SAND2021-7561C

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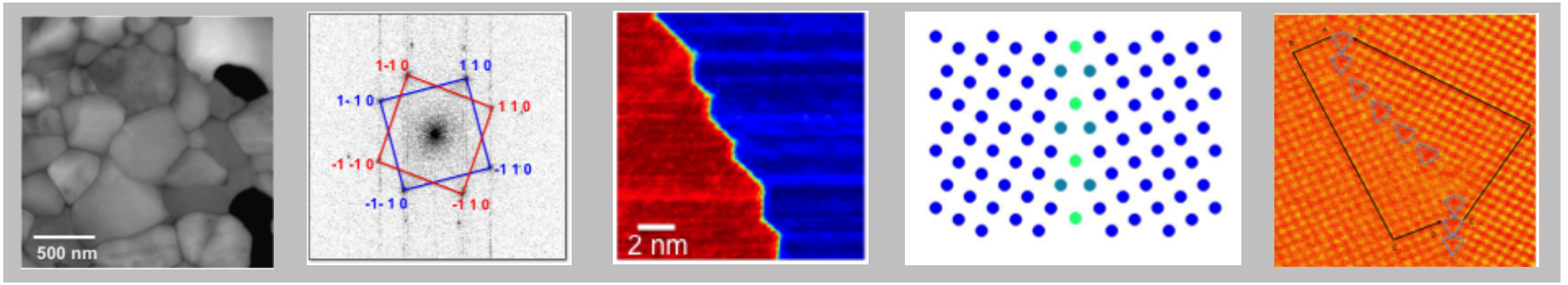

Defect Character at Grain Boundary Facet Junctions: *A combined HRSTEM and Atomistic Modeling Study of a Σ=5 GB in Fe*

D.L. Medlin[1], K. Hattar[2], J.A. Zimmerman[2], F. Abdeljawad[2], S.M. Foiles[2]

[1]Sandia National Laboratories, Livermore, CA

[2]Sandia National Laboratories, Albuquerque, NM

U.S. DEPARTMENT OF ENERGY

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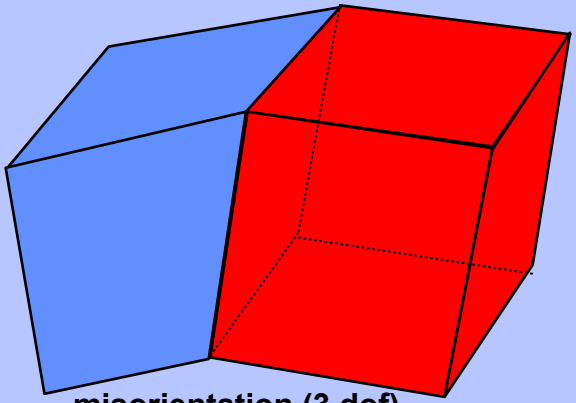
How to connect between atomistic and continuum descriptions of grain boundaries?

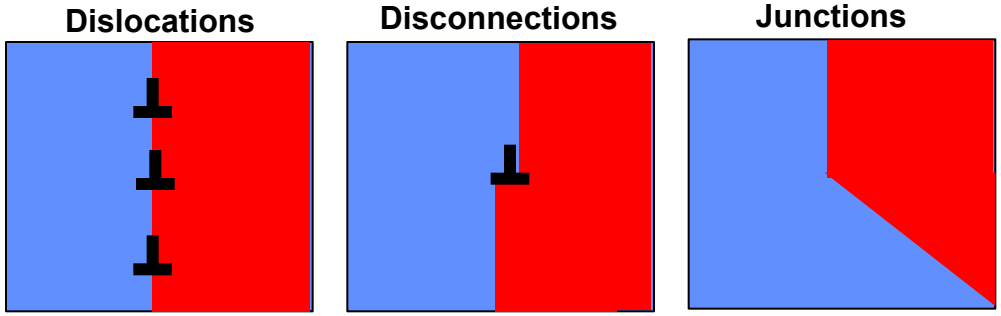
Grain boundary geometry characterized by 5 "macroscopic" degrees of freedom



misorientation (3 dof)
inclination (2 dof)

Our approach:

Focus on arrangements and interactions of elementary interfacial line defects



Atomistic scale microscopy and modeling

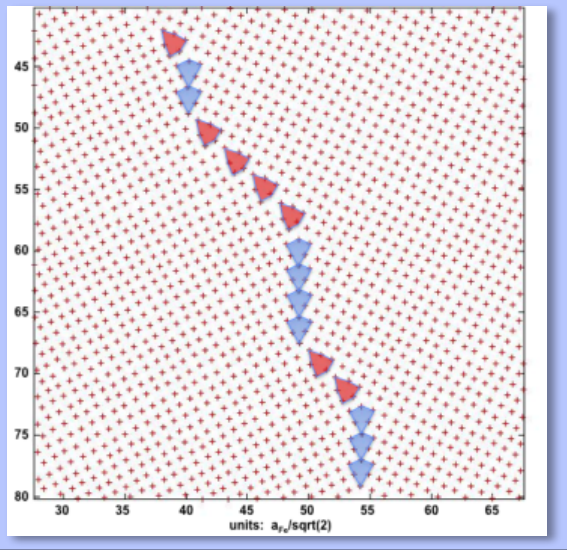
Focus for Today's talk

-Observations and calculations of a Σ=5 Grain boundary in BCC Fe

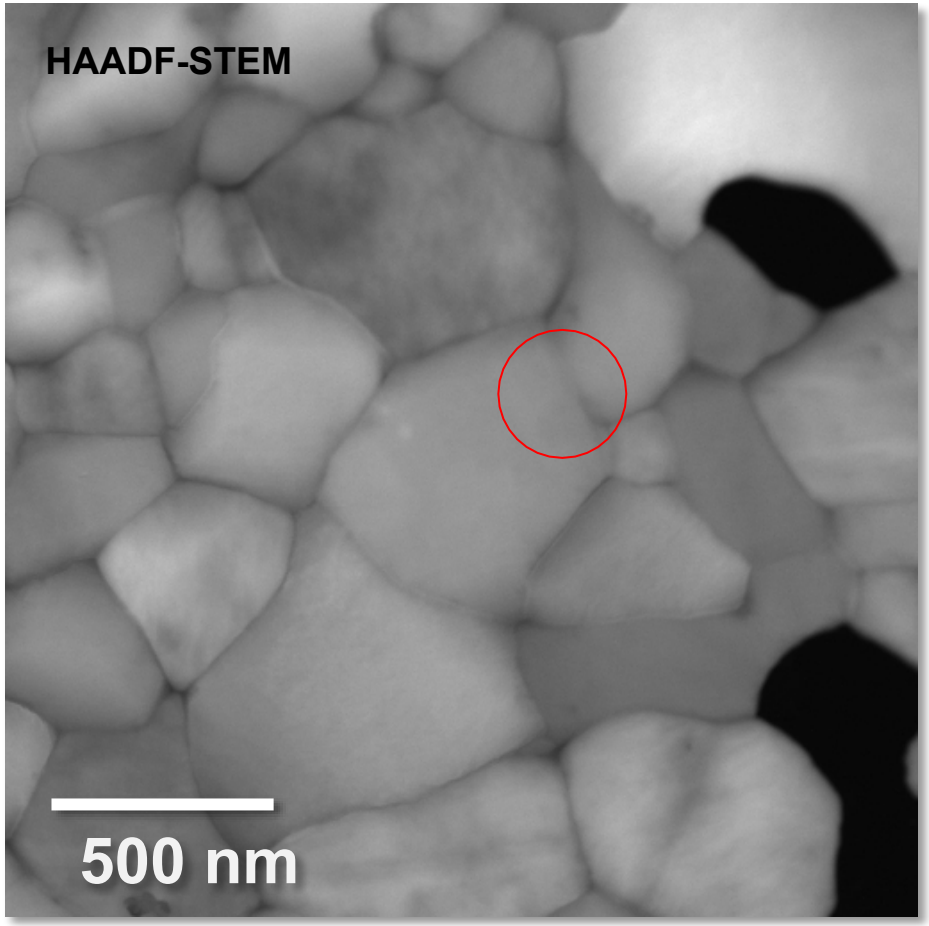
-Deviation from symmetric inclination and ideal misorientation:

