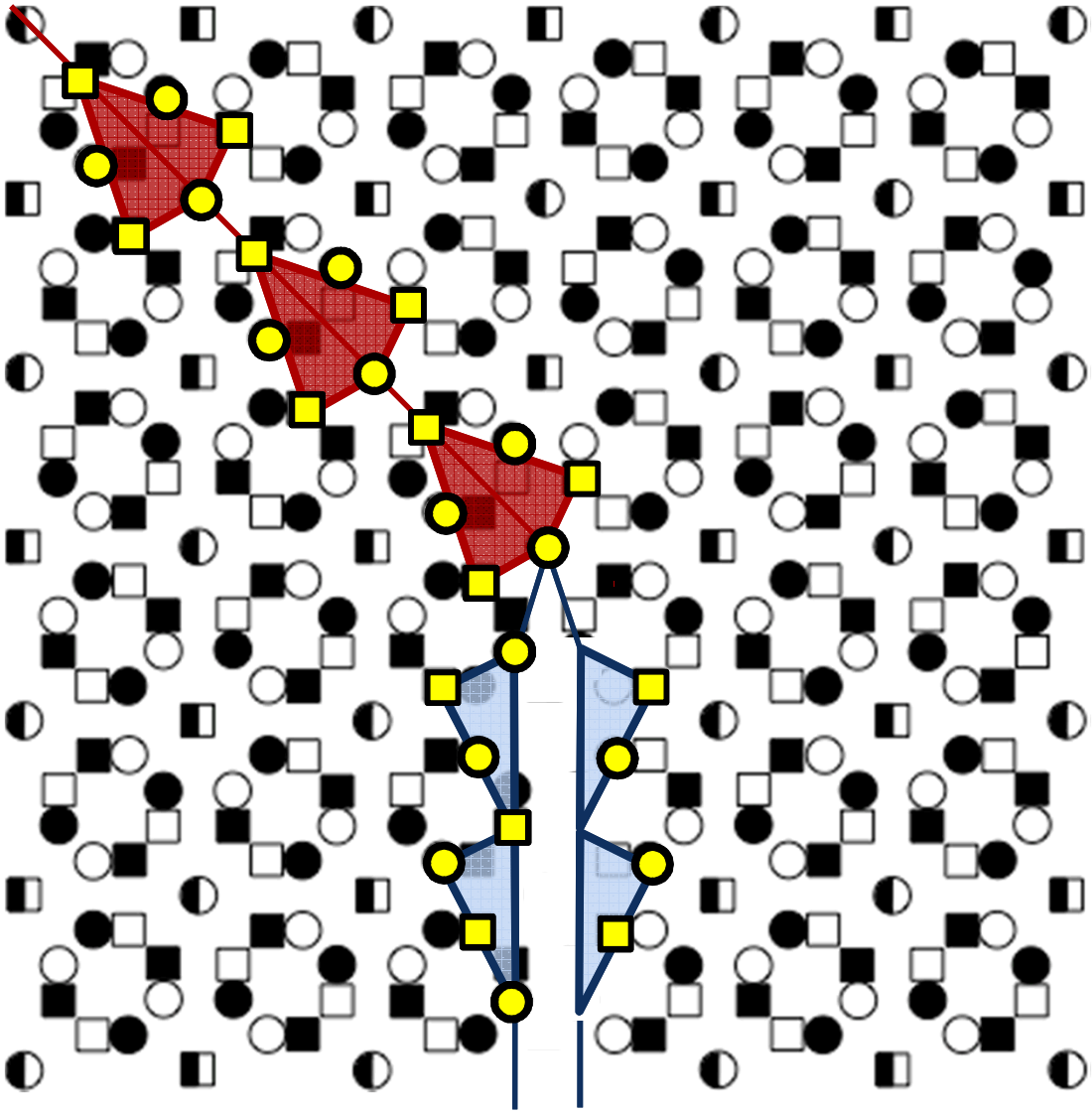
Remove material from half-plane of width (1/5)[310]

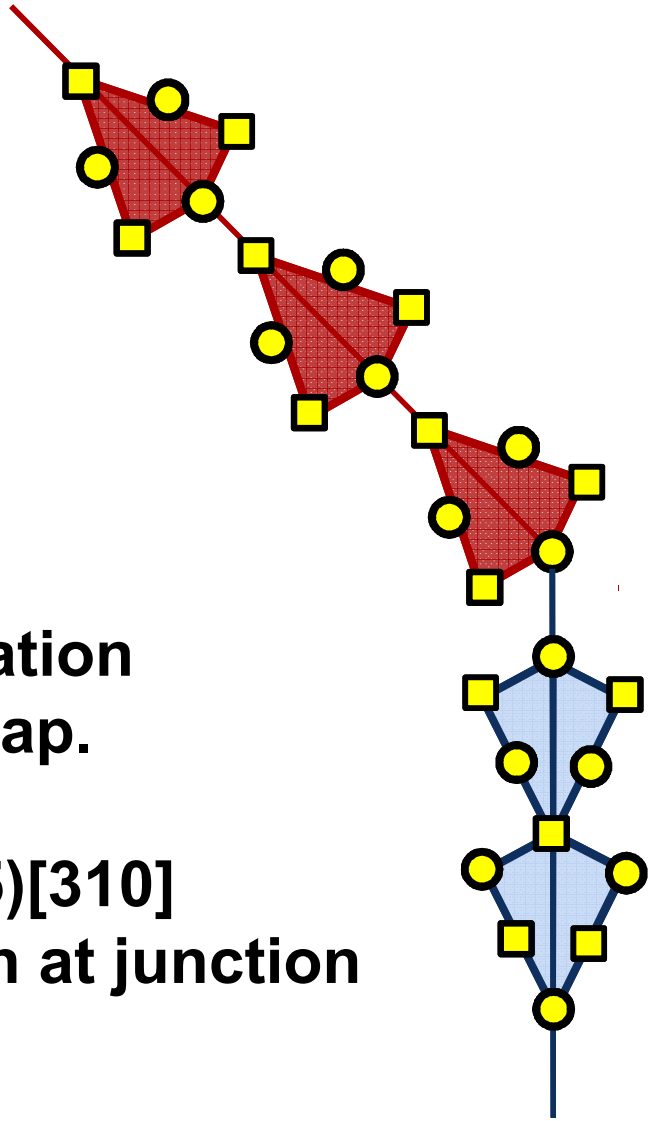


Geometric origin of the junction structure

Sandia National Laboratories



Geometric origin of the junction structure



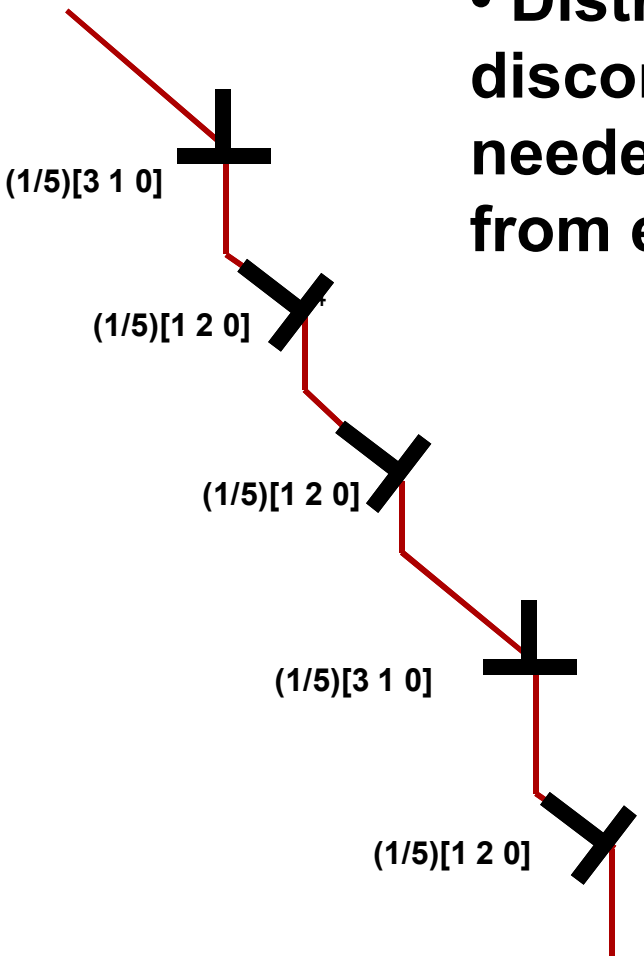
Kites are now off-set

Volterra operation
to close the gap.

Creates a (1/5)[310]
disconnection at junction

Similar
construction for
(1/5)[120]
disconnection

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.

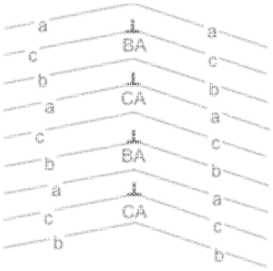
- Suggests that facet length scale here is tied to misorientation/inclination via dislocation content.

