Defect Character at Grain Boundary Facet Junctions:

A combined HRSTEM and Atomistic Modeling Study of a Σ=5 Grain Boundary in Fe

SAND2014-18751C

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U.S. DEPARTMENT OF ENERGY

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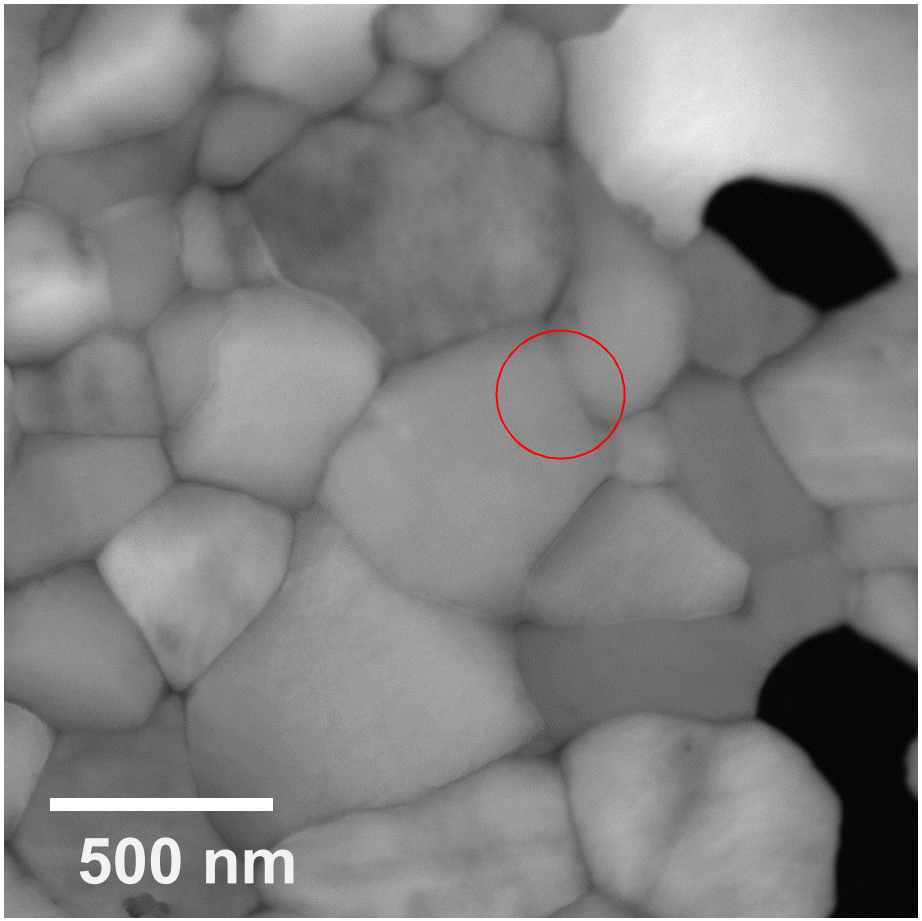
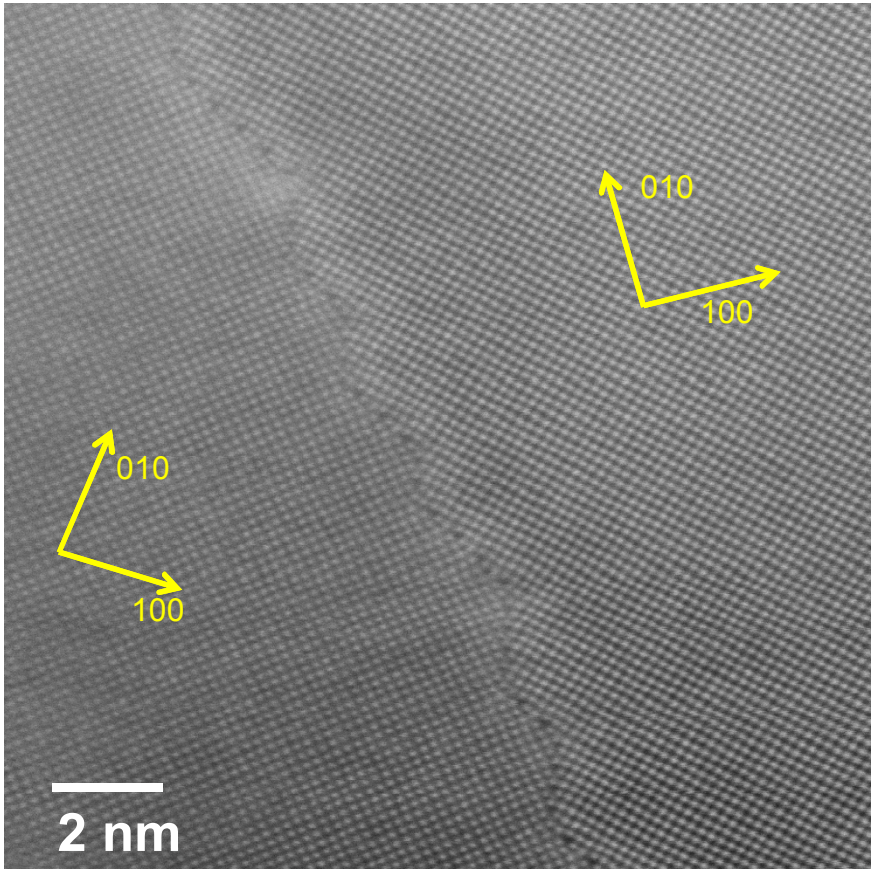
Observations: polycrystalline Fe thin film