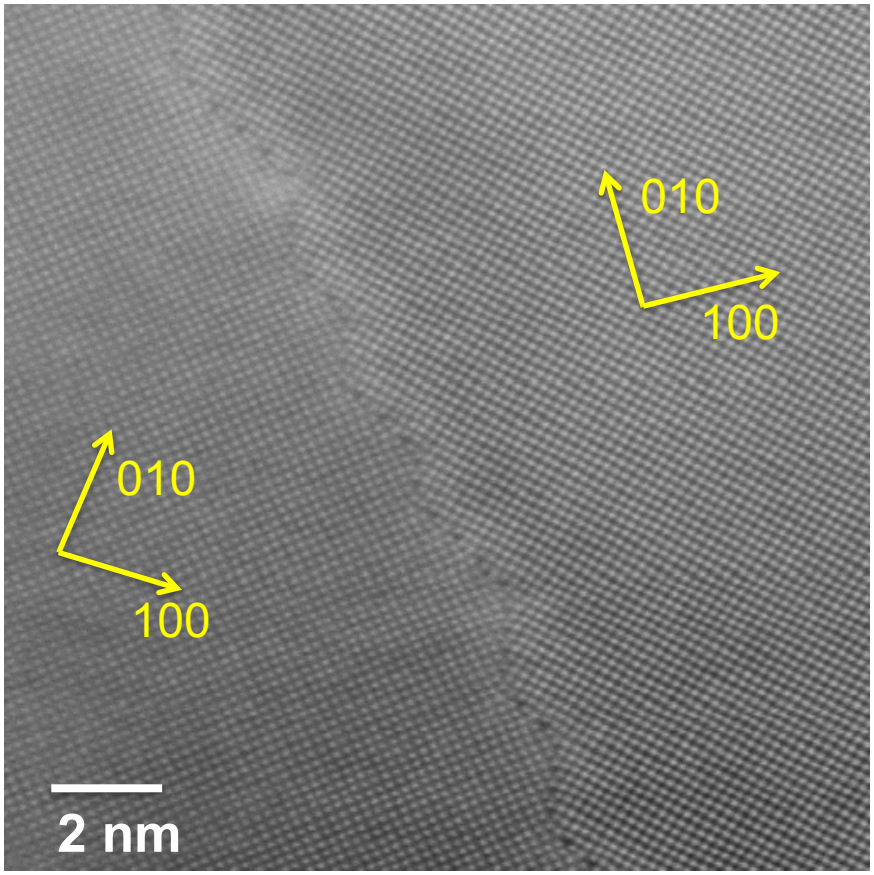
-nanoscale faceting

-interfacial dislocations



Observations: Polycrystalline BCC Fe film

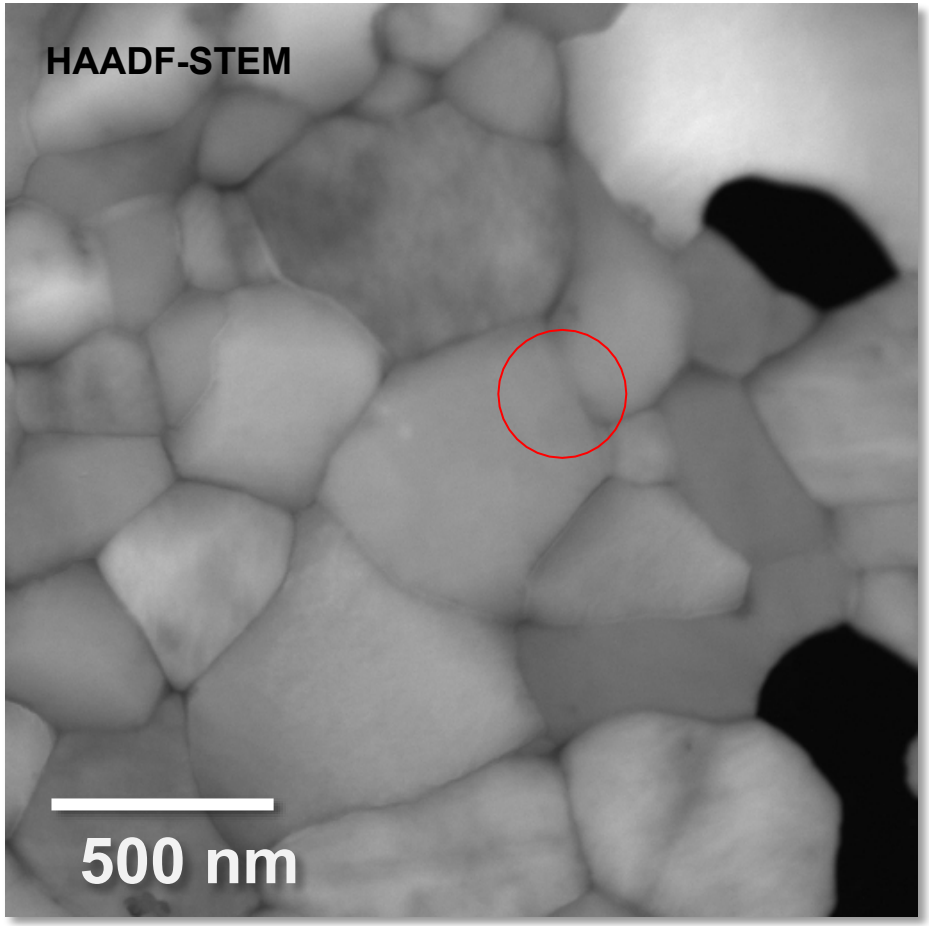


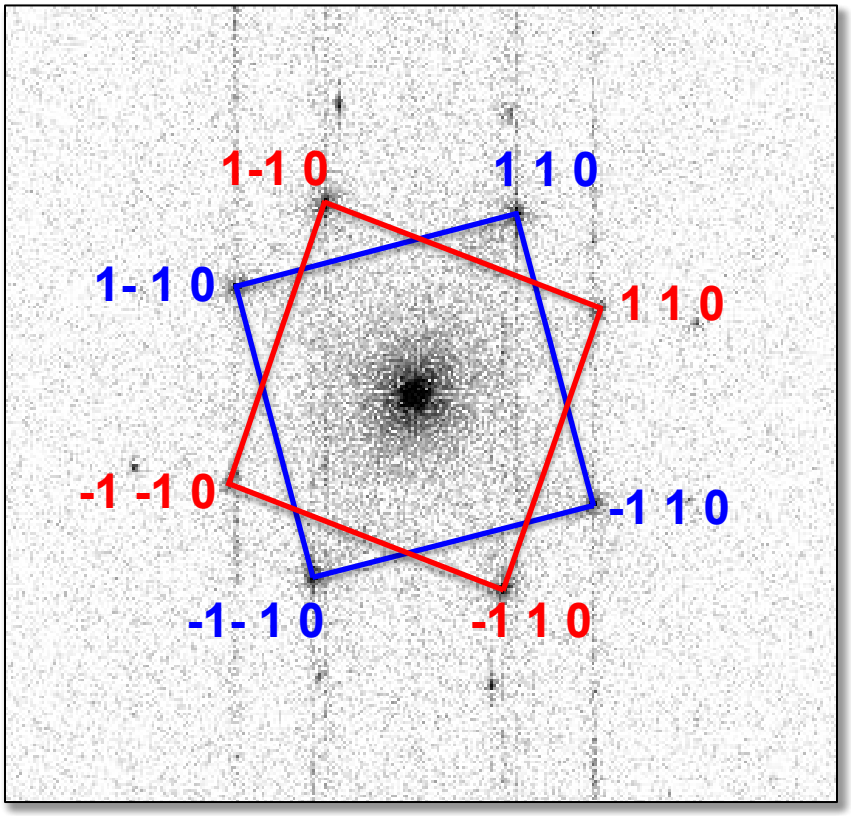


Pulsed Laser Deposited Fe on Rocksalt (NaCl). 36 nm thickness.
Specimen released and annealed on Mo grid 675°C, 2 hours.
under vacuum

HAADF-STEM
FEI-200 keV probe corrected Titan

Observations: polycrystalline Fe thin film

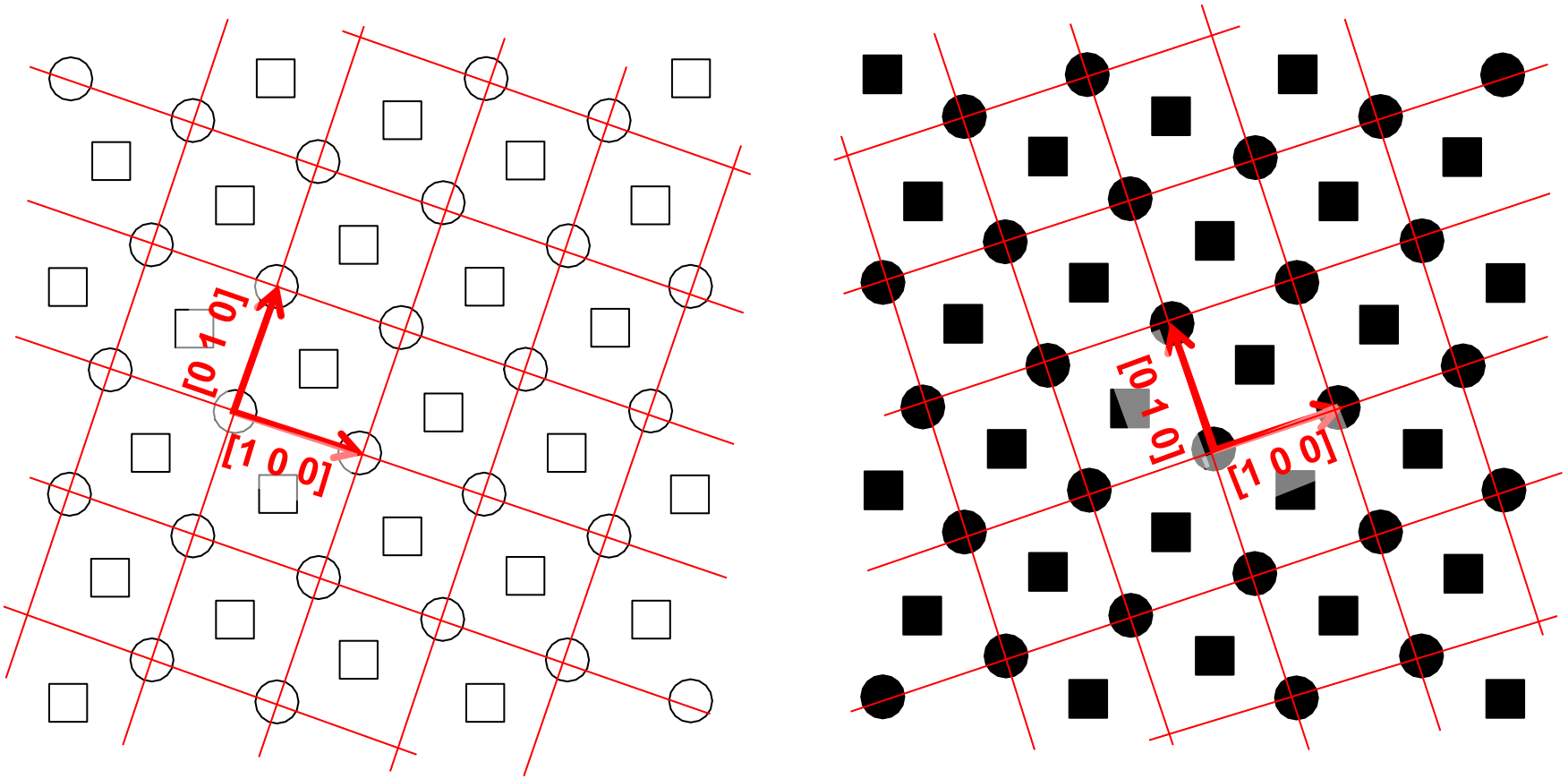




Pulsed Laser Deposited Fe on Rocksalt (NaCl). 36 nm thickness.
Specimen released and annealed on Mo grid 675°C, 2 hours.
under vacuum