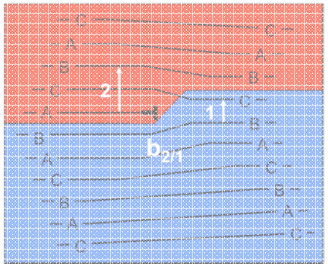
Outline

Background on Interfacial Line defects

-Overview of defect types

-Examples from low and high angle GBs.

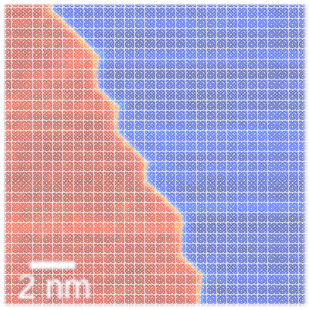


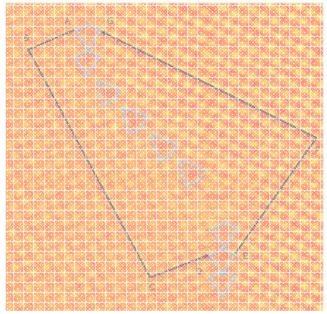


GB disconnections and facet junctions

-Asymmetric Σ=5 GB in BCC Fe

-Interplay of facet junctions and grain boundary disconnections

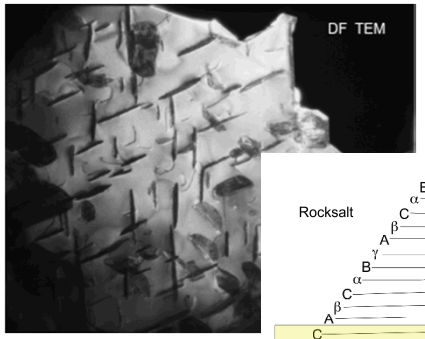




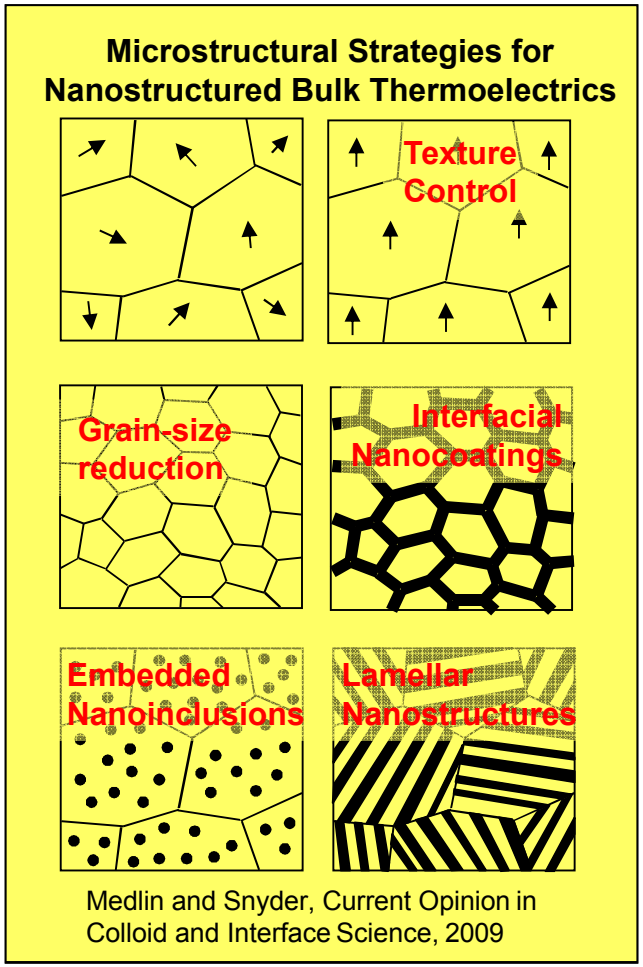
Disconnections at heterophase interfaces

-Telluride precipitates in thermoelectric alloy.

-Role of disconnections in transformation mechanism and interfacial strain relief.



Bulk Thermoelectrics: Control of Microstructure to Improve Performance



TE Energy Conversion Efficiency: Figure of Merit

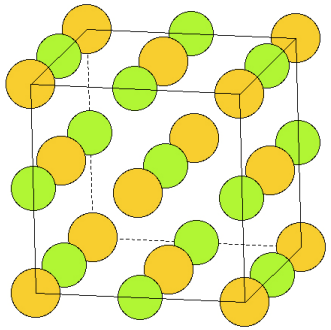
Seebeck Coefficient, Electrical Conductivity, Thermal Conductivity

$$zT = \frac{S^2\sigma}{\kappa}T$$

- **Variety of microstructural strategies for bulk thermoelectrics employ embedded interfaces to decouple thermal and electronic transport**
- **What are the atomic mechanisms that govern interface formation and stability?**

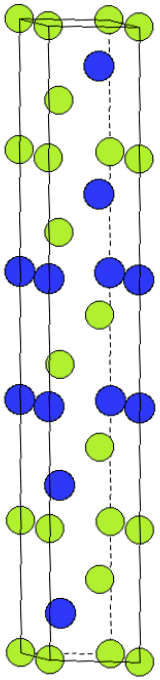
Heterophase Rocksalt/Tetradymite Telluride Interfaces

Rock-Salt
($PbTe$, $AgSbTe_2$)



Fm-3m

Tetradymite
(Bi_2Te_3,Sb_2Te_3)



R-3m

What happens at interface?
How do transformations occur?
Misfit accommodation?

-Interest in forming thermoelectric nanocomposites of rock-salt and tetradymite tellurides:

-Possibility for well ordered interfaces.

-Transformations provide bulk route to synthesis.

Ikeda, et al., Chem Mater. 2007

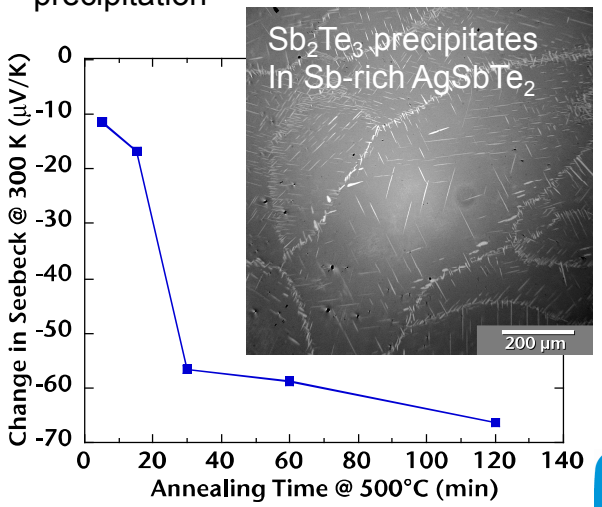
Snyder and Toberer, Nature Materials 2008

-$AgSbTe_2$:

-Constituent of TAGS $(GeTe)_x(AgSbTe_2)_{1-x}$ and LAST $(PbTe)_x(AgSbTe_2)_{1-x}$ zT ~ 1.8

-High performance TE material: zT > 1.2

-Degradation of Seebeck coefficient with Sb_2Te_3 precipitation



Sharma, Sugar, Medlin J. Appl. Phys. 2010

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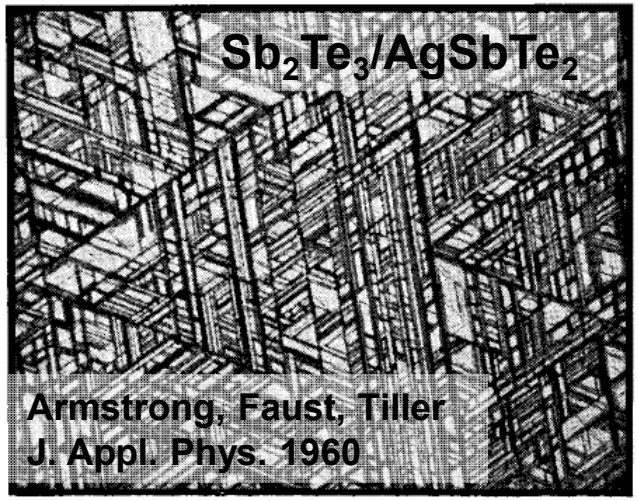
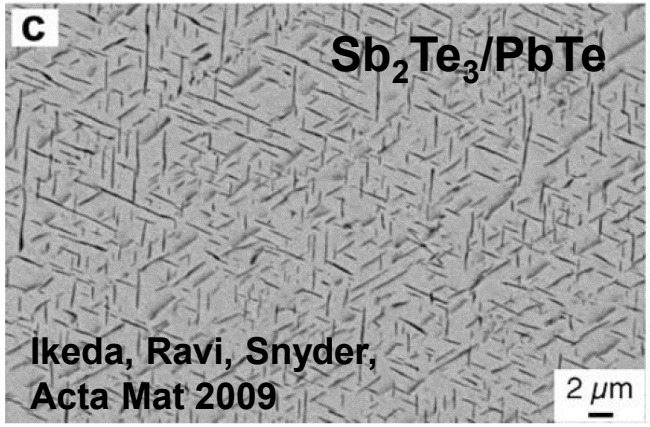
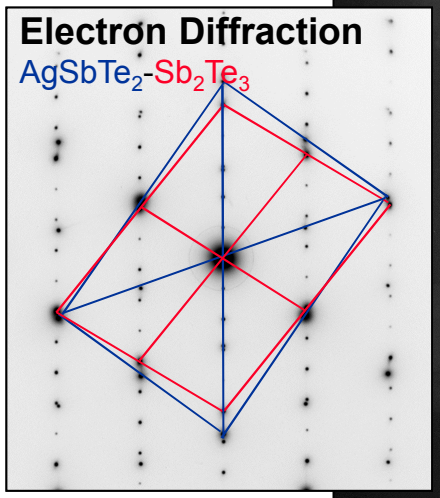
Crystallographic alignment between rocksalt and tetradymite phases