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

HAADF-STEM
FEI-200 keV probe corrected Titan

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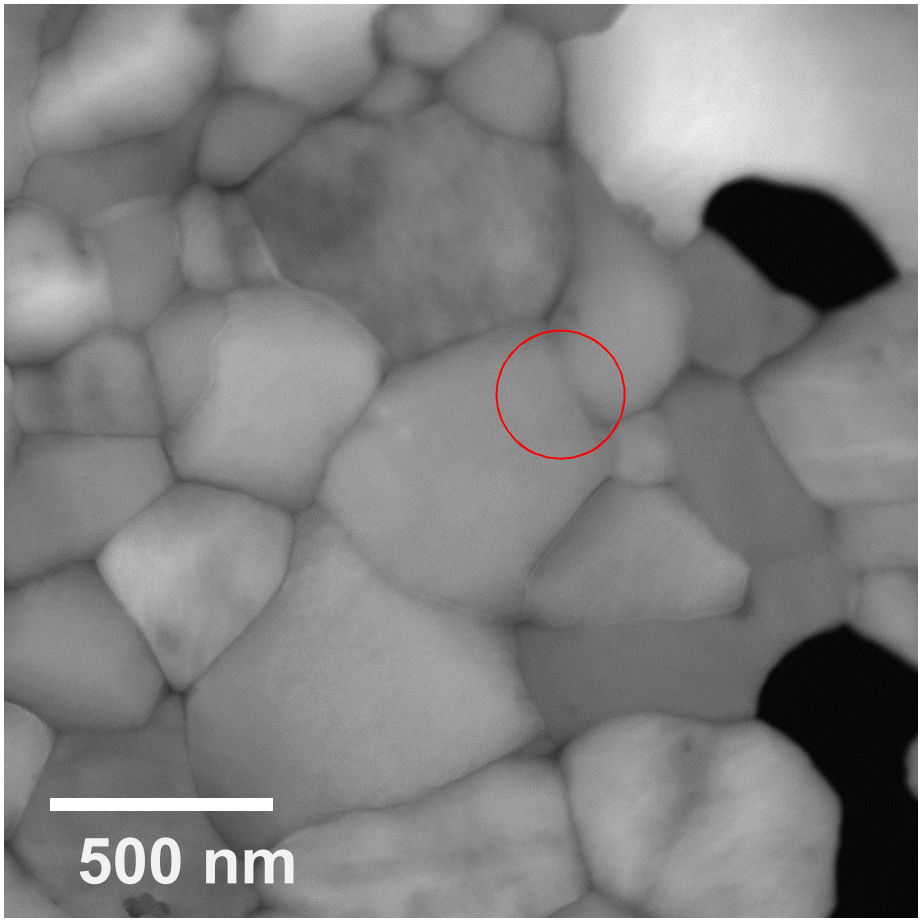
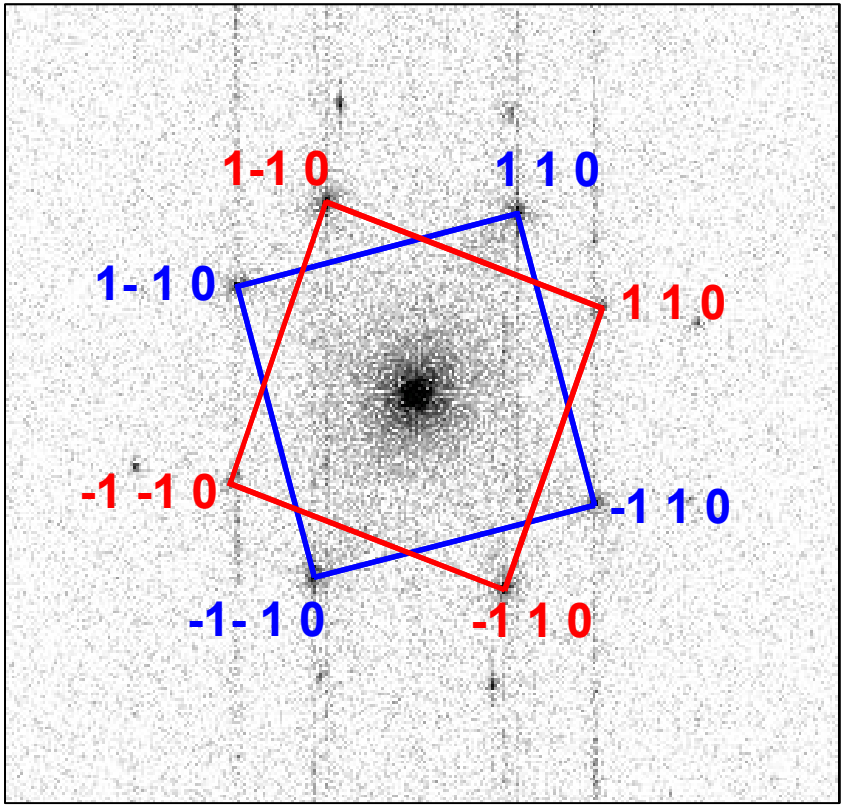
Observations: polycrystalline Fe thin film





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

Measured Disorientation: 34.5˚ ± 0.7˚
Very close to Σ=5: $\theta_{\Sigma=5}$=36.87˚

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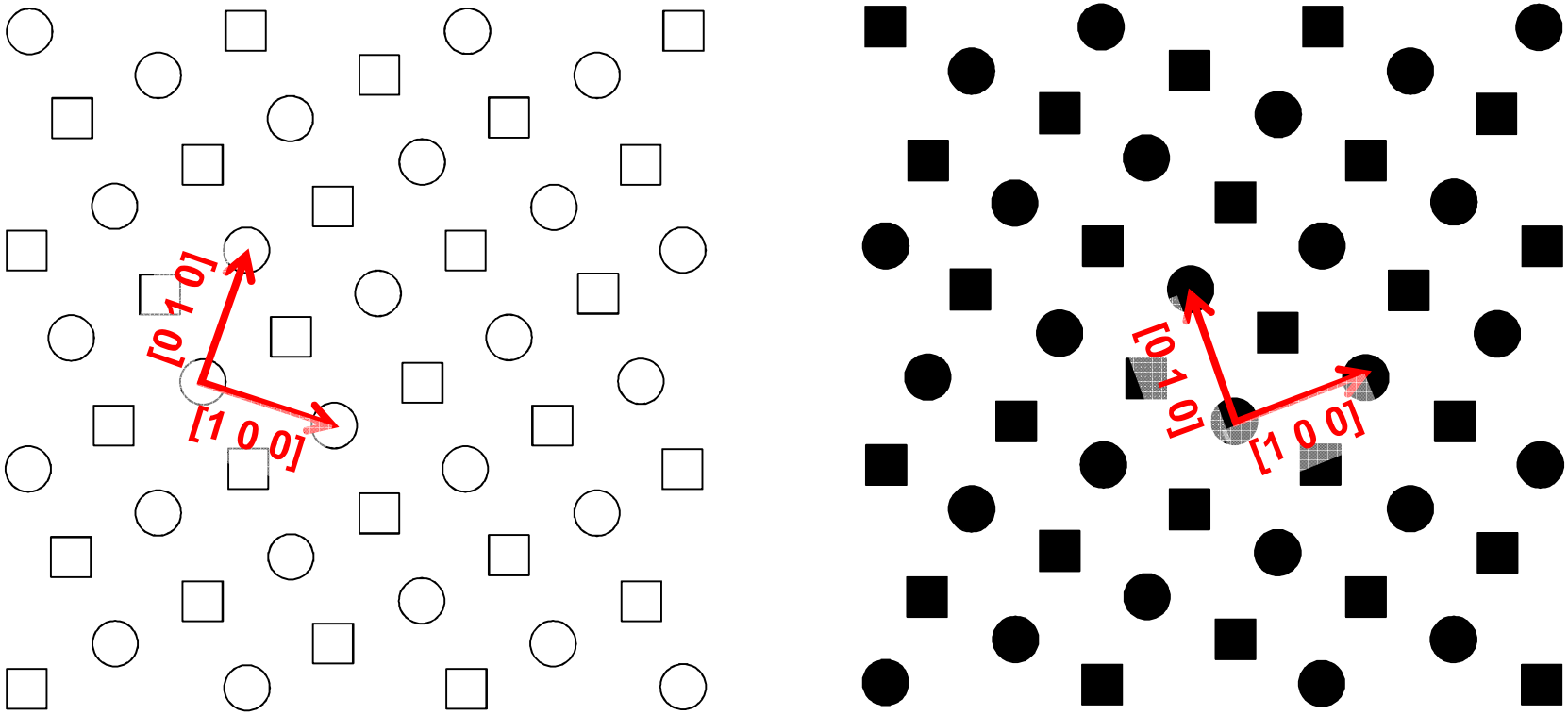
BCC Σ=5 [001]: Interfacial Crystallography