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

BCC Σ=5 [001]: Interfacial Crystallography



36.87° Rotation about [001]

BCC Σ=5 [001]: Interfacial Crystallography

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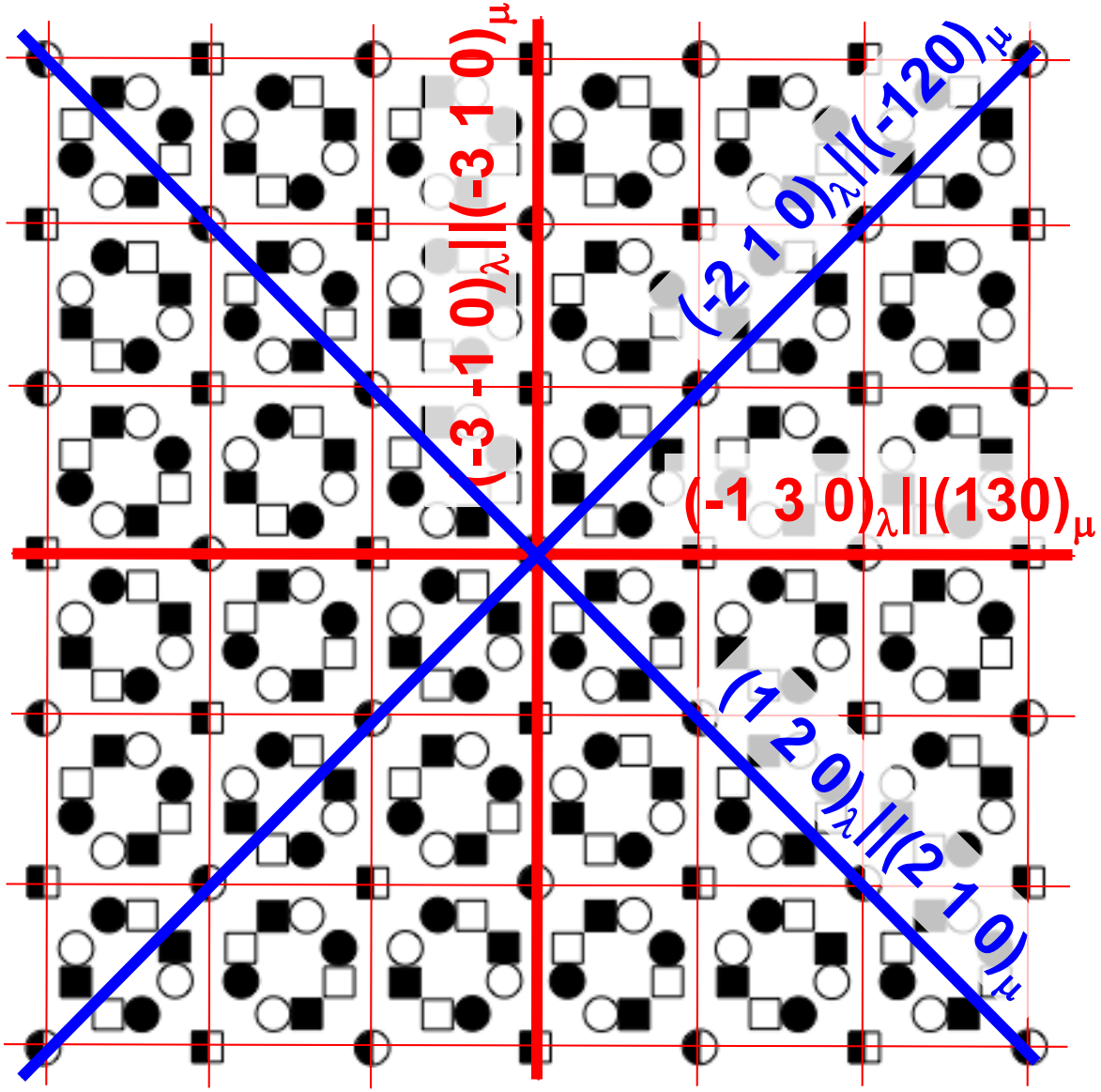
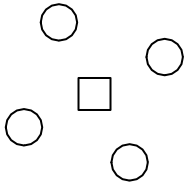
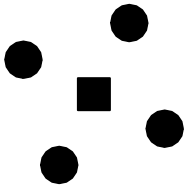
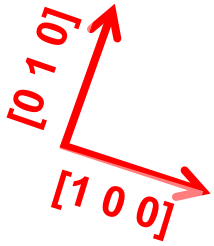
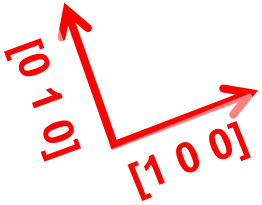
Dichromatic Pattern











HRSTEM shows nanoscale faceting at Grain boundary

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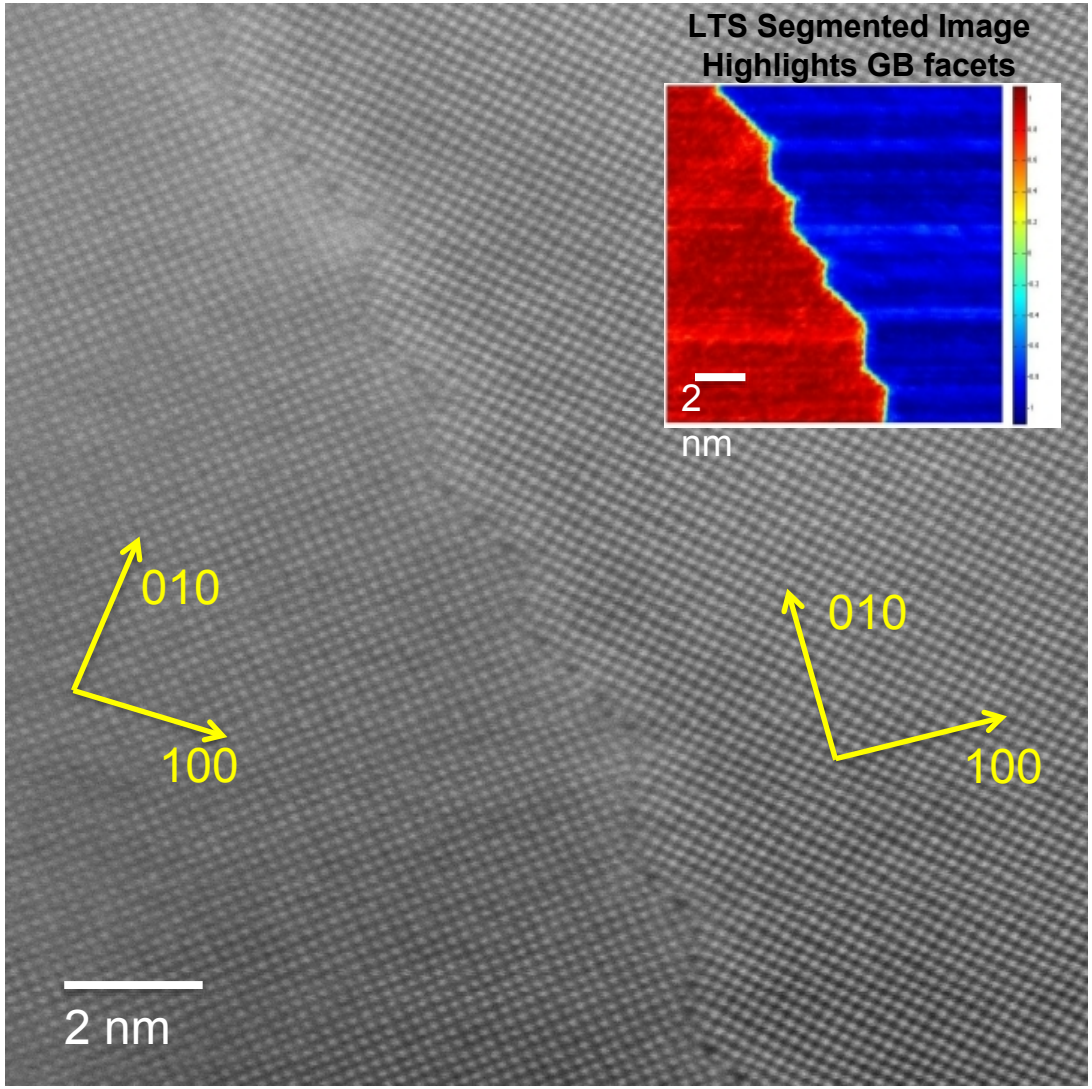
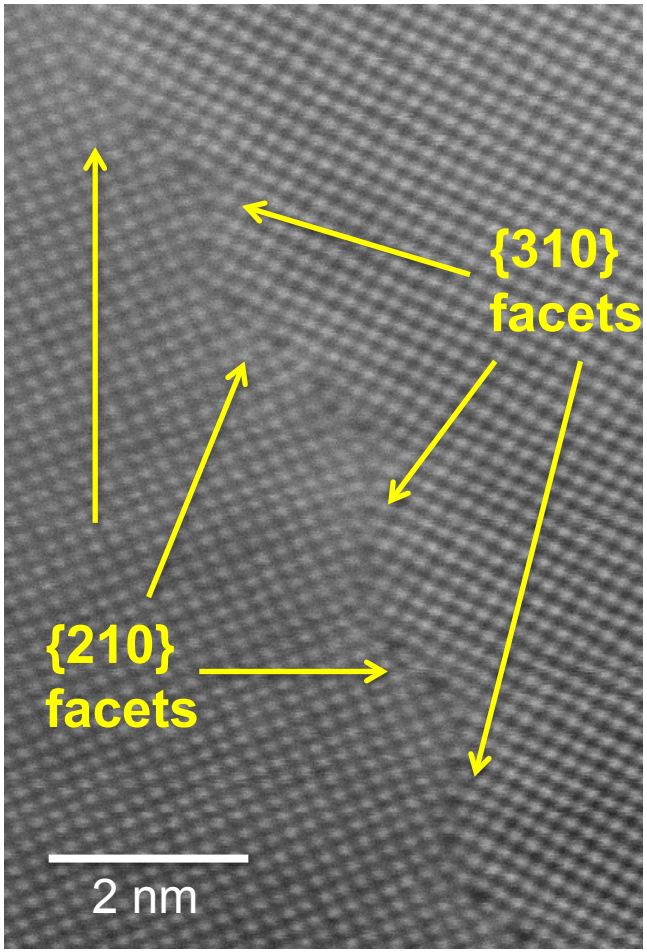
HAADF-STEM Σ=5 <001> Boundary in Fe