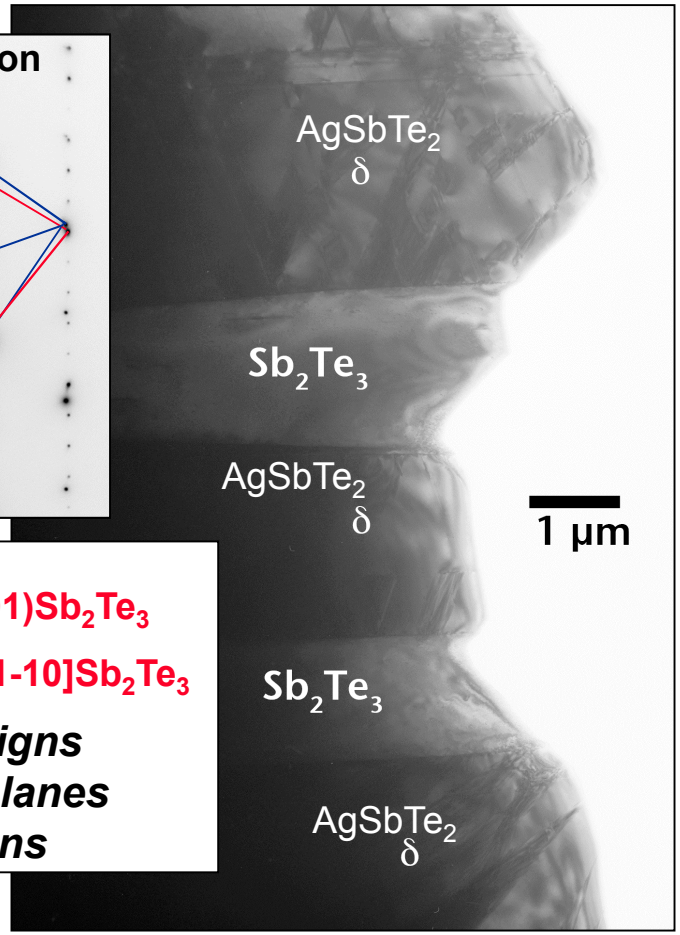
Widmanstätten plates





TEM $Sb_2Te_3/AgSbTe_2$





(111)$AgSbTe_2$ // (0001)Sb_2Te_3

[-101]$AgSbTe_2$ // [2-1-10]Sb_2Te_3

Orientation aligns close-packed planes and directions

Medlin and Sugar,
Scripta Mat 2010

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How to convert between the rocksalt and tetradymite structures?

Rocksalt

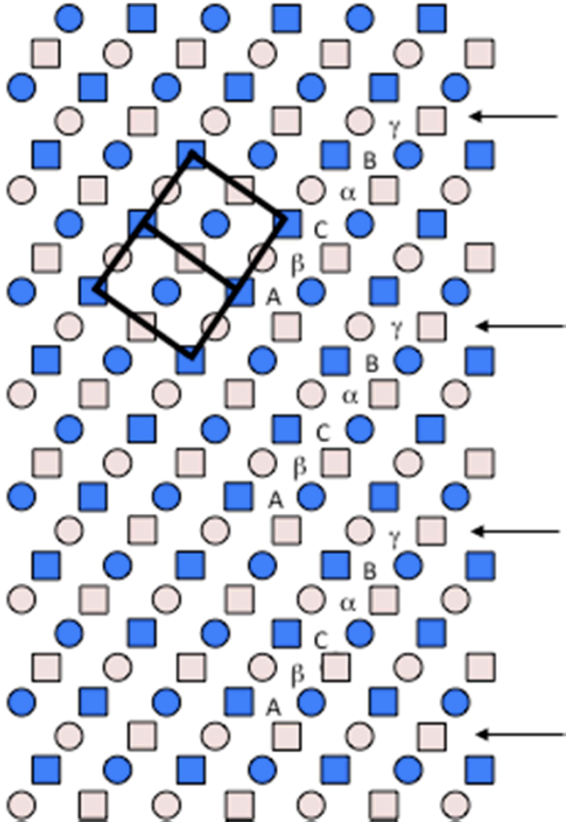
(MTe)

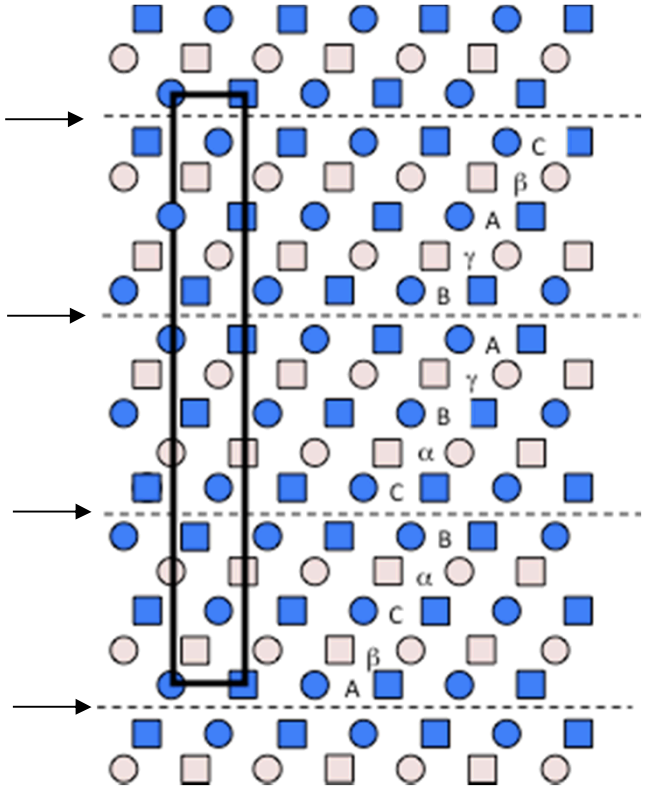
Tetradymite

(M_2Te_3)

Te

Metal





-Remove metal plane every 6 layers

-Shear blocks by 1/3<10-10> (or 1/6<112> relative to cubic coordinates)