36.87° Rotation about [001]

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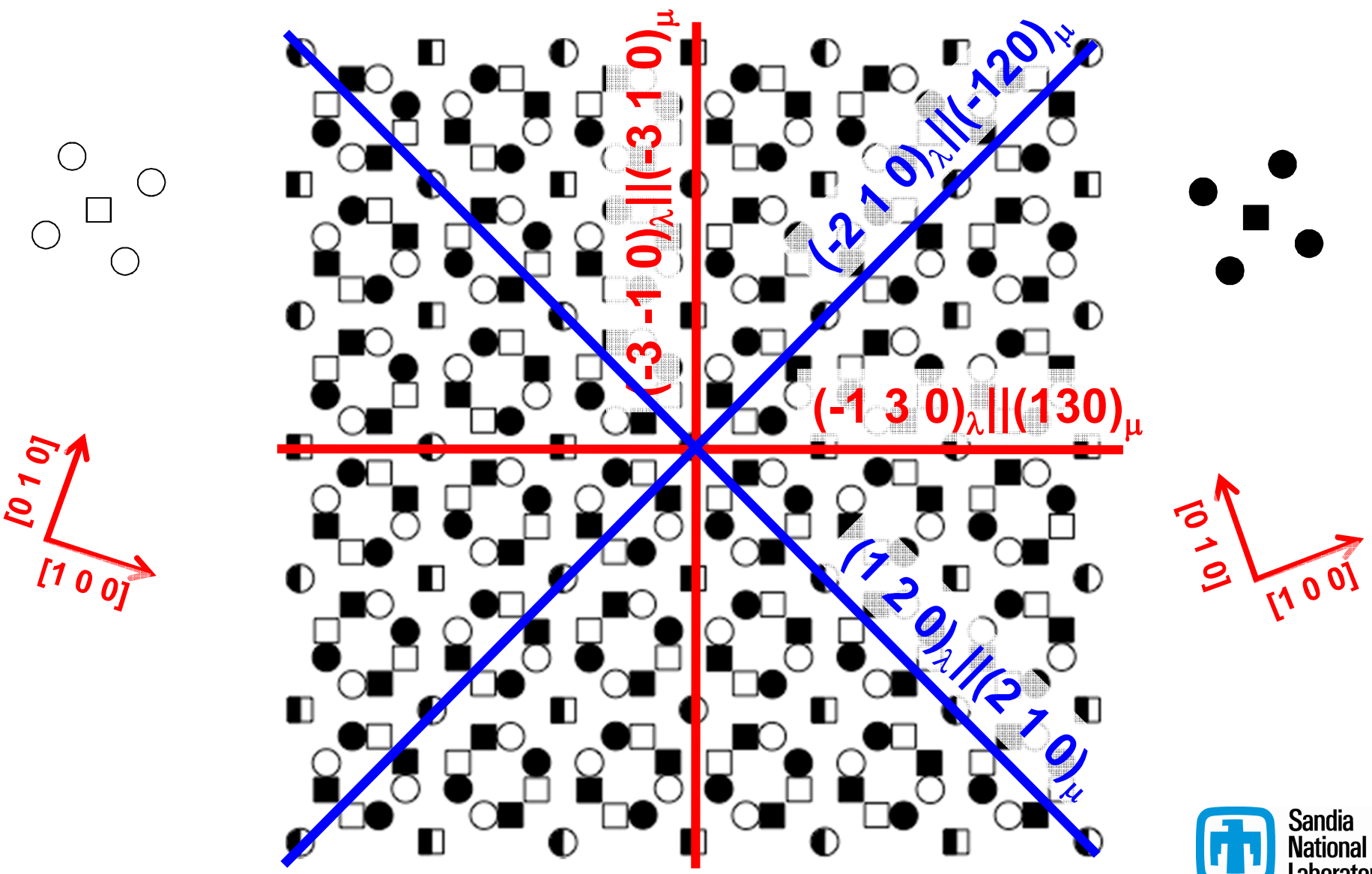
BCC Σ=5 [001]: Interfacial Crystallography

Dichromatic Pattern



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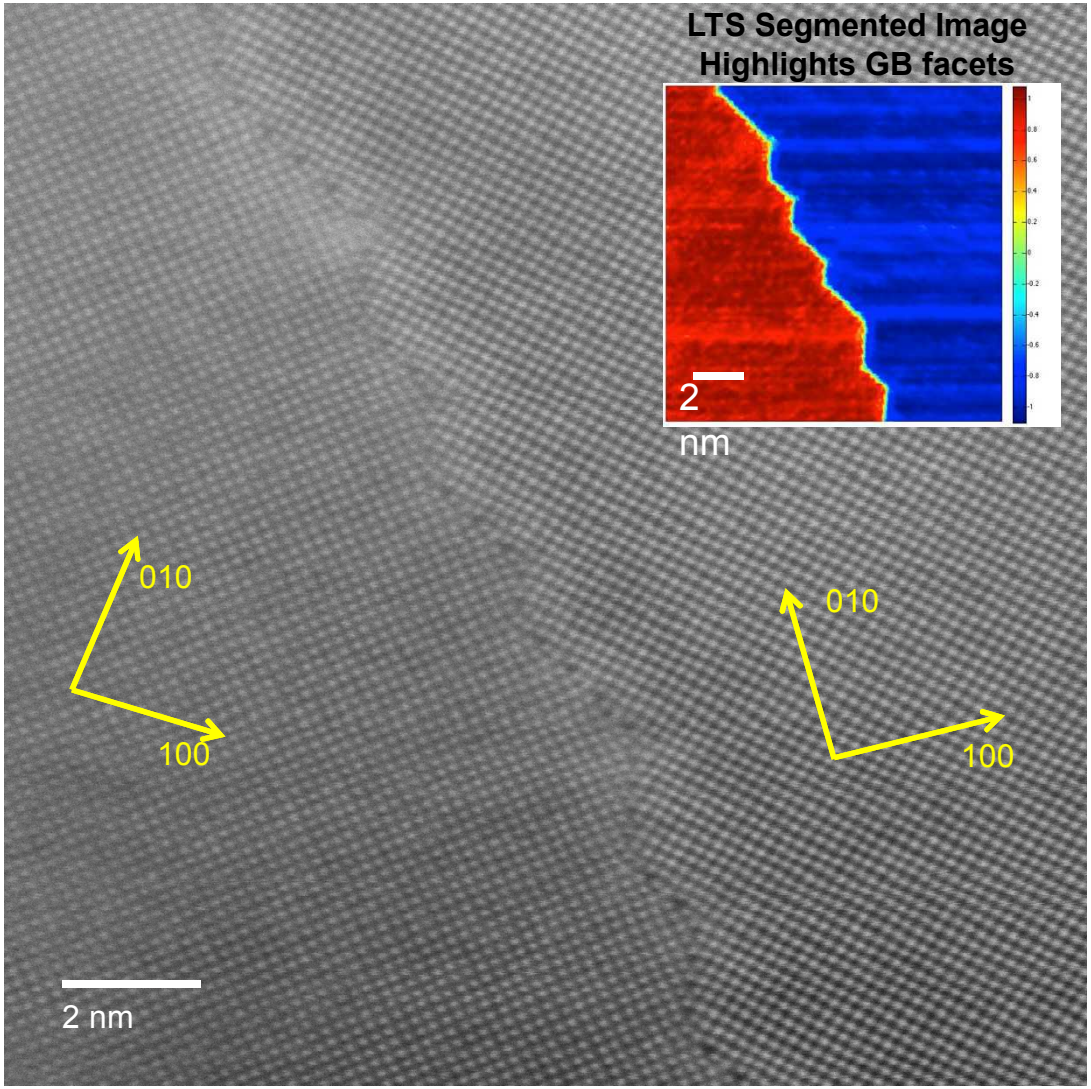
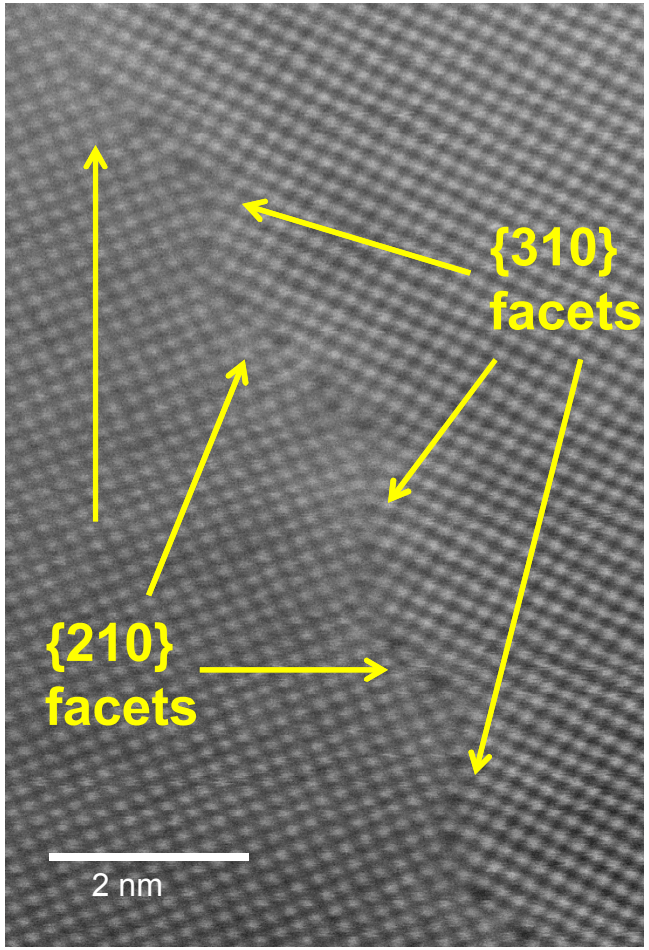
HRSTEM Shows Nanoscale Faceting at Grain Boundary