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



Inclination from {310}: ≈25°

Faceting: Signature of anisotropic interfacial energy

- **Driving force (μ) for interface evolution:**

H: mean curvature
V_m: molar volume
γ: interface energy

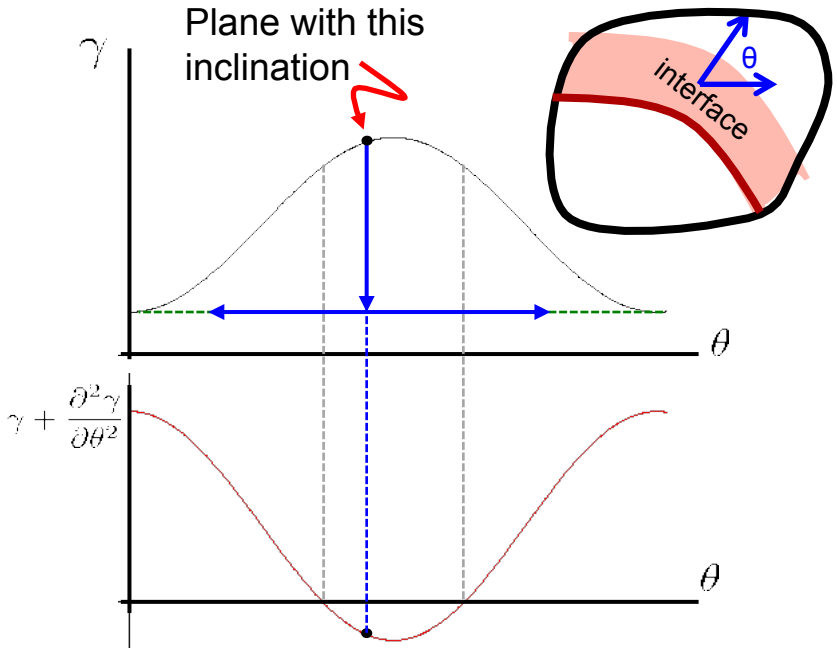
$$\mu \sim v_m \left(\gamma + \frac{\partial^2 \gamma}{\partial \theta^2} \right) H$$

W. W. Mullins (1963)

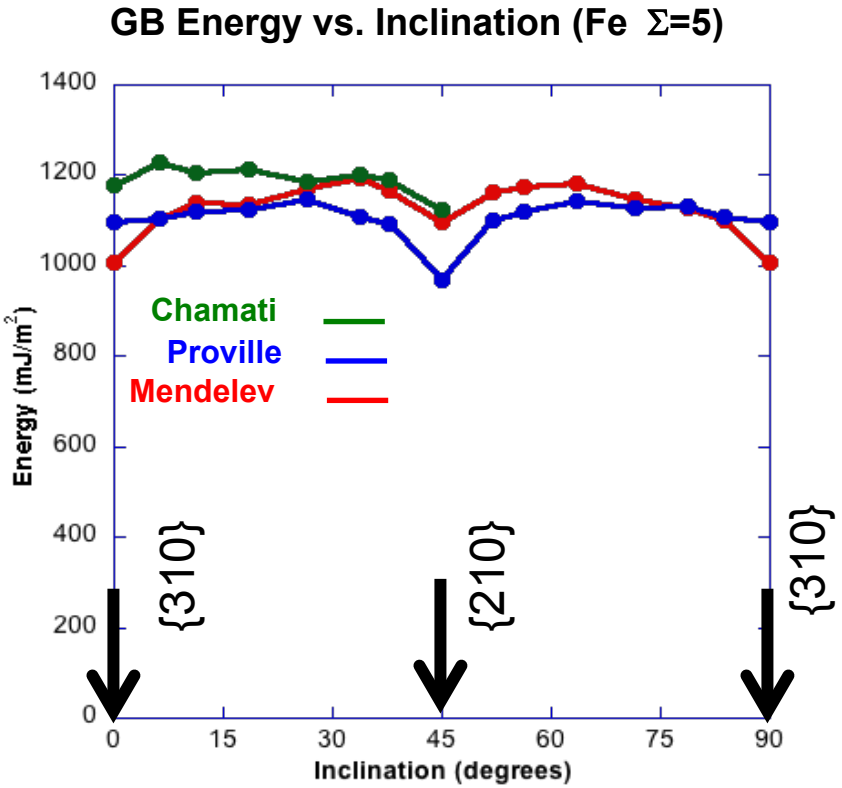
Interface stiffness

-Inclinations with negative interface stiffness break into facets with minimum energy orientations.

-"interface spinodals": analogous to phase separation in bulk materials.



Frank (1963), Cabrera (1964), Stewart (1992), Liu (1993)



Σ=5 {310} Structures with different Potentials

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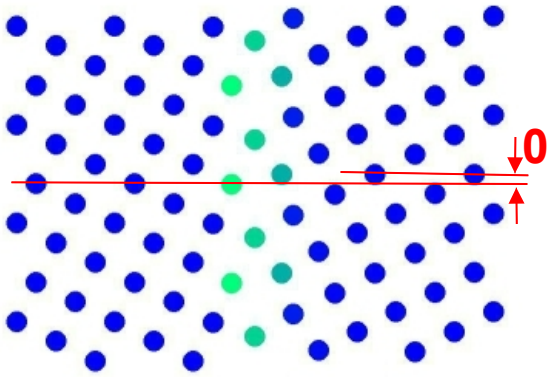
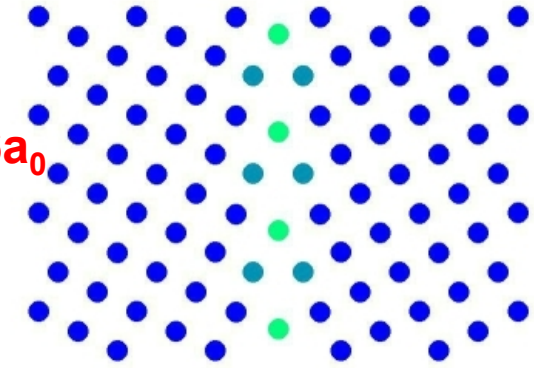
Asymmetric



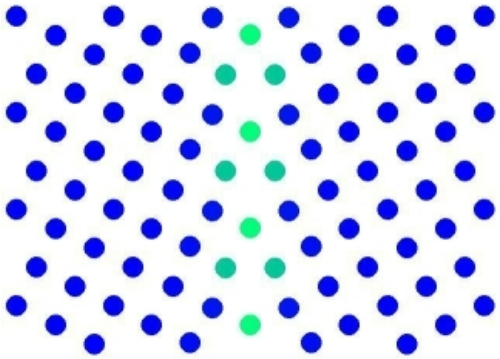
Potential: Chamati, 2006

Symmetric



Potential: Mendelev, 2003

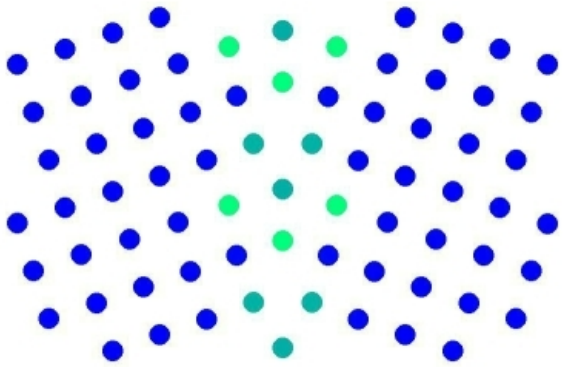
Symmetric



Potential: Proville, 2012

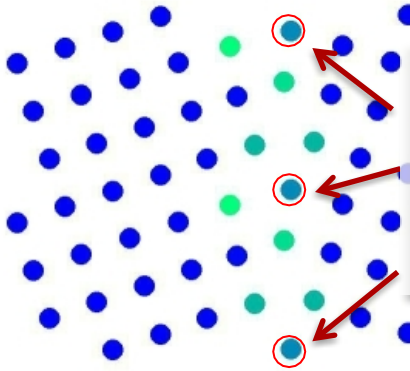
Σ=5 {210} Structures with different Potentials