N. Frangis et al., J. Solid State Chemistry 84 (1990)

Transformation can be accomplished by motion of disconnections

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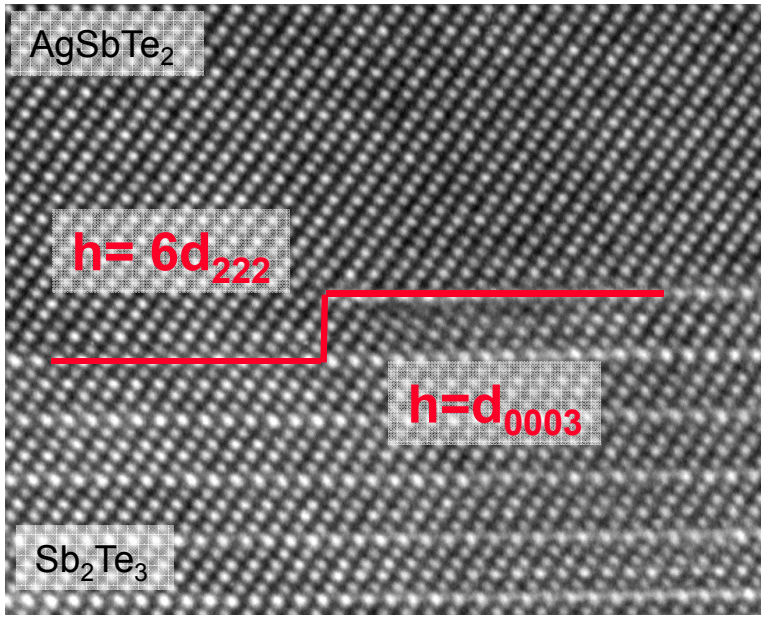
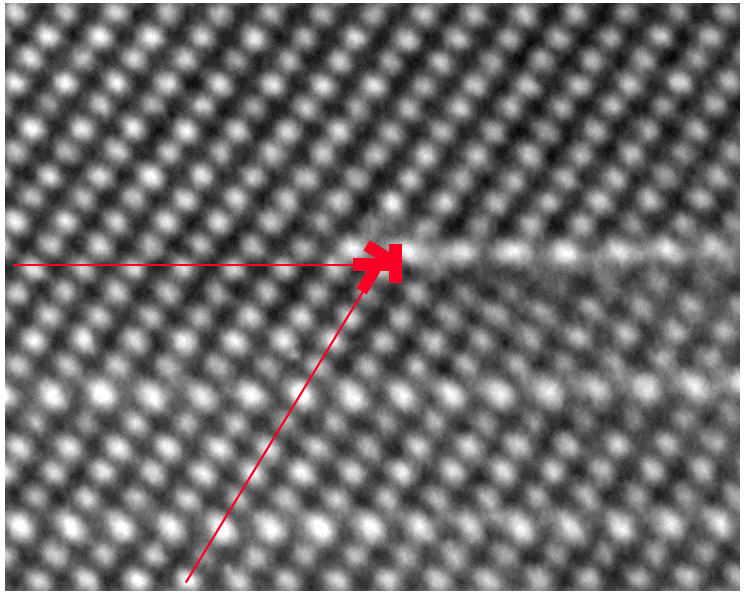
HRTEM : Step at $AgSbTe_2/Sb_2Te_3$ Interface





JEOL 4000EX HRTEM

Defect has both step and dislocation character.

-Interfacial "Disconnection" (e.g. Hirth and Pond, Acta Mat 1996).

-Geometric properties of disconnections control mass flux and structural rearrangements of phase transformations.

Step joins 6 {222} planes in $AgSbTe_2$ with 5 {000 15} planes in Sb_2Te_3

Complex dislocation configuration.

Medlin and Sugar, Scripta Materialia, 2010.

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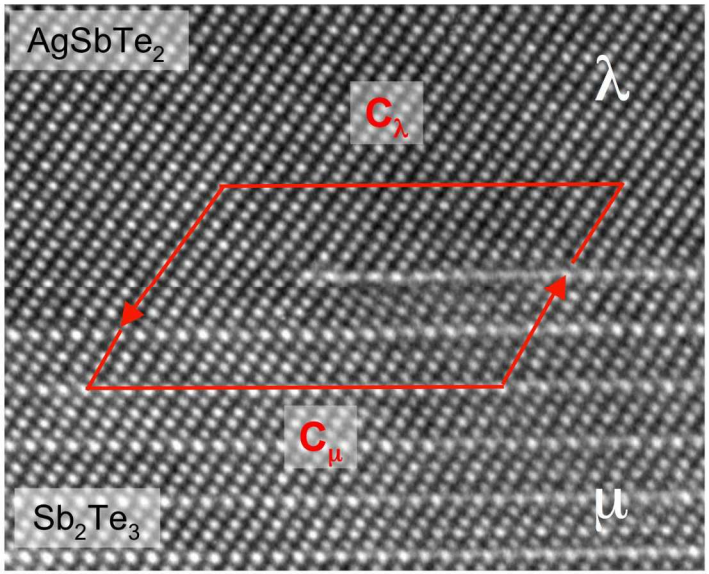
Role of defect in precipitate growth:

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

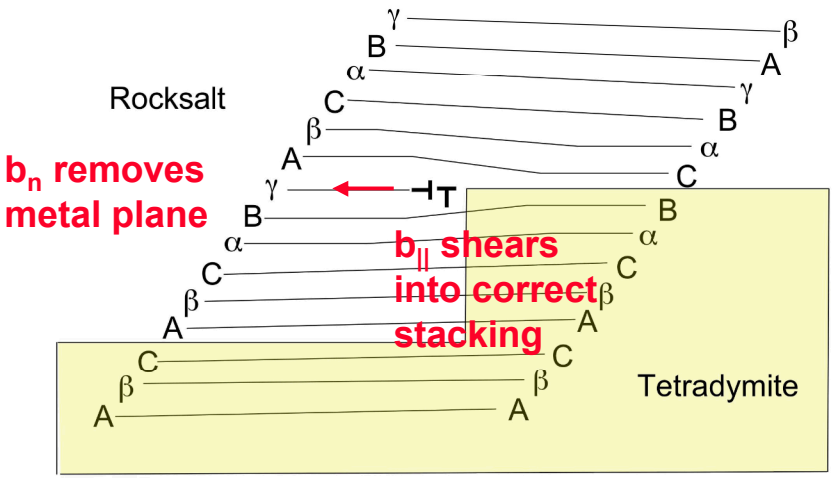
Resolve b into components normal and parallel to interface

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

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

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

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



Medlin and Sugar, Scripta Materialia, 2010.

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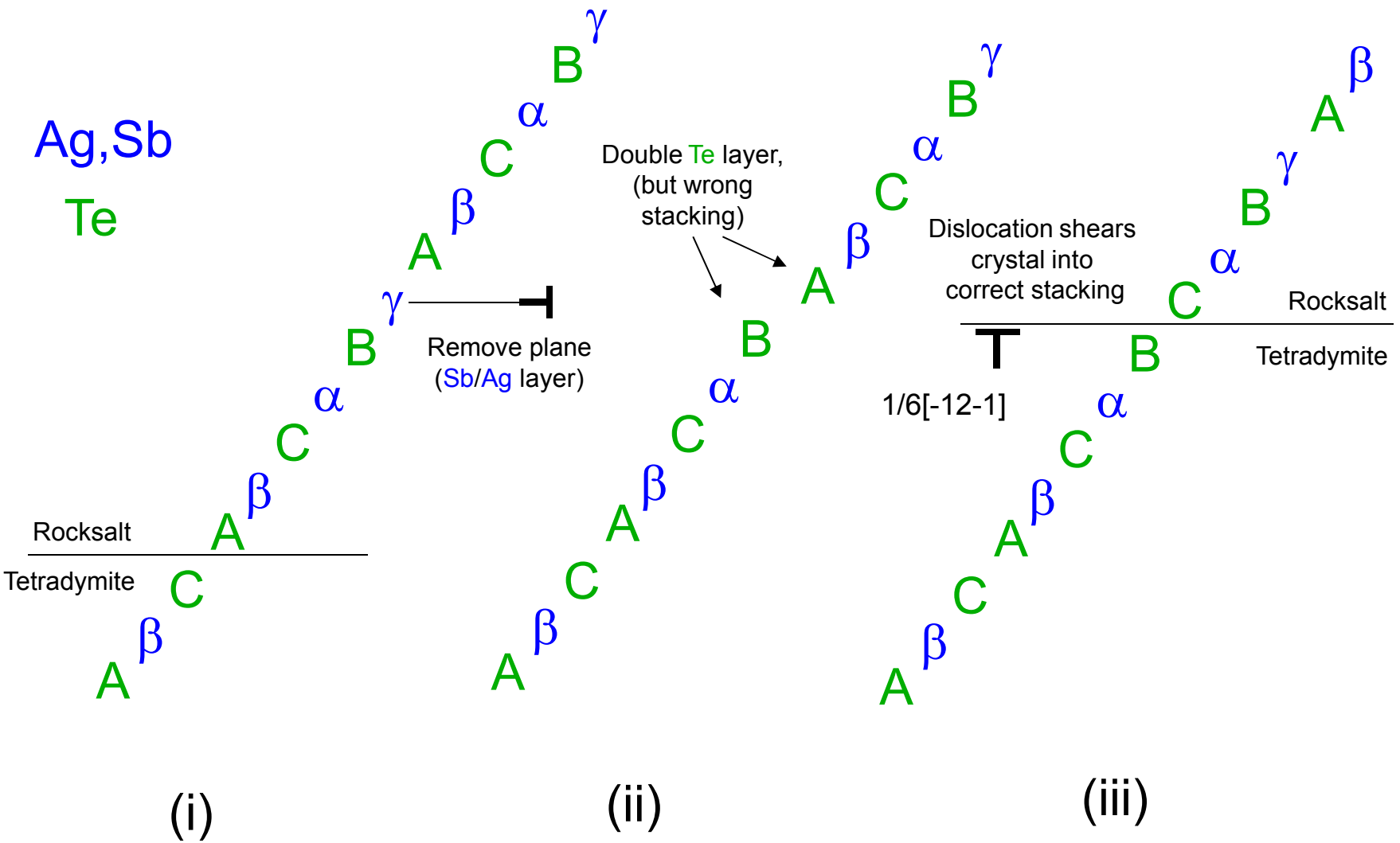
Schematic of Transformation Sequence



Medlin and Sugar, Scripta Materialia, 2010.