HAADF-STEM Σ=5 <001> Boundary in Fe



Boundary is faceted on
{210} and {130} type inclinations



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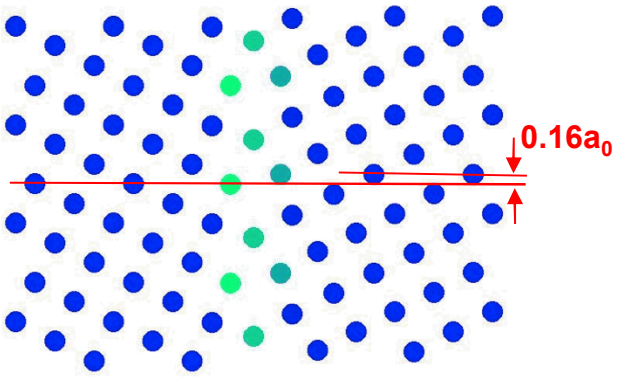
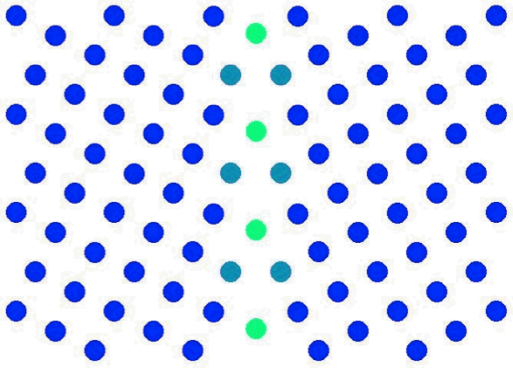
Σ=5 {310} Structures with different Potentials

Asymmetric



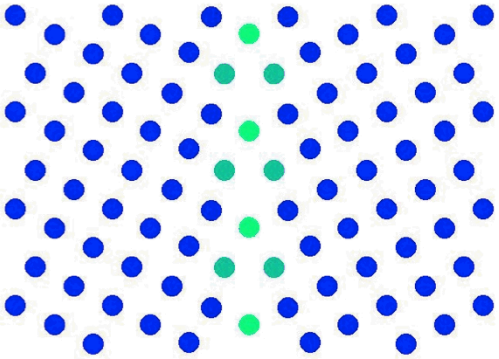
Potential: Chamati, 2006

Symmetric



Potential: Mendelev, 2003

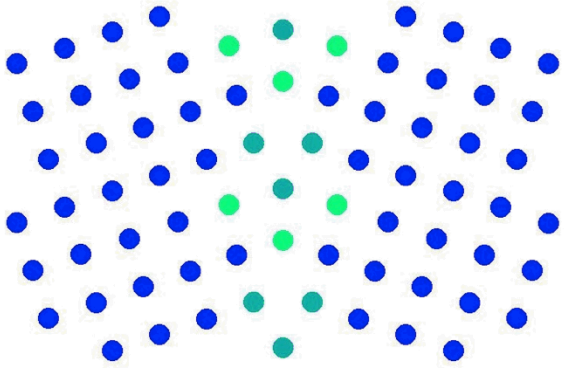
Symmetric



Potential: Proville, 2012

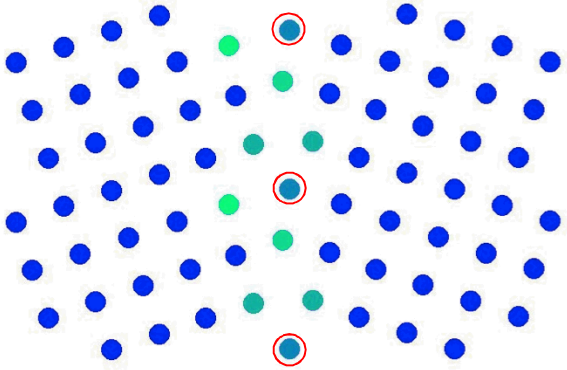
Σ=5 {210} Structures with different Potentials