Symmetric



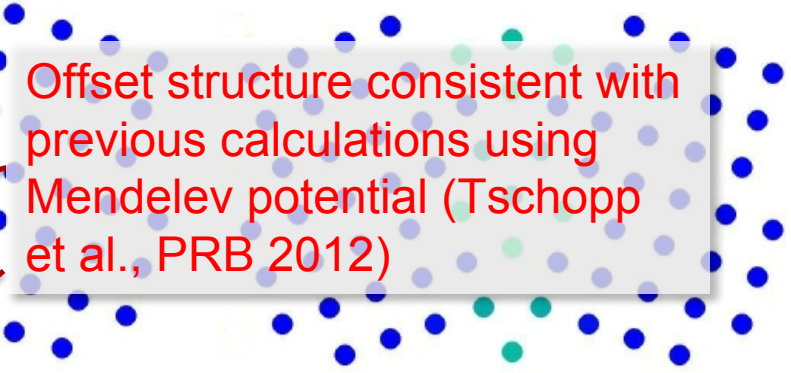
Potential: Chamati, 2006

Asymmetric



Potential: Mendelev, 2003

Symmetric



Potential: Proville, 2012

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

Quantifying the GB Images: Peak Location

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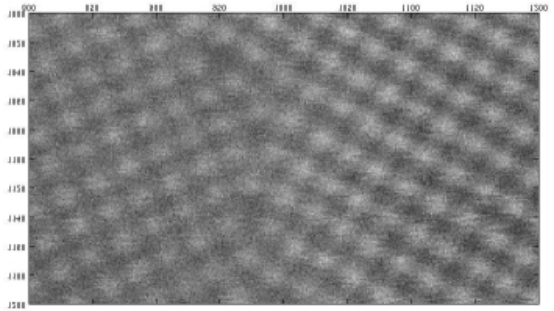
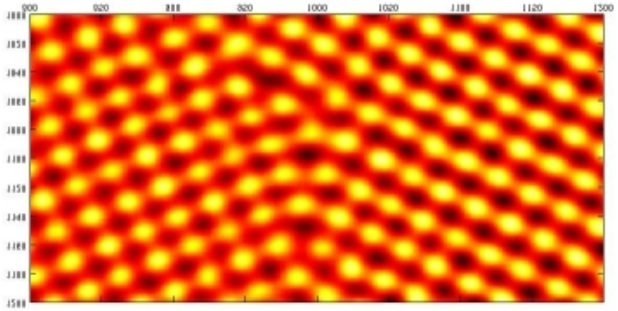
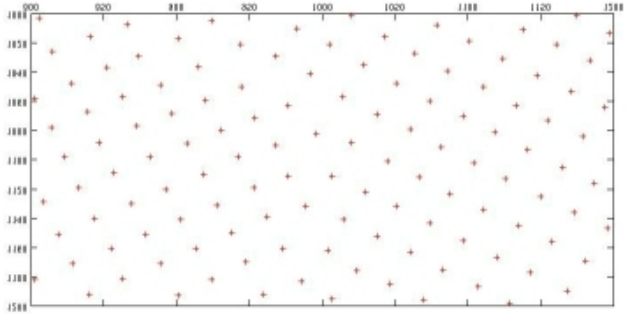
Raw HAADF STEM Image

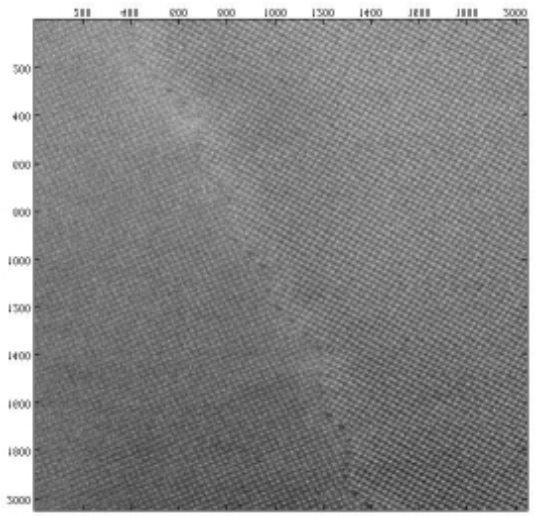


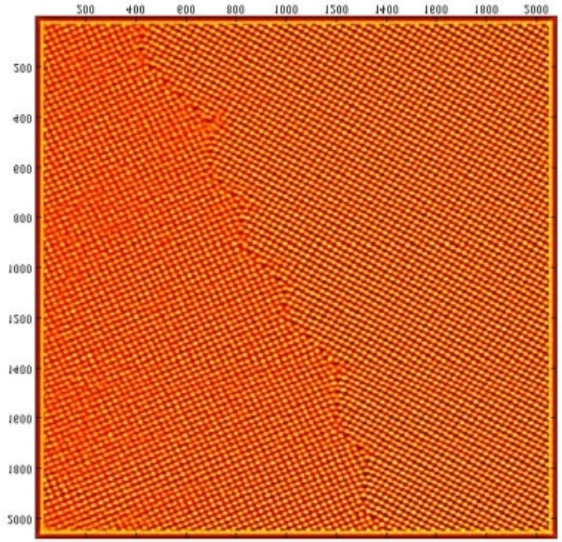
Correlation Image-Guassian

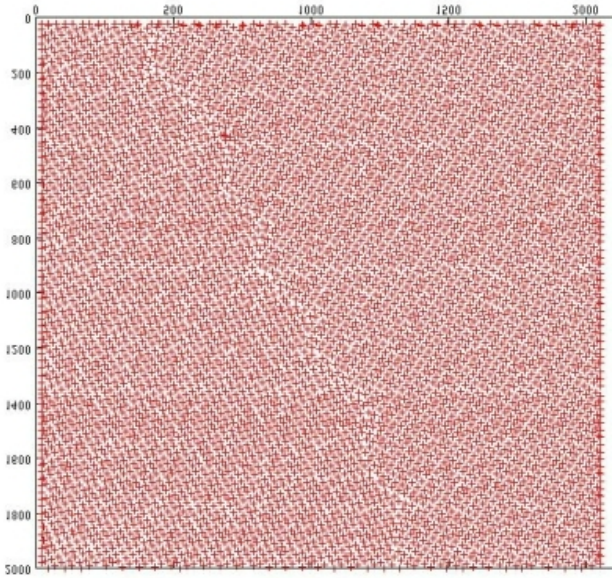


Peak Positions

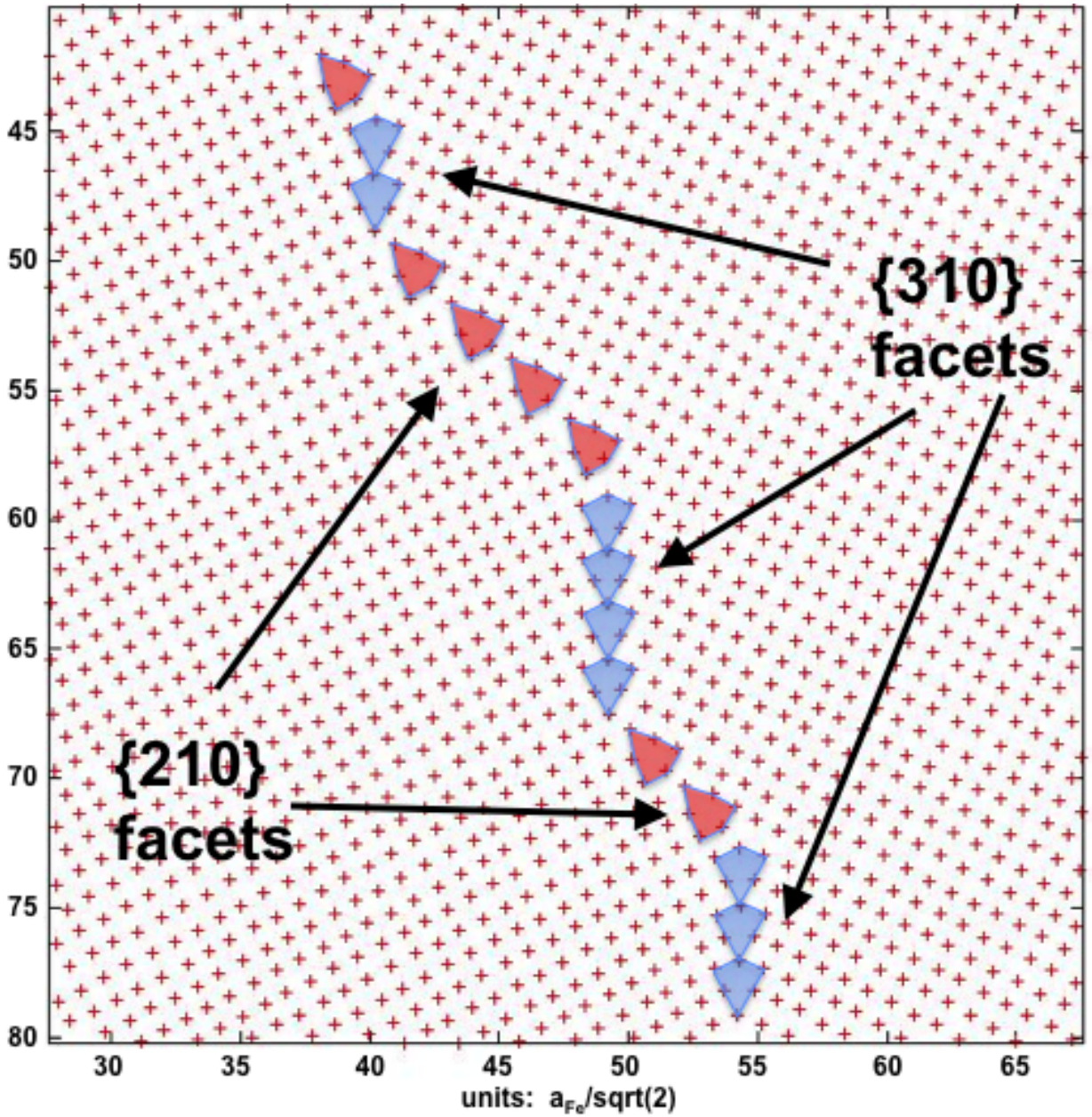








Shear distortion due to specimen drift during image acquisition.
Corrected by affine transformation to peak position array.