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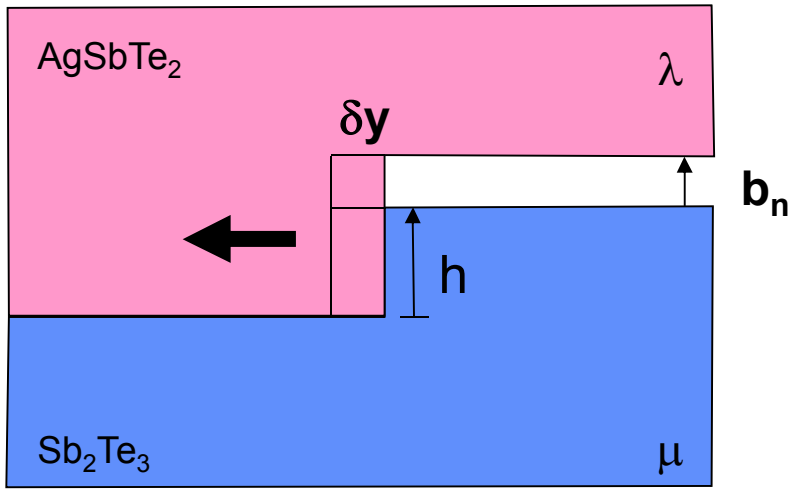
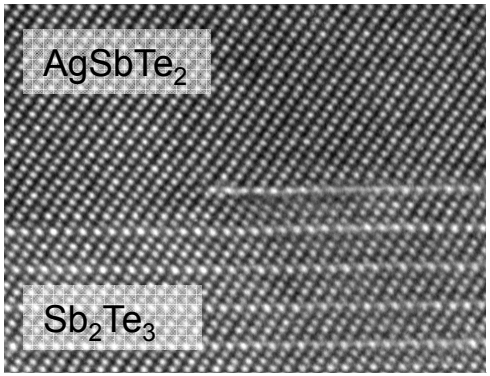
Defect properties give local mass flux required for transformation

Partition flux for defect motion into step and dislocation components





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

Hirth & Pond, Acta Mat 1996

Species	Step flux (atoms/Å²)	Dislocation flux (atom/Å²)	Total flux (atom/Å²)
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.

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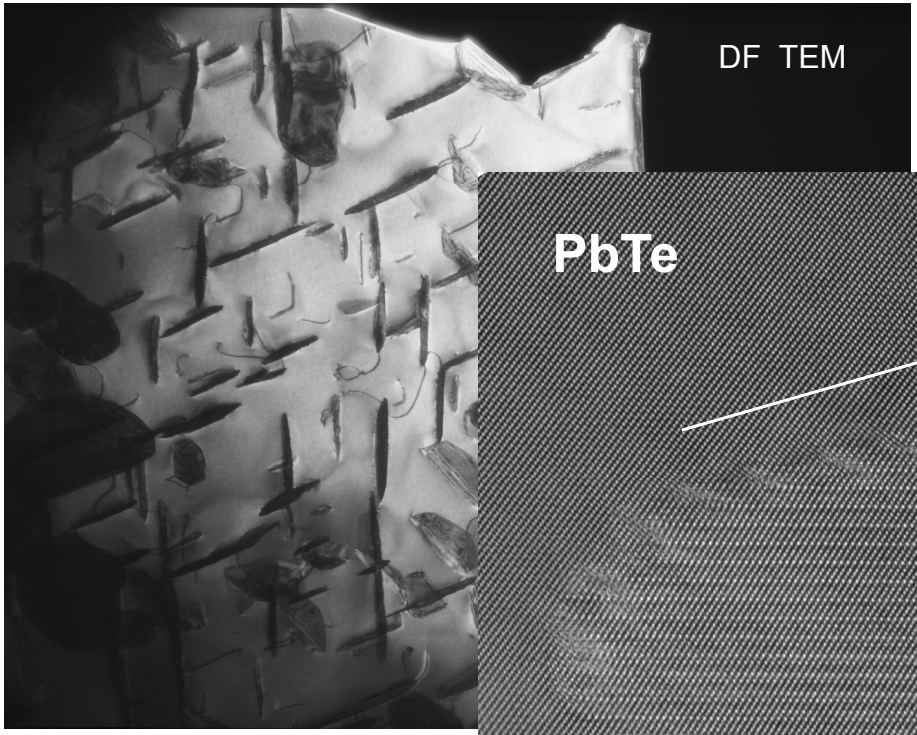
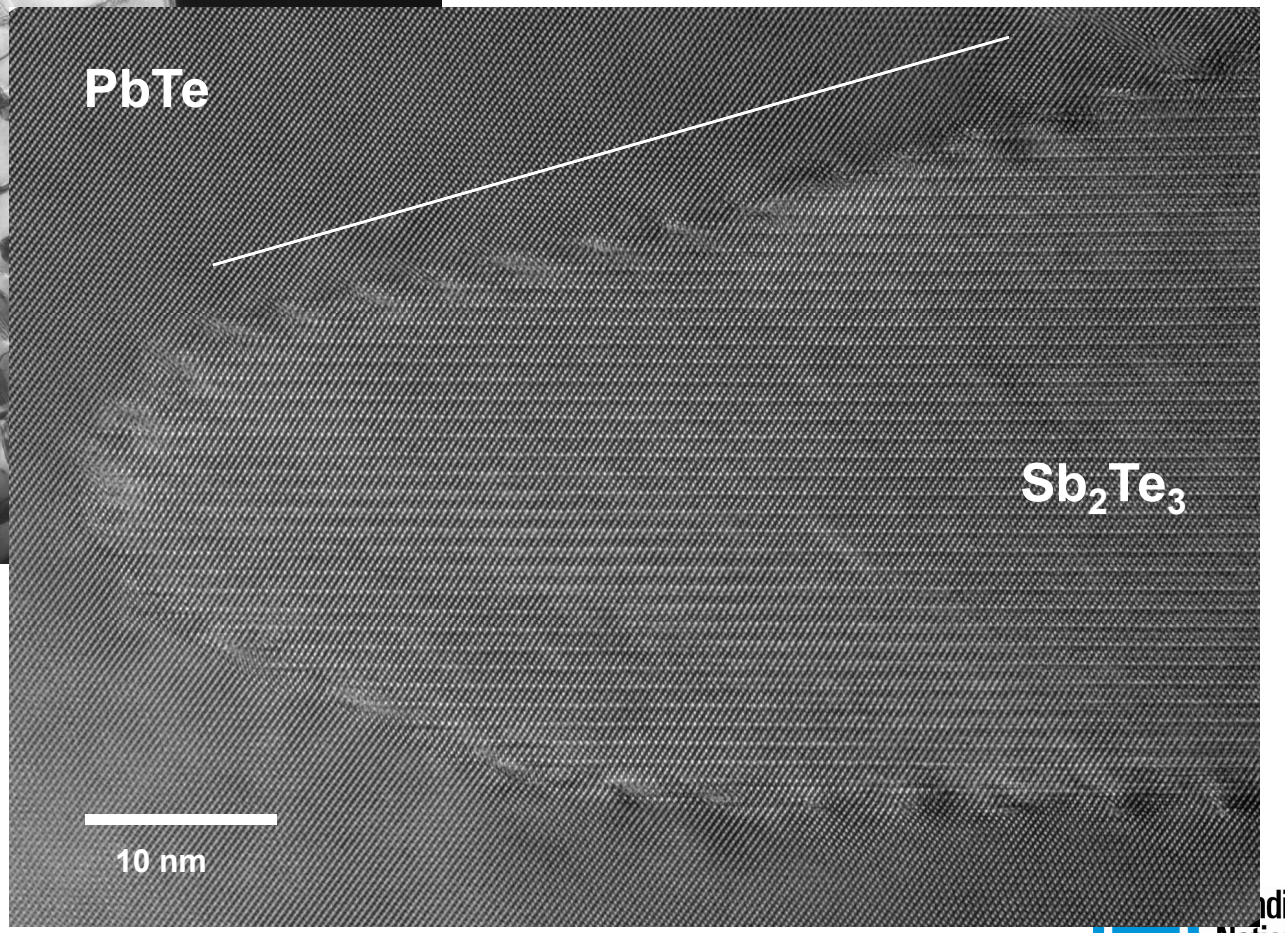
A system with larger misfit: $PbTe/Sb_2Te_3$