Symmetric



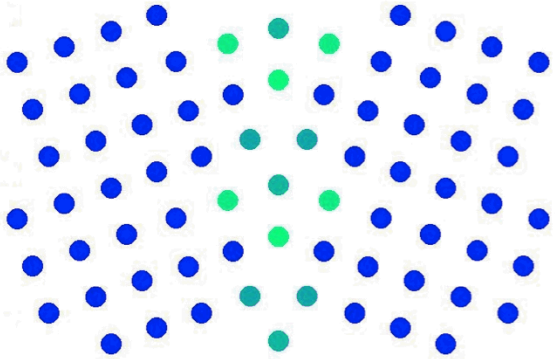
Potential: Chamati, 2006

Asymmetric



Potential: Mendelev, 2003

Symmetric



Potential: Proville, 2012

Atoms shaded by centrosymmetry parameter

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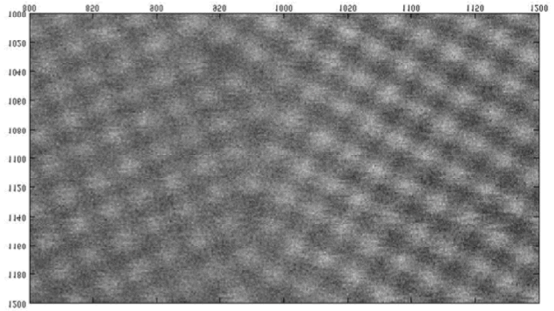
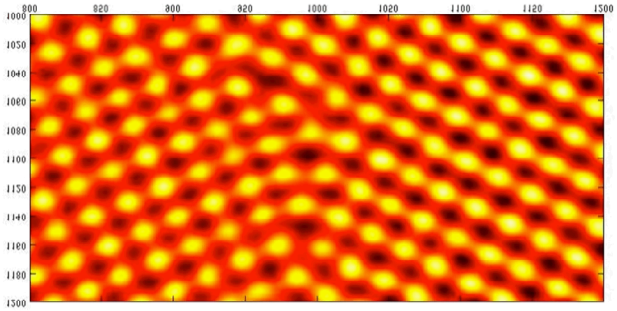
Quantifying the GB Images: Peak Location