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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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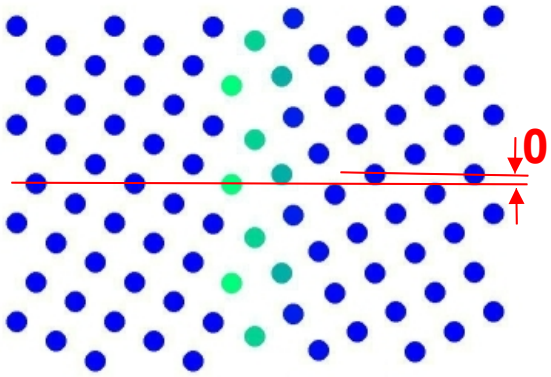
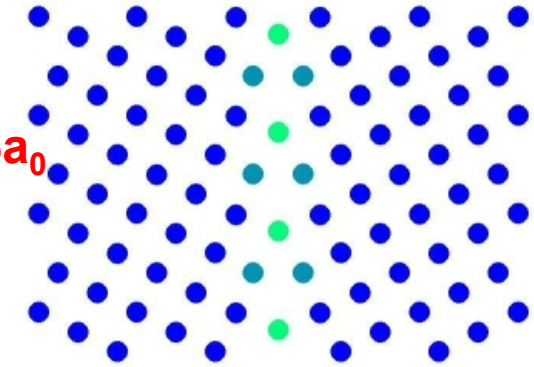
Asymmetric



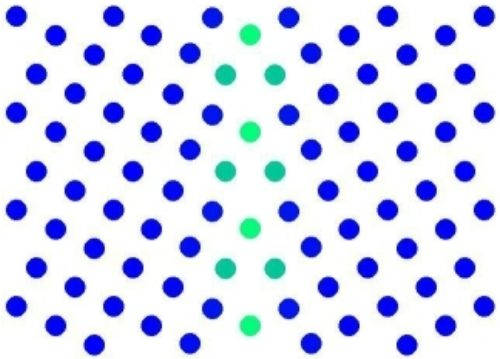
Potential: Chamati, 2006

Symmetric



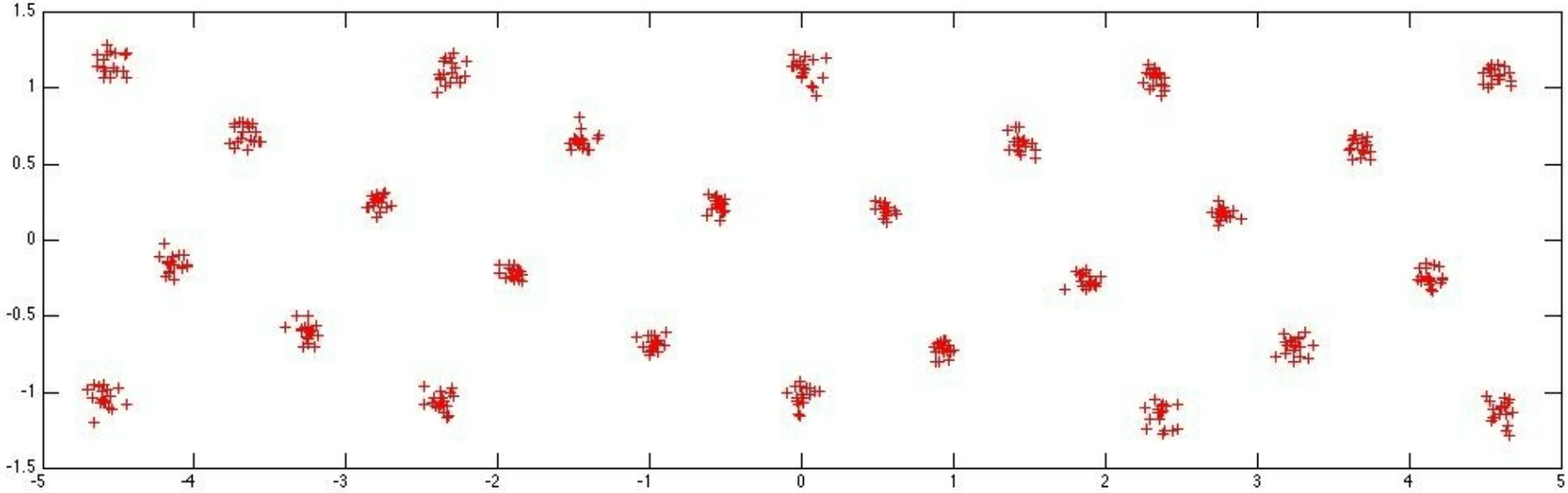
Potential: Mendelev, 2003

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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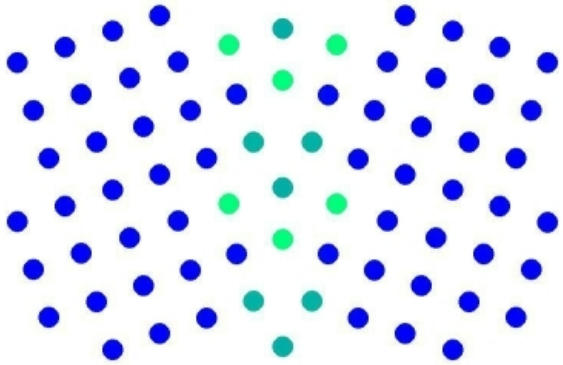
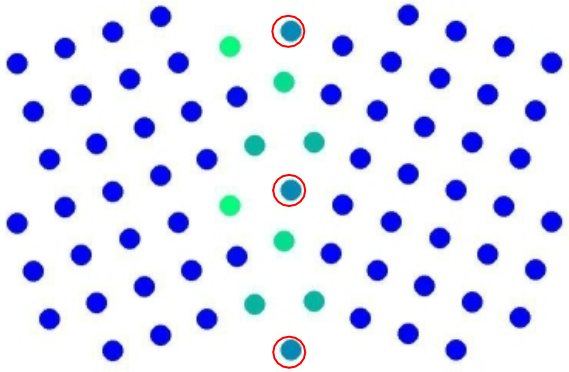
Symmetric



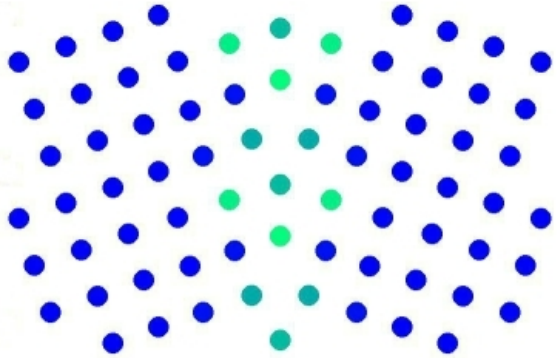
Potential: Chamati, 2006

Asymmetric



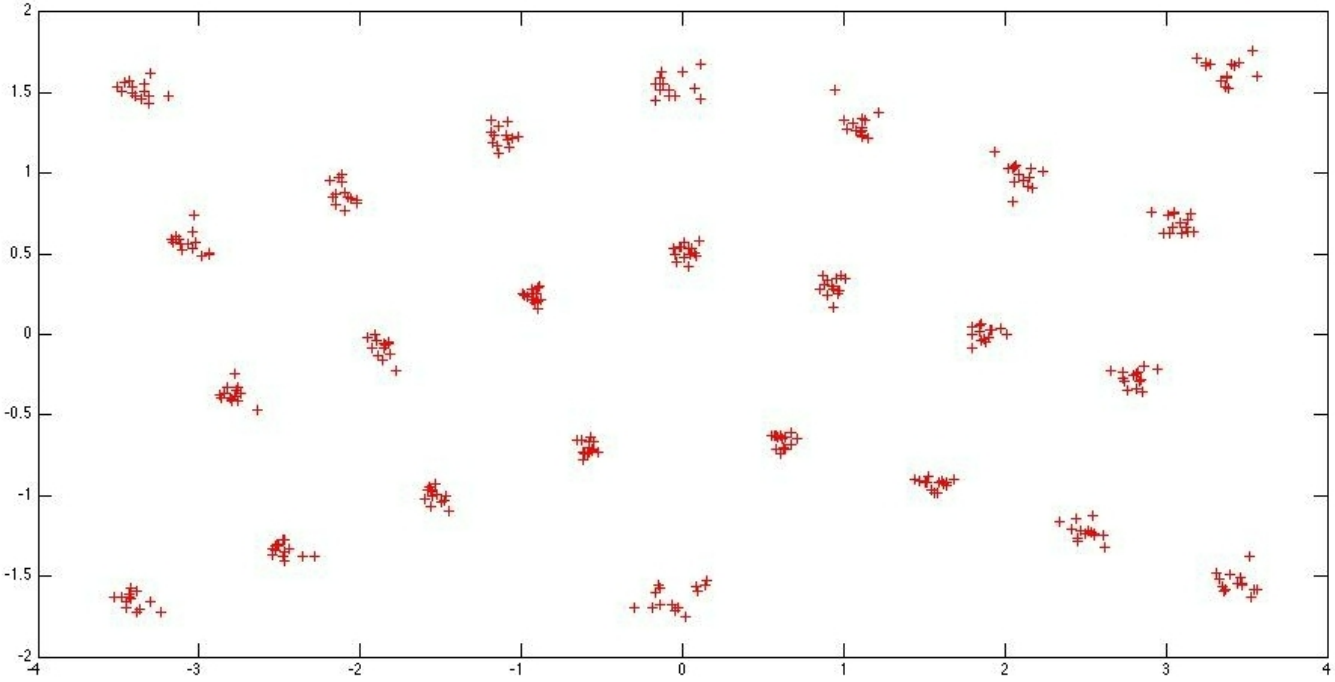
Potential: Mendelev, 2003

Symmetric



Potential: Proville, 2012

Experimental Peak Positions (HAADF STEM)