Sb_2Te_3 Precipitates in PbTe

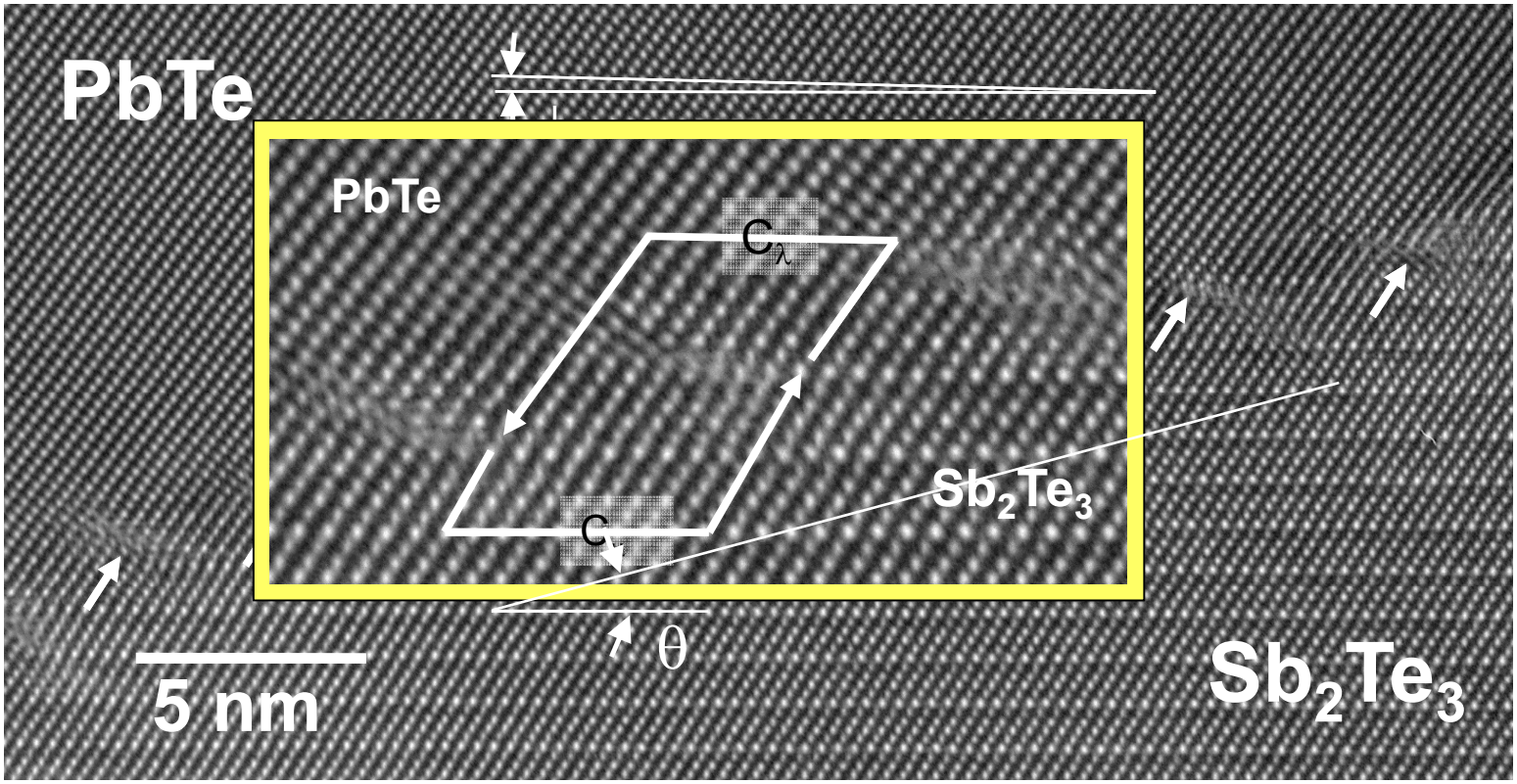


$AgSbTe_2(111)/Sb_2Te_3(0001)$
Misfit: +0.79%



Heinz, Ikeda, Snyder, Medlin, Acta Materialia (2011)

Inclined Section of interface Composed of Disconnections



HRTEM JEOL 4000EX

Circuit Analysis:

Defects identical to the "6/5" disconnections observed in $AgSbTe_2/Sb_2Te_3$

Interface Geometry:

Inclination: θ =14.8° Lattice rotation: ϕ = 1.1° to 1.4°

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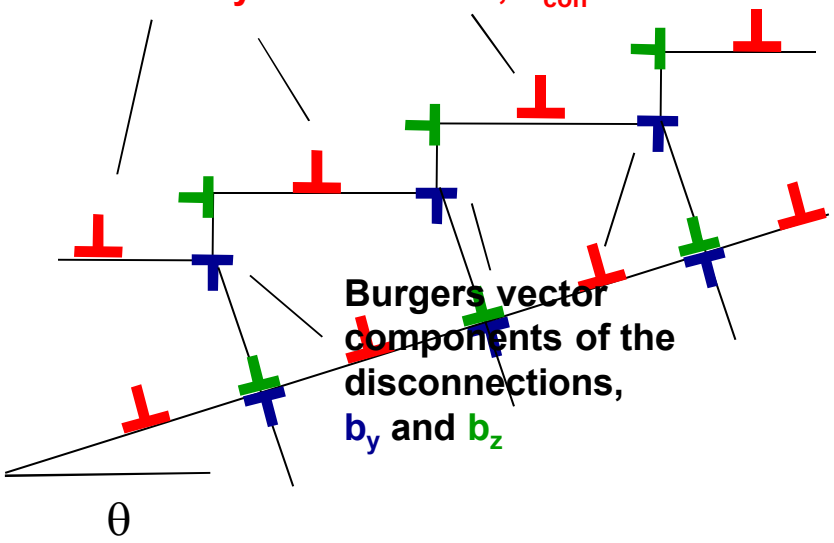
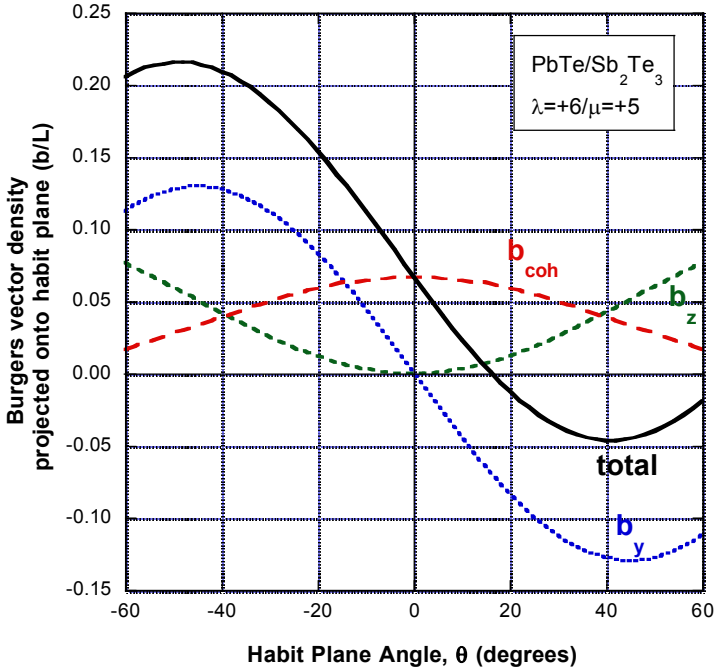
Interplay between Misfit Accommodation and Interface Inclination

Project components on inclined interface plane

Adjust spacing to cancel (ε_{yy} = 0)

Coherency strain on terraces as "coherency" dislocations, b_{coh}





$$-\varepsilon = (b_y \tan\theta + b_z \tan^2\theta)h^{-1}$$ ➔ θ=16.2°

Pond, Celotto, Hirth, Acta Mater. 2003

Out of plane **b** components produce small rigid body crystal rotation,

$$\phi = 2\sin^{-1}[(b_z \cos\theta - b_y \sin\theta - \varepsilon h \cos\theta)\sin\theta / 2h]$$ ➔ ϕ=1.7°

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

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Summary

- **Analysis of interfacial defects provides insights concerning structure and mechanisms.**
  - Complex core structures for defects and grain boundaries.
  - Junction-defect interactions.
  - Mechanisms underpinning phase transformations.

- **Interfacial defects: bridge between atomistic scale observations and simulations and mesoscale scientific understanding**
  - Establishing the defect geometry (step and Burgers vector) is critical.