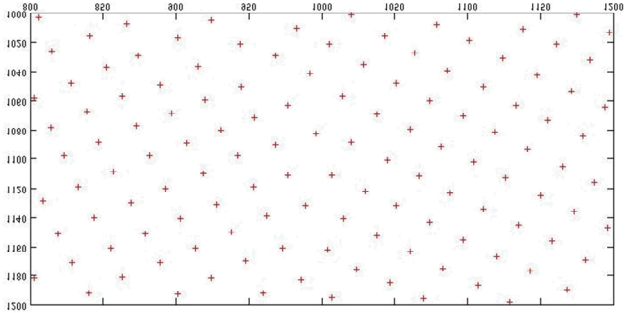
Raw HAADF STEM Image

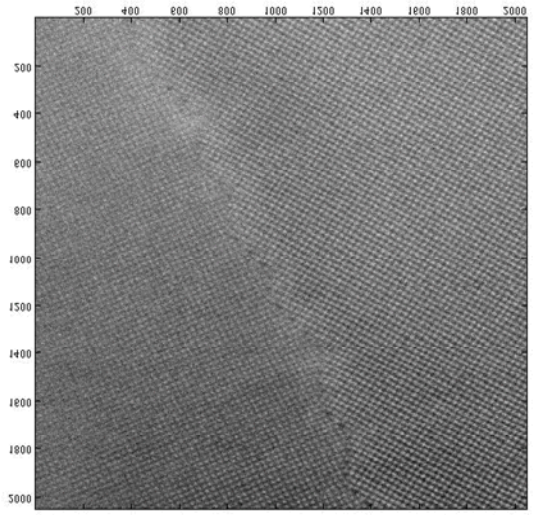


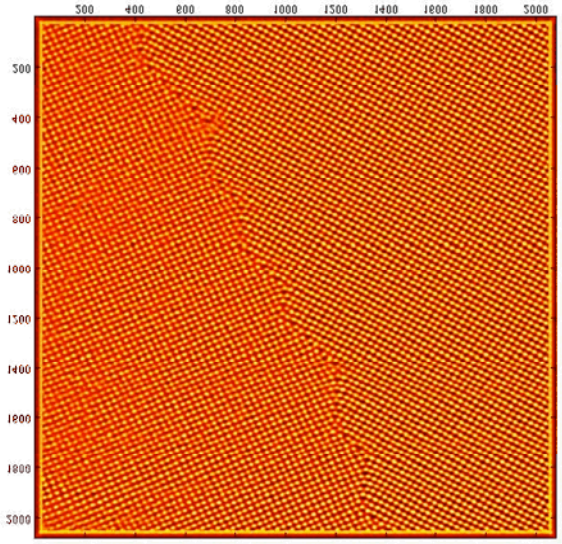
Correlation Image-Guassian

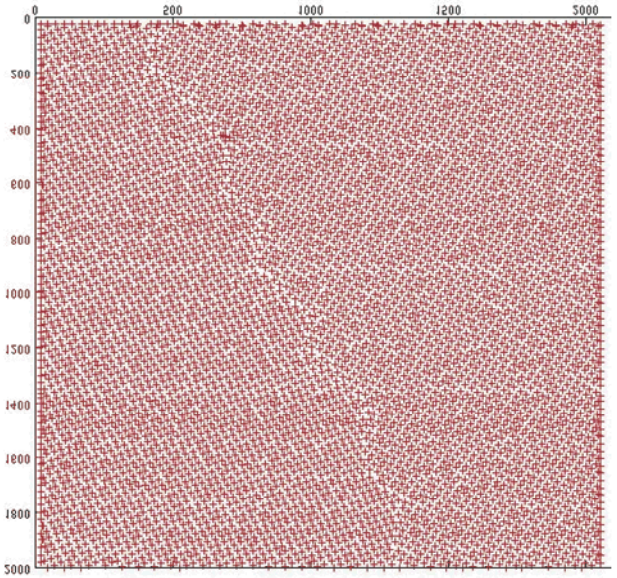


Peak Positions









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

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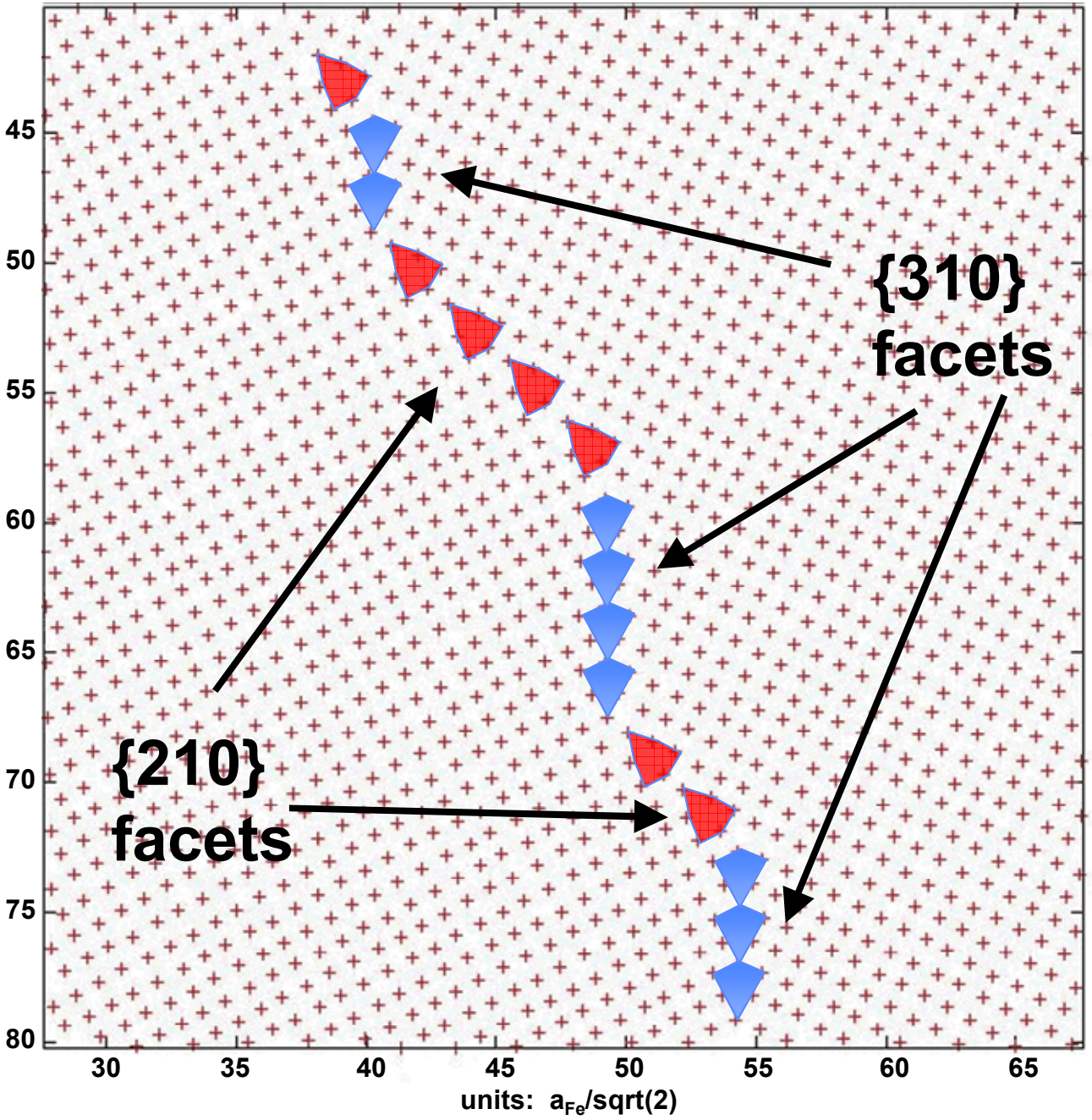

Intensity peak positions from HAADF-STEM of Fe Σ=5 grain boundary

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

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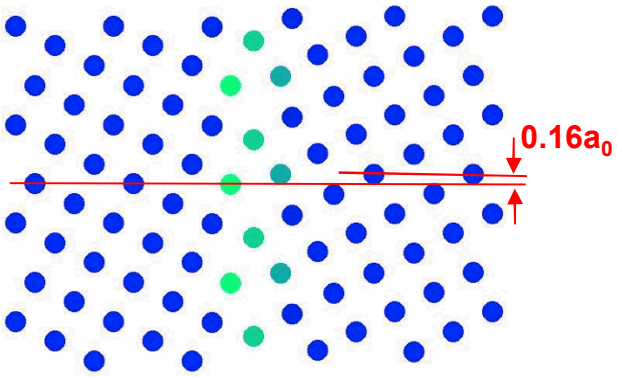
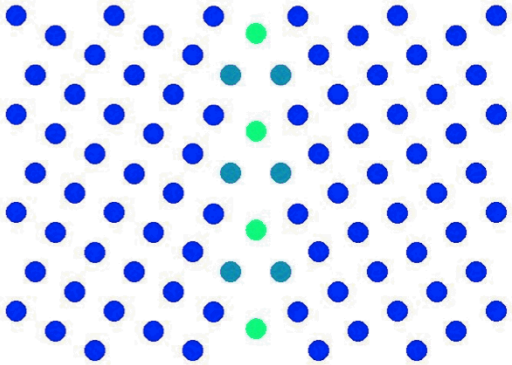
Σ=5 {310} Structures with different Potentials

Asymmetric



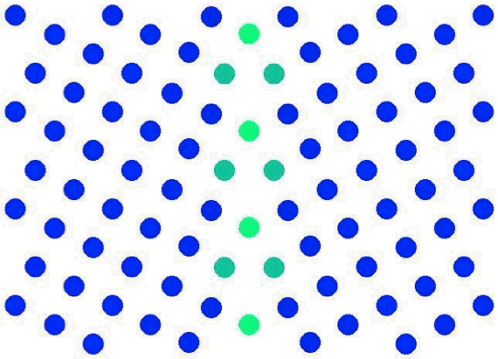
Potential: Chamati, 2006

Symmetric



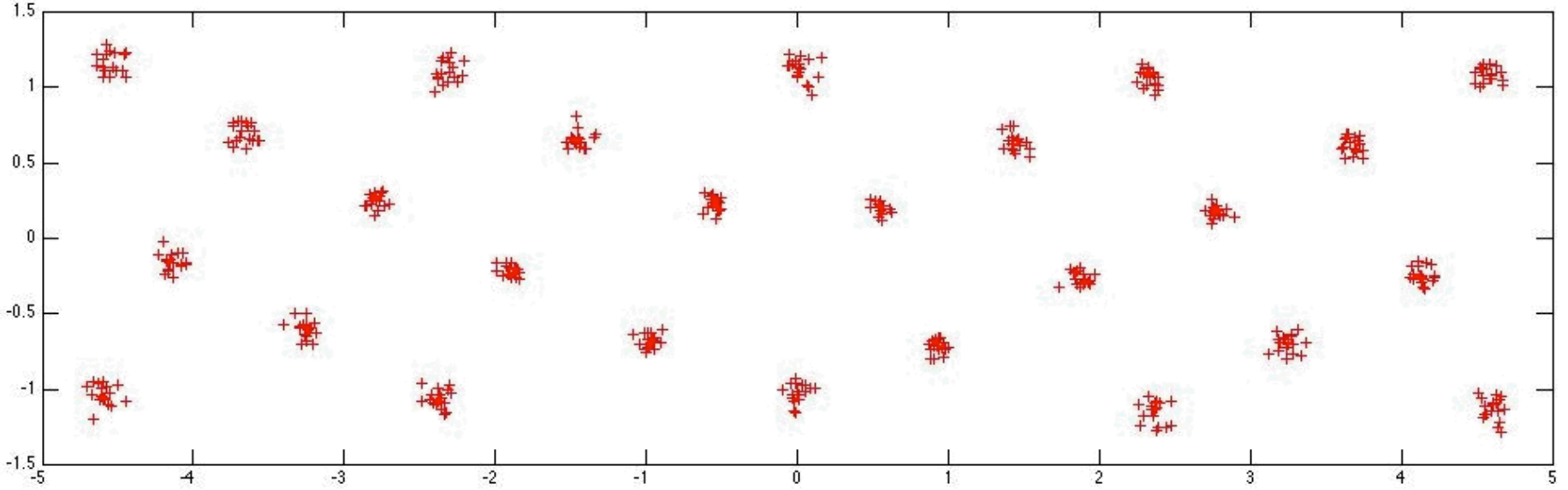
Potential: Mendelev, 2003

Symmetric



Potential: Proville, 2012

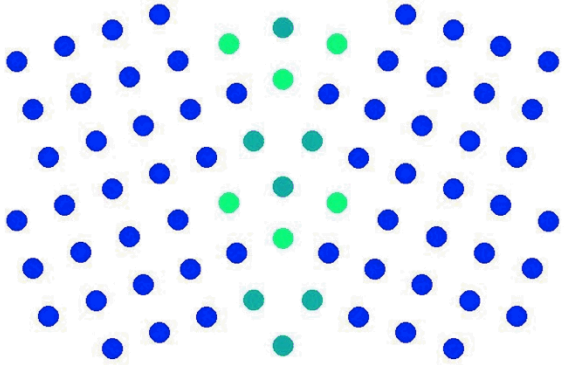
Experimental Peak Positions (HAADF STEM)