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

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

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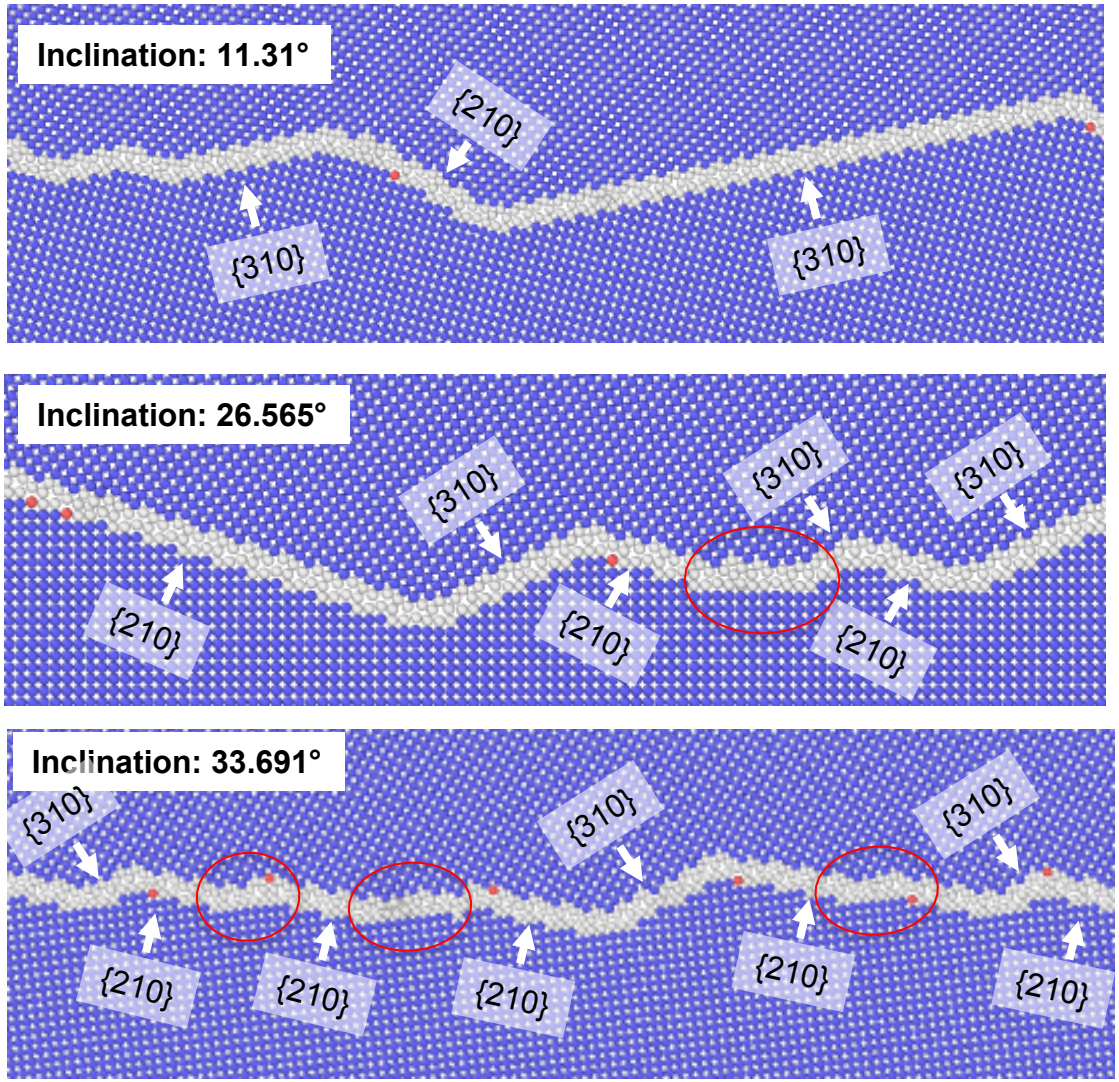
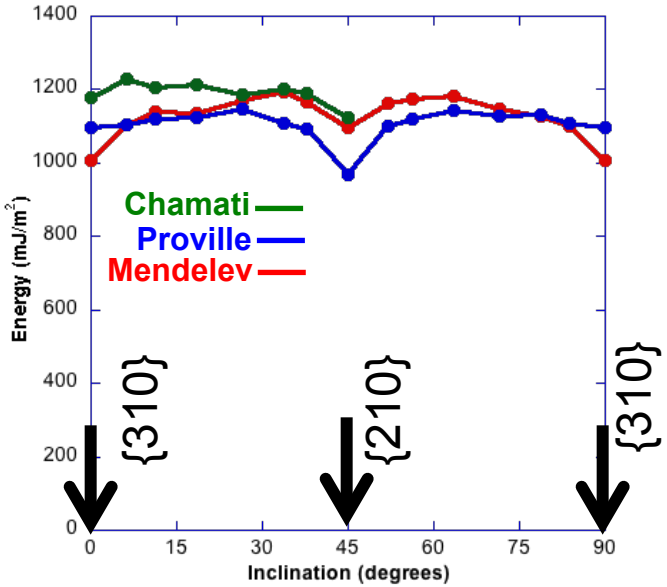


Mendelev Potential

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

Are Grain Boundary Dislocations Present?

Boundary is misoriented from exact Σ=5 ($\Delta\theta$=-2.38°)

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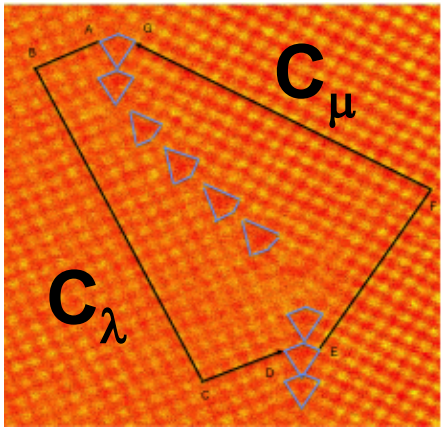
Determine defect content by Circuit Mapping over all facet junctions



Path in μ crystal

Path in λ crystal

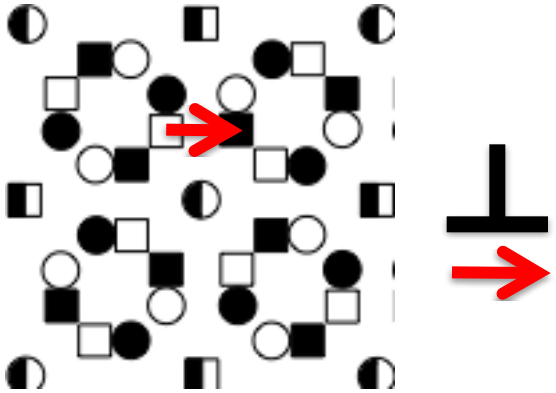
$$\mathbf{b} = -(C_\lambda + \mathbf{P}C_\mu)$$

Burgers vector

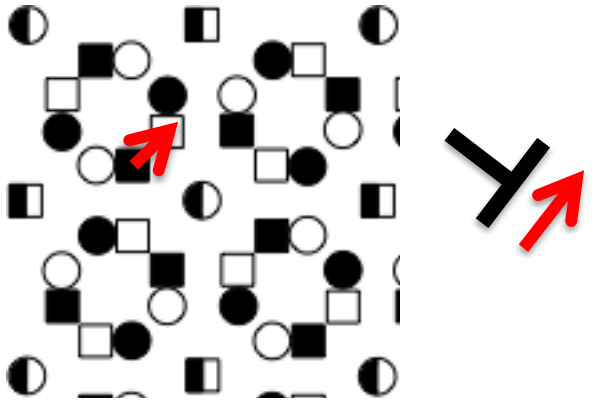
Re-express μ path in λ crystal coordinates.

Two types of defect observed:

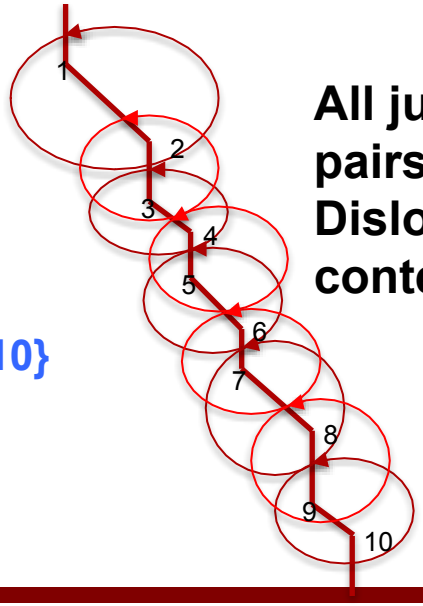
b=(1/5)[3,1,0]



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

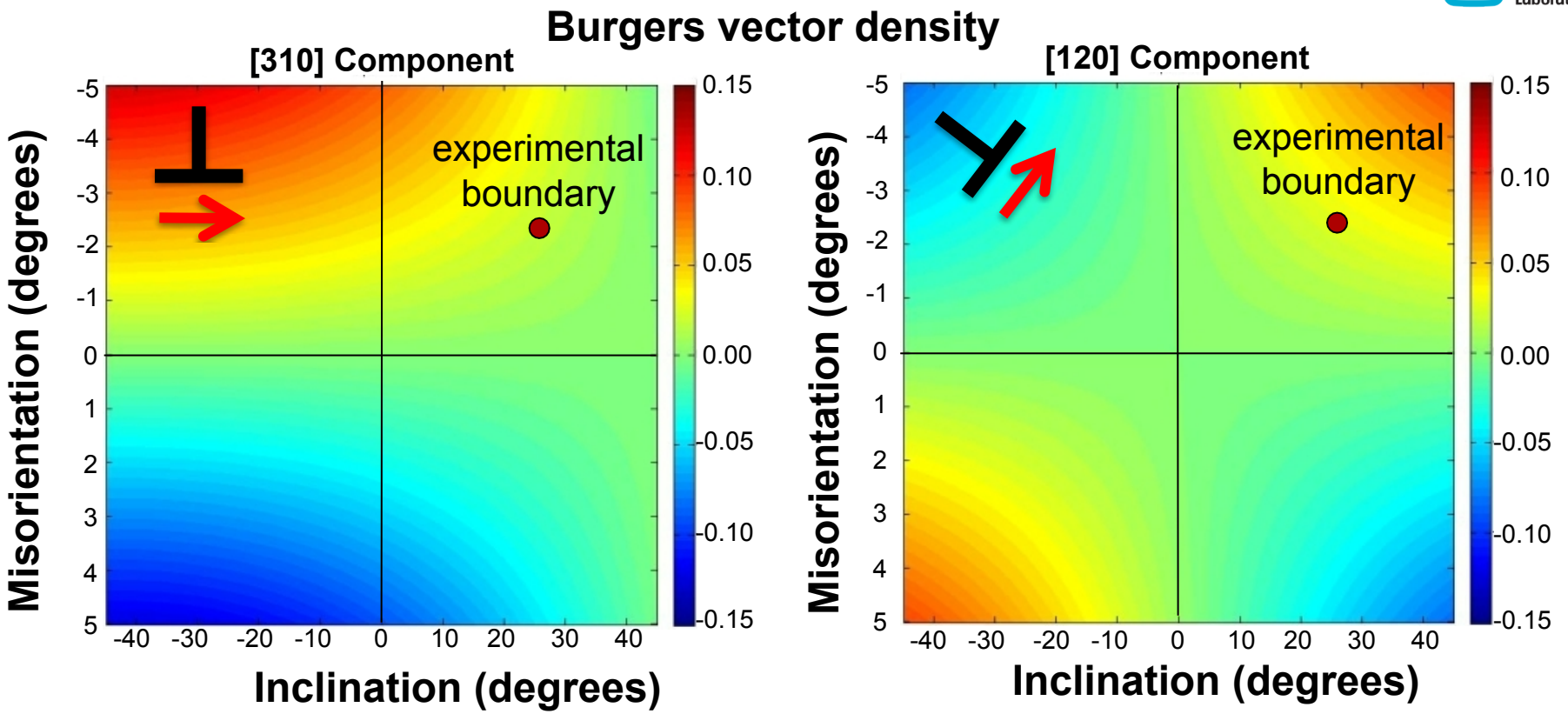


-Circuits must cross at equivalent GB sites
-Every circuit then includes 2 junctions.
-Alternate between circuits on {210} and {310} inclinations