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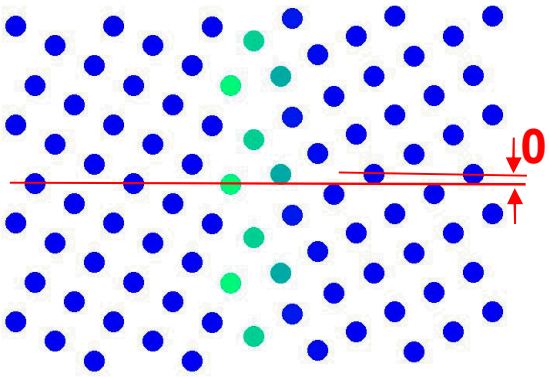
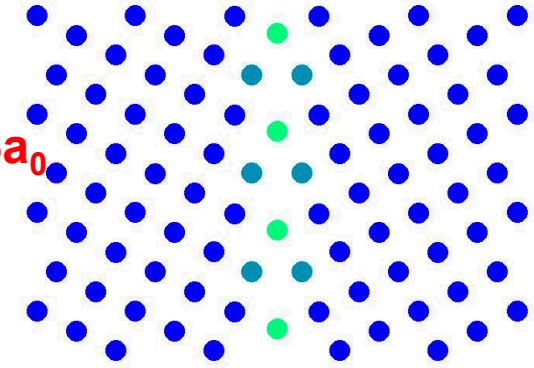
Σ=5 {310} Structures with different Potentials

Asymmetric



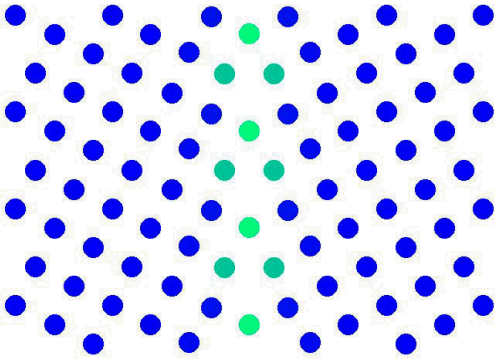
Potential: Chamati, 2006

Symmetric



Potential: Mendelev, 2003

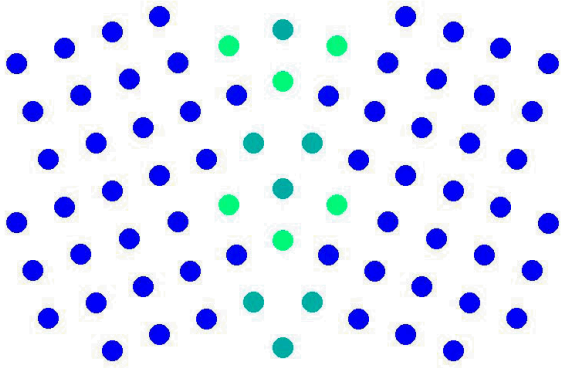
Symmetric



Potential: Proville, 2012

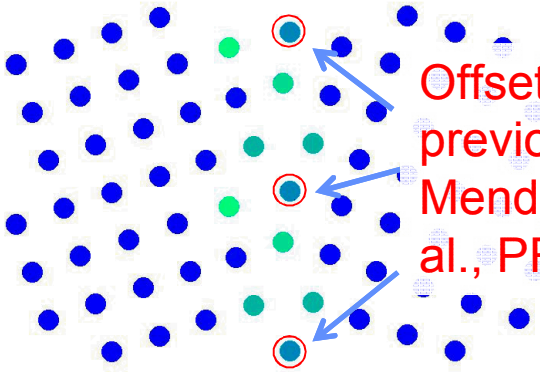
Σ=5 {210} Structures with different Potentials

Symmetric



Potential: Chamati, 2006

Asymmetric



Potential: Mendelev, 2003

Symmetric

Potential: Proville, 2012

Offset structure consistent with previous calculations using Mendelev potential (Tschopp et al., PRB 2012)

Atoms shaded by centrosymmetry parameter

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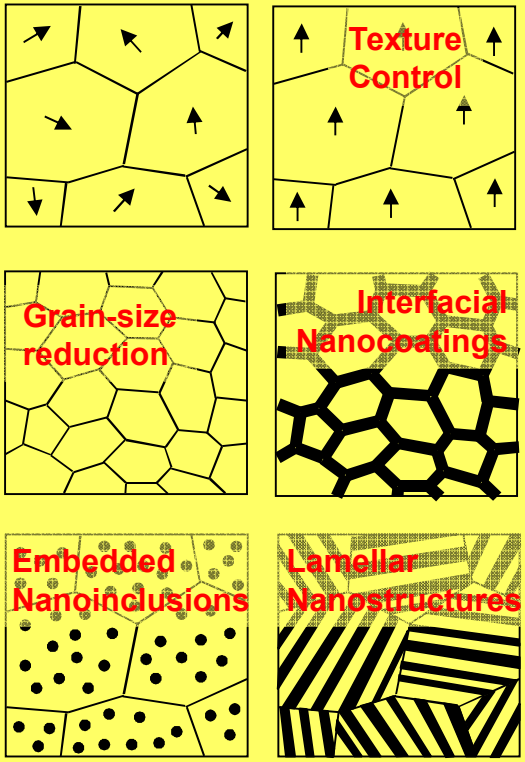
Bulk Thermoelectrics: Control of Microstructure to Improve Performance