Laboratories

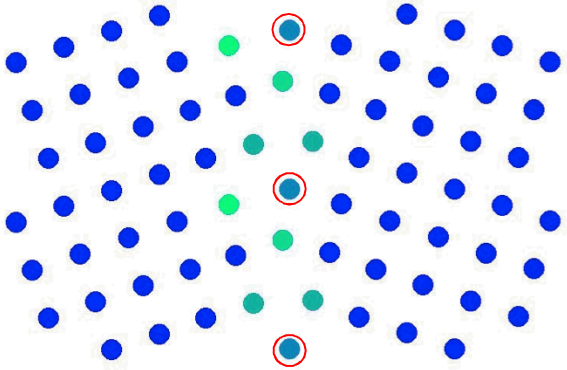
Σ=5 {210} Structures with different Potentials

Symmetric



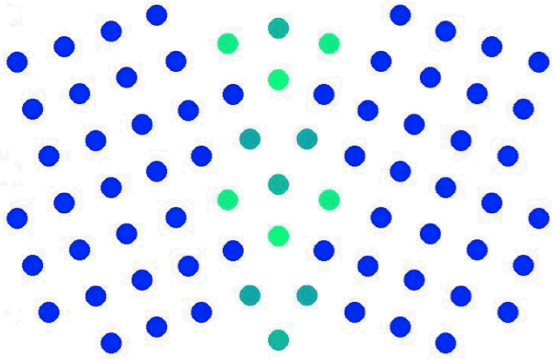
Potential: Chamati, 2006

Asymmetric



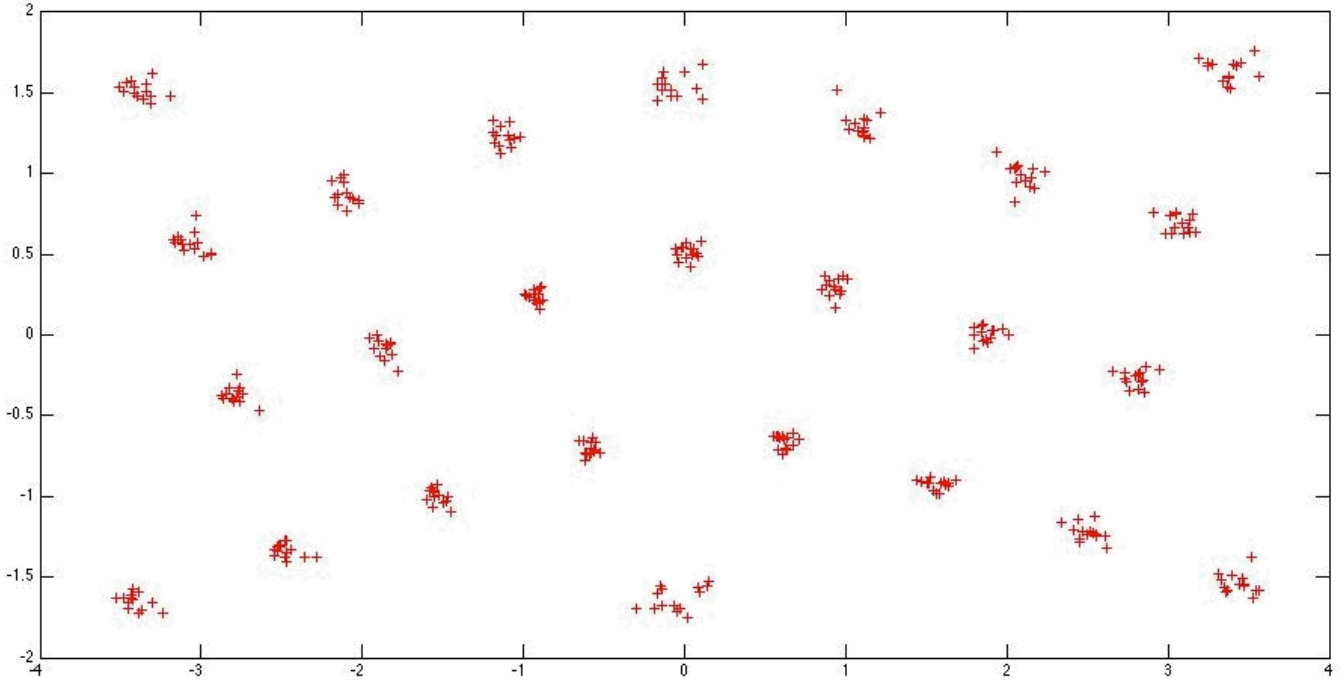
Potential: Mendelev, 2003

Symmetric



Potential: Proville, 2012

Experimental Peak Positions (HAADF STEM)



