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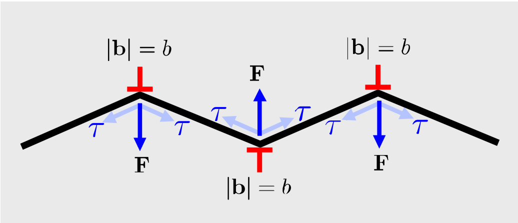

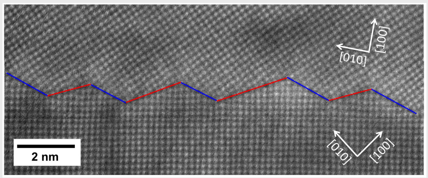

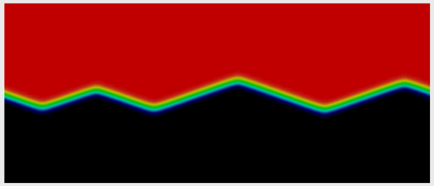