Microstructural Strategies for Nanostructured Bulk Thermoelectrics



Medlin and Snyder, Current Opinion in Colloid and Interface Science, 2009

TE Energy Conversion Efficiency: Figure of Merit

Example: Ag_2Te nanoprecipitates in PbTe

Phonon scattering on Ag_2Te precipitates lowers κ_l

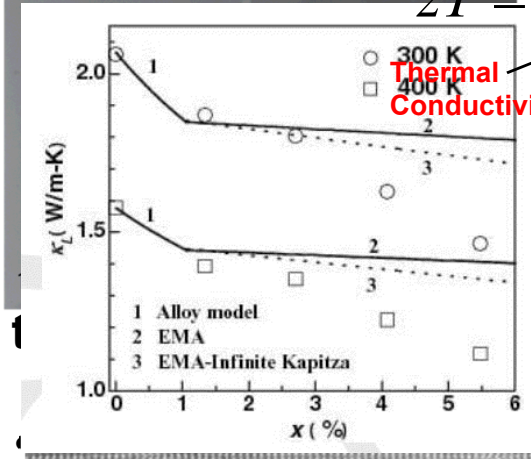
$$zT = \frac{S^2 \sigma}{\kappa} T$$

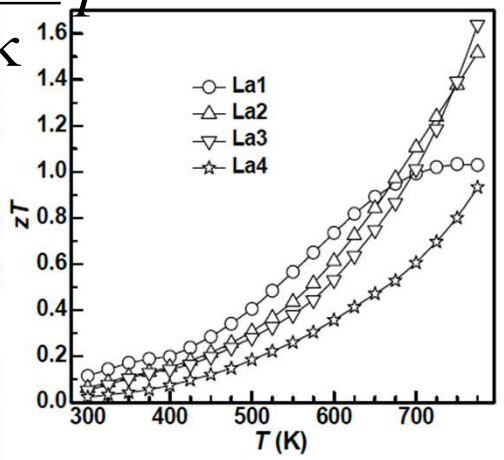
Seebeck Coefficient

Electrical Conductivity

Thermal Conductivity

T as high as 1.6 with suitable doping





Y. Pei, J. Lensch-Falk, E.S. Toberer, D.L. Medlin, G.J. Snyder, *Advanced Functional Materials* (2010).

J. Lensch-Falk, J. Sugar, M. Hekmaty, D. Medlin, Journal of Alloys and Compounds (2010)

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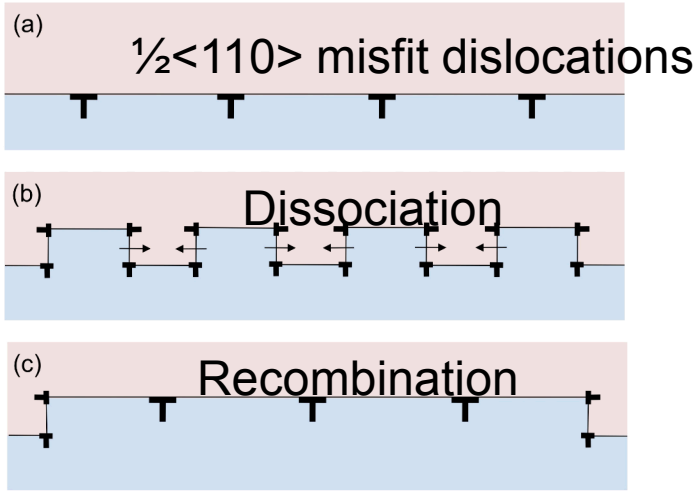
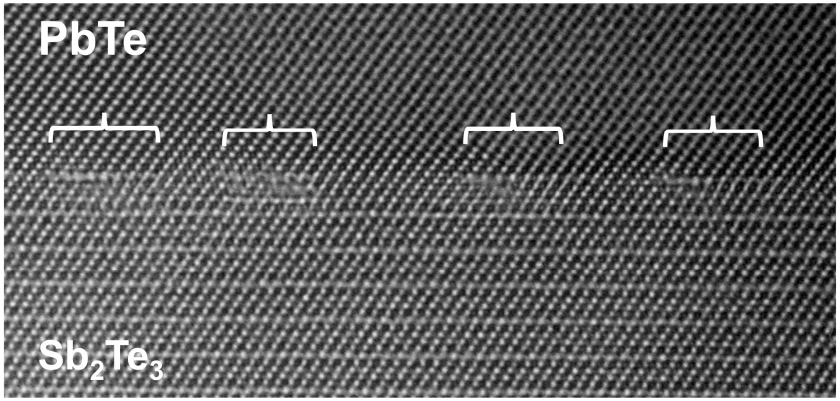
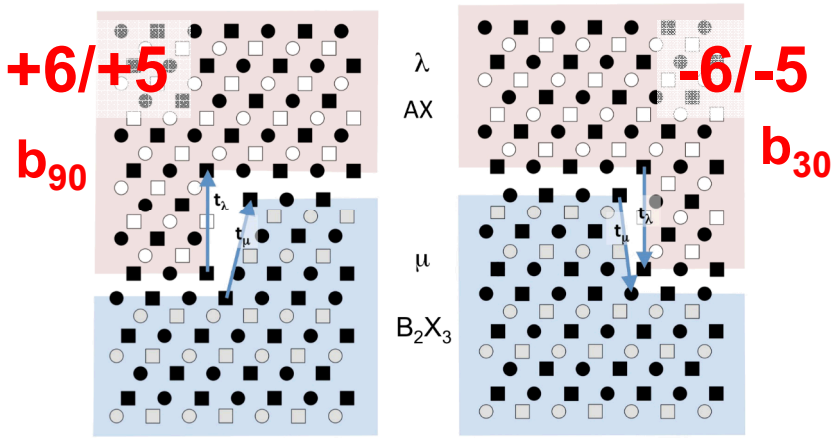
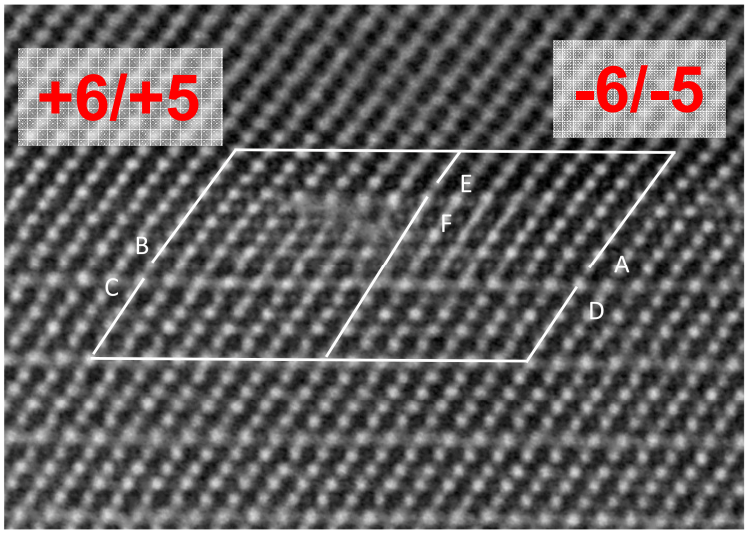
How might these defects form?

Dissociation of ½<110> misfit dislocations at flat sections of interface into disconnections









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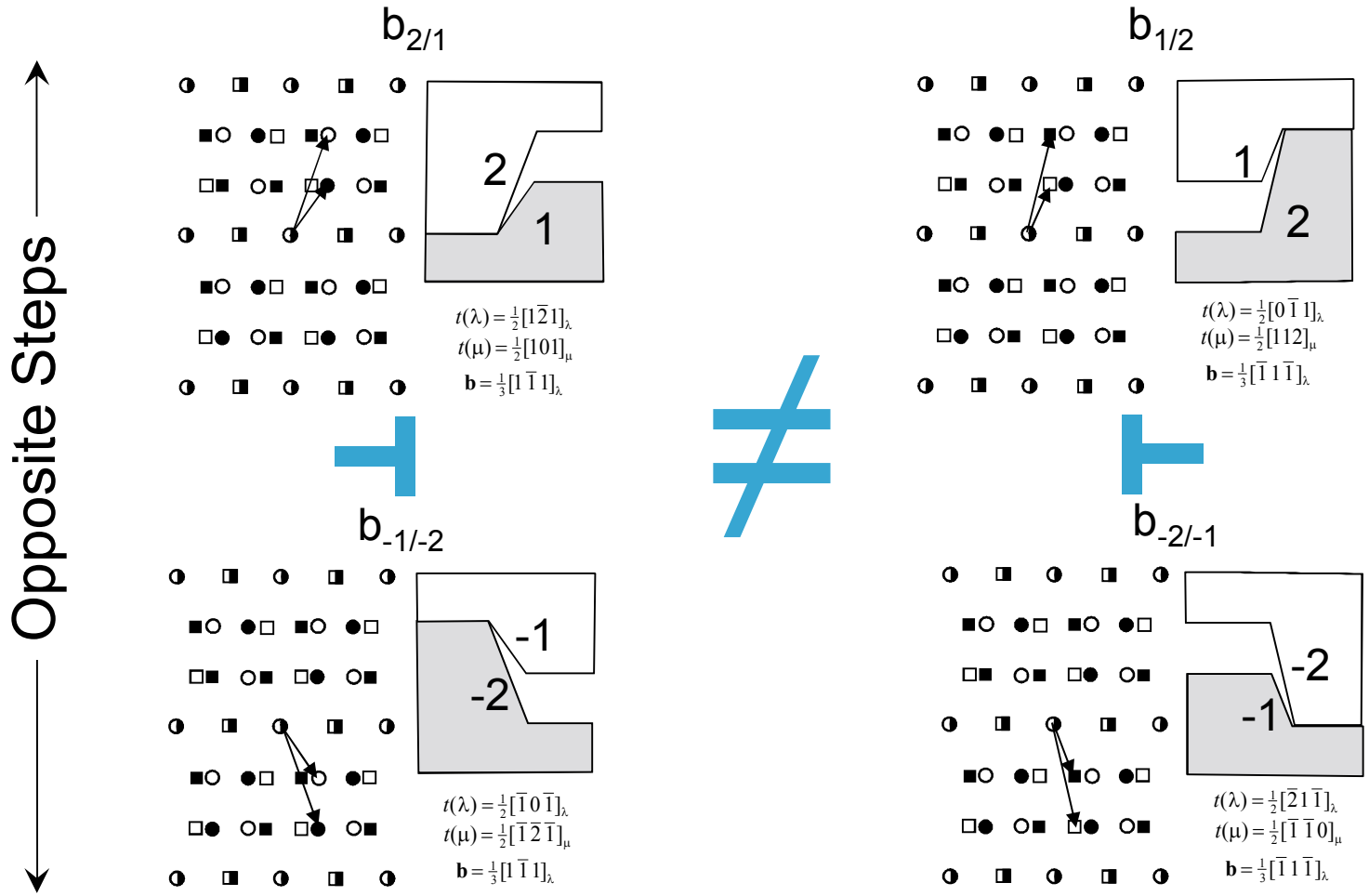
Variants of the 1/3<111> Disconnection



← Opposite Burgers Vectors →

Classical Distinction between High and Low Angle Boundaries

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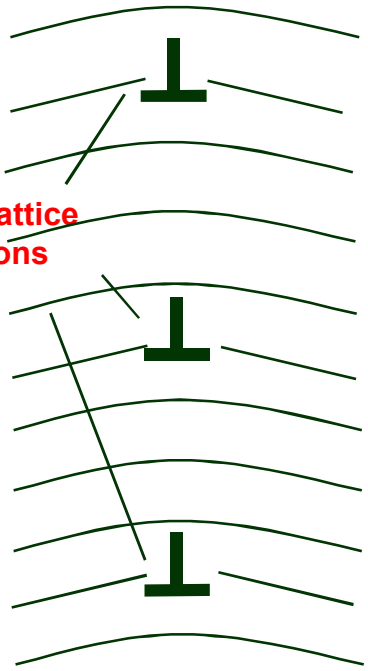
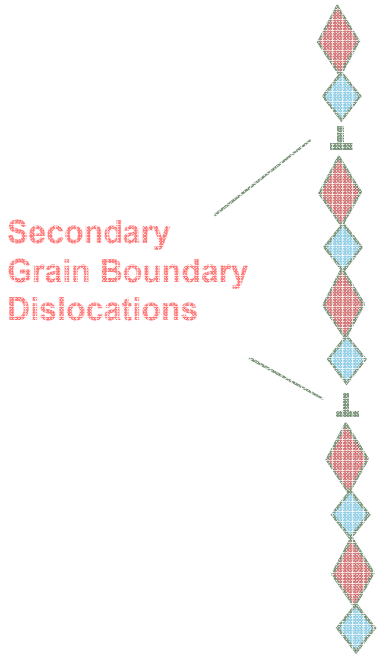
Low Angle GB



Perfect Lattice Dislocations

Reference Frame:
Single Crystal

High Angle GB



Secondary Grain Boundary Dislocations

Reference Frame:
Low Energy GB Structure