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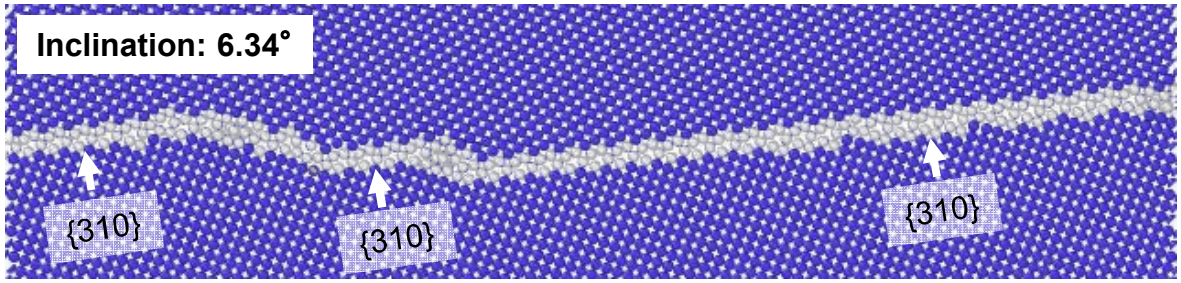
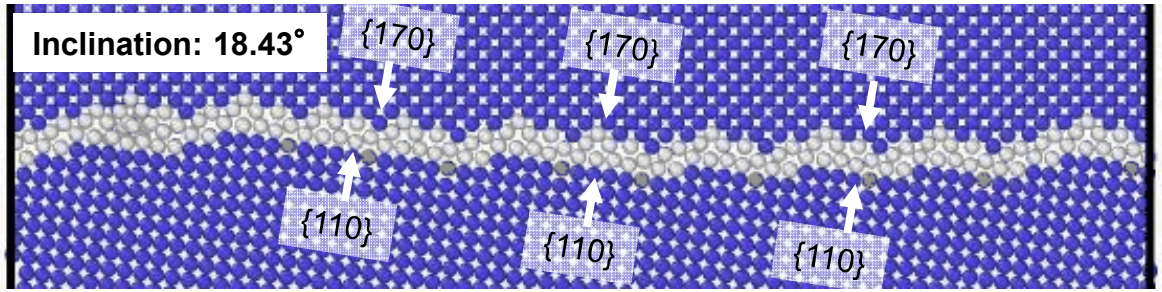
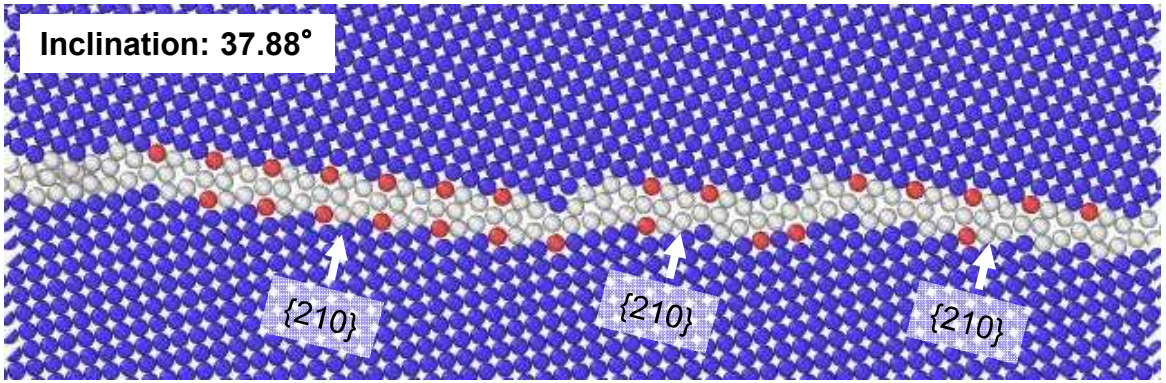
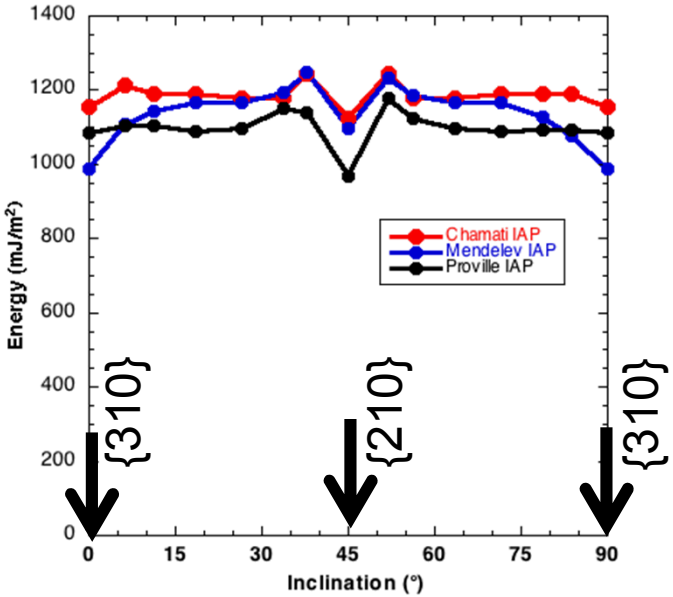
Atomistic Simulations of Σ=5 Boundaries: Variation of Boundary Inclination Angle







Atoms shaded by CNA



Contrary to experiment, the atomistics do not show co-existence of both {310} and {210} facets for intermediate inclinations

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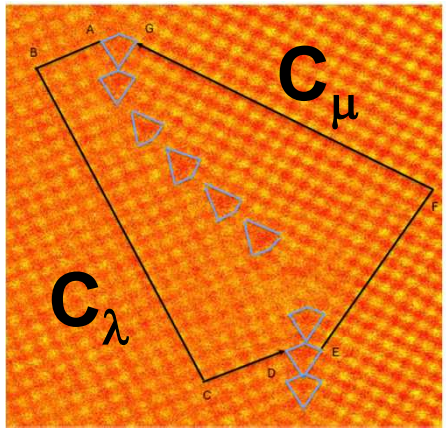
Are Grain Boundary Dislocation Present?

Determine defect content by Circuit Mapping over all facet junctions



Path in μ crystal

Path in λ crystal

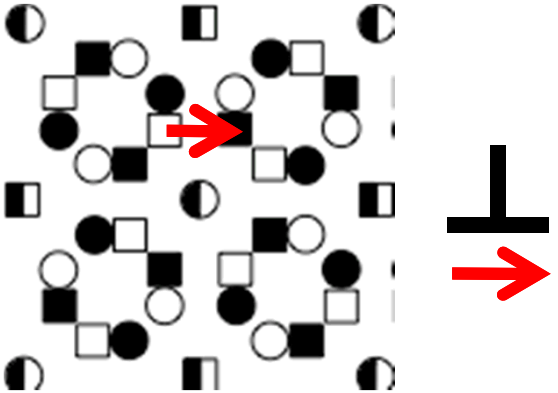
$$\mathbf{b} = -(C_\lambda + \mathbf{P}C_\mu)$$

Burgers vector

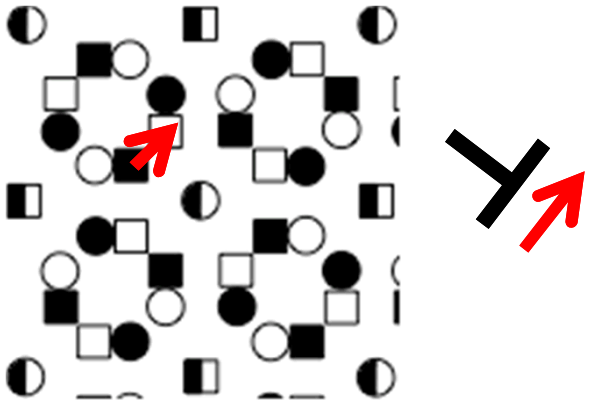
Re-express μ circuit in λ crystal coordinates.

Two types of defect observed:

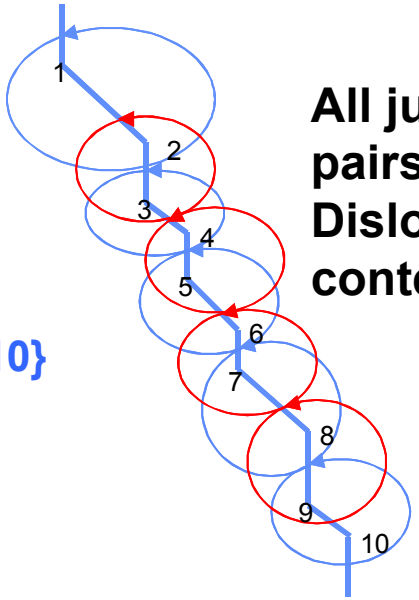
b=(1/5)[3,1,0]



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

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Conclusions.

- 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 S=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).

  - -Inclusion of grain-boundary dislocations may play a role in stabilizing the faceting.