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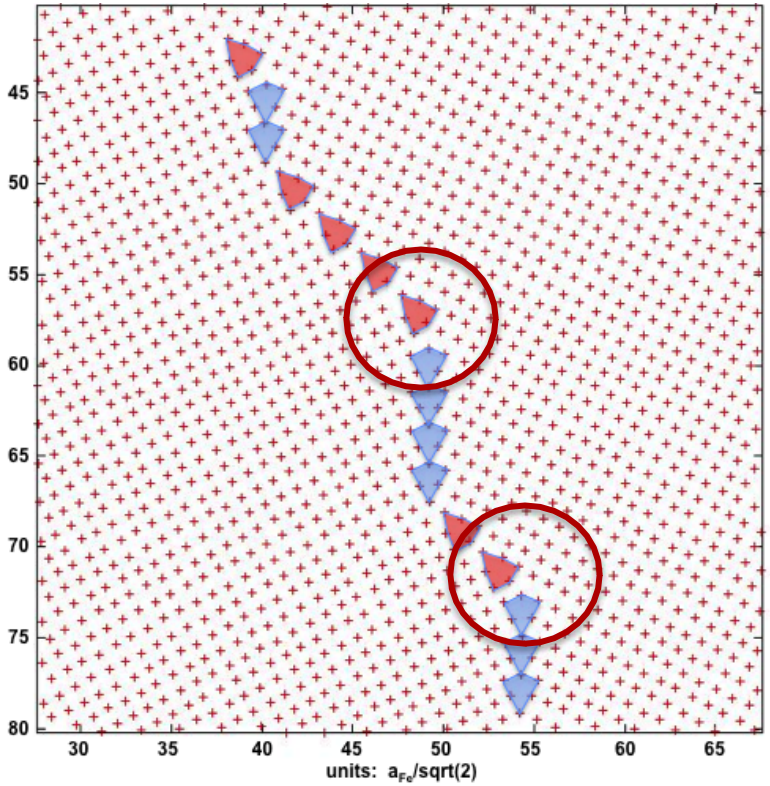
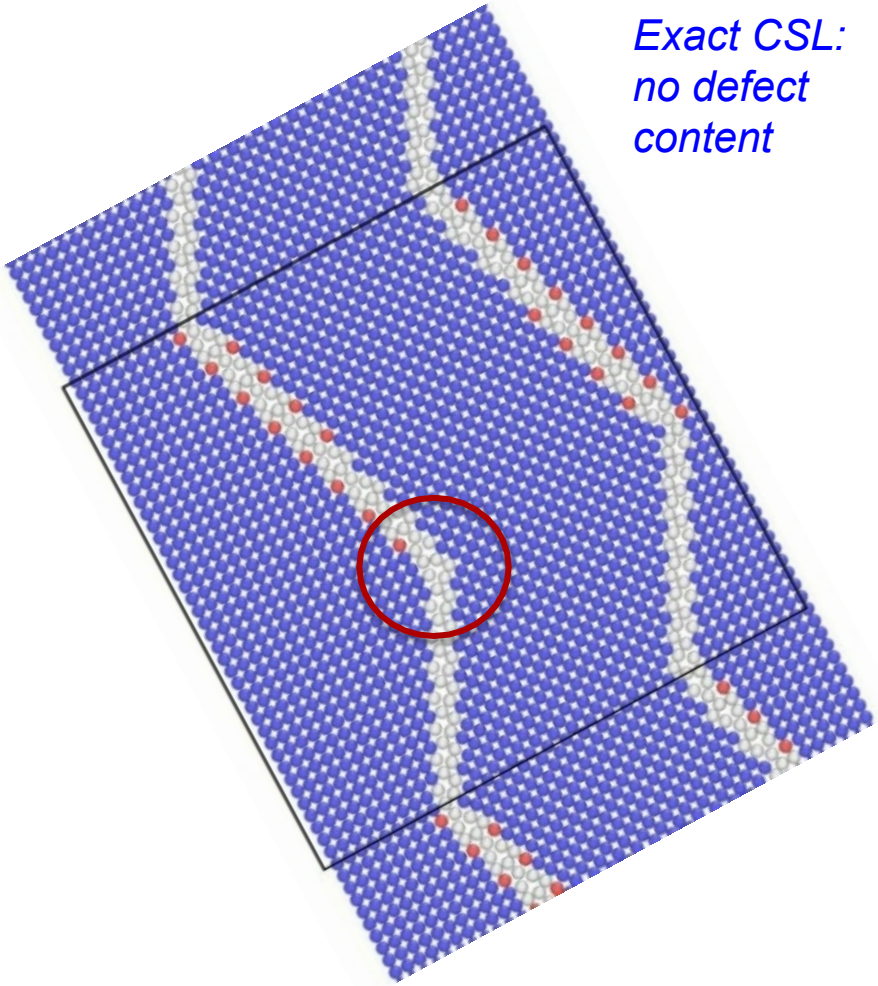
Experimental Junctions
b=(1/5)(120) and (1/5)(310)



Relaxed Periodic Atomistic Structure

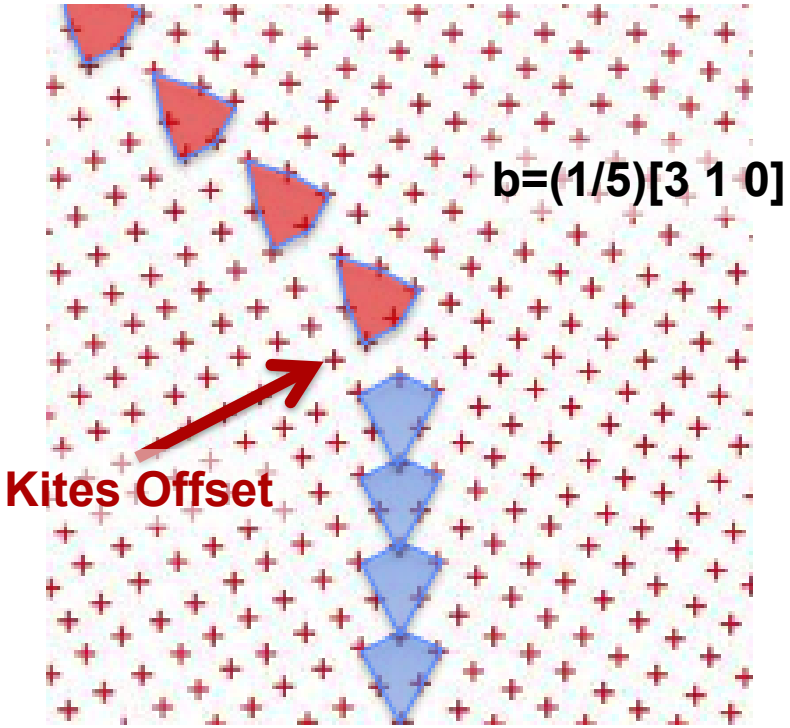


Exact CSL: no defect content

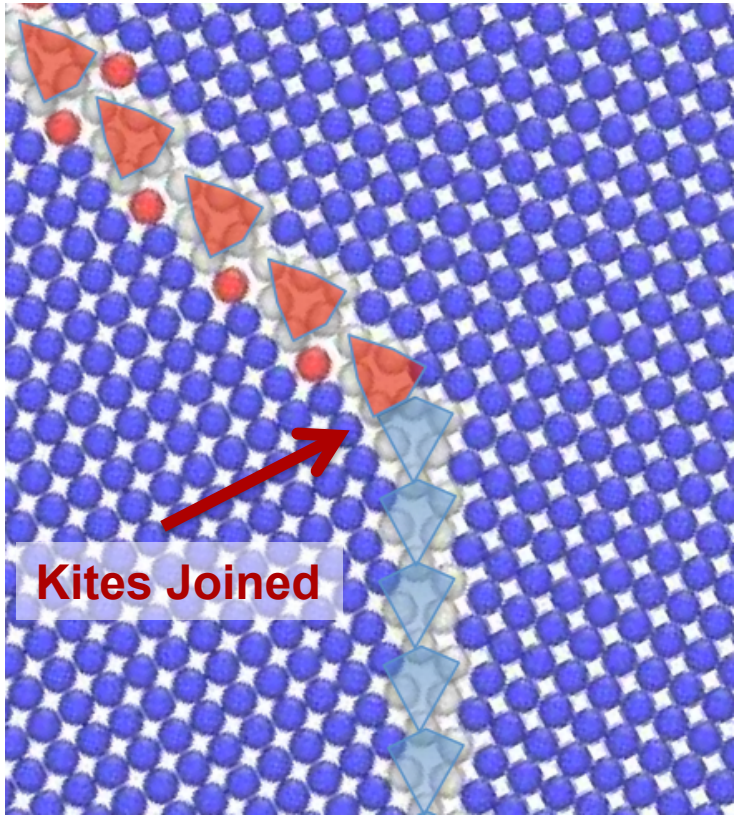
How are the grain boundary dislocations manifested in the junction structure?

Sandia National Laboratories

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



Relaxed Periodic Atomistic Structure



Conclusions.

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- **HRSTEM observations of a Σ=5 <001> Boundary in Fe shows nanoscale faceting**
  - **-Facets are on {310} and {210} planes, which correspond to the mirror symmetry planes for the Σ=5 dichromatic pattern.**

- **The atomic structures observed along the {310} and {210} facets are consistent with predictions of atomistic calculations.**

- **Circuit analysis shows presence of grain boundary dislocations at all facet junction pairs.**
  - **-two types of defect observed:**
    b=(1/5)(3,1,0) and b=(1/5)(1,2,0).
  - **-Defect density accommodates misorientation/inclination.**

- ***Open question: Does the distribution of grain boundary dislocations dictate the facet length scale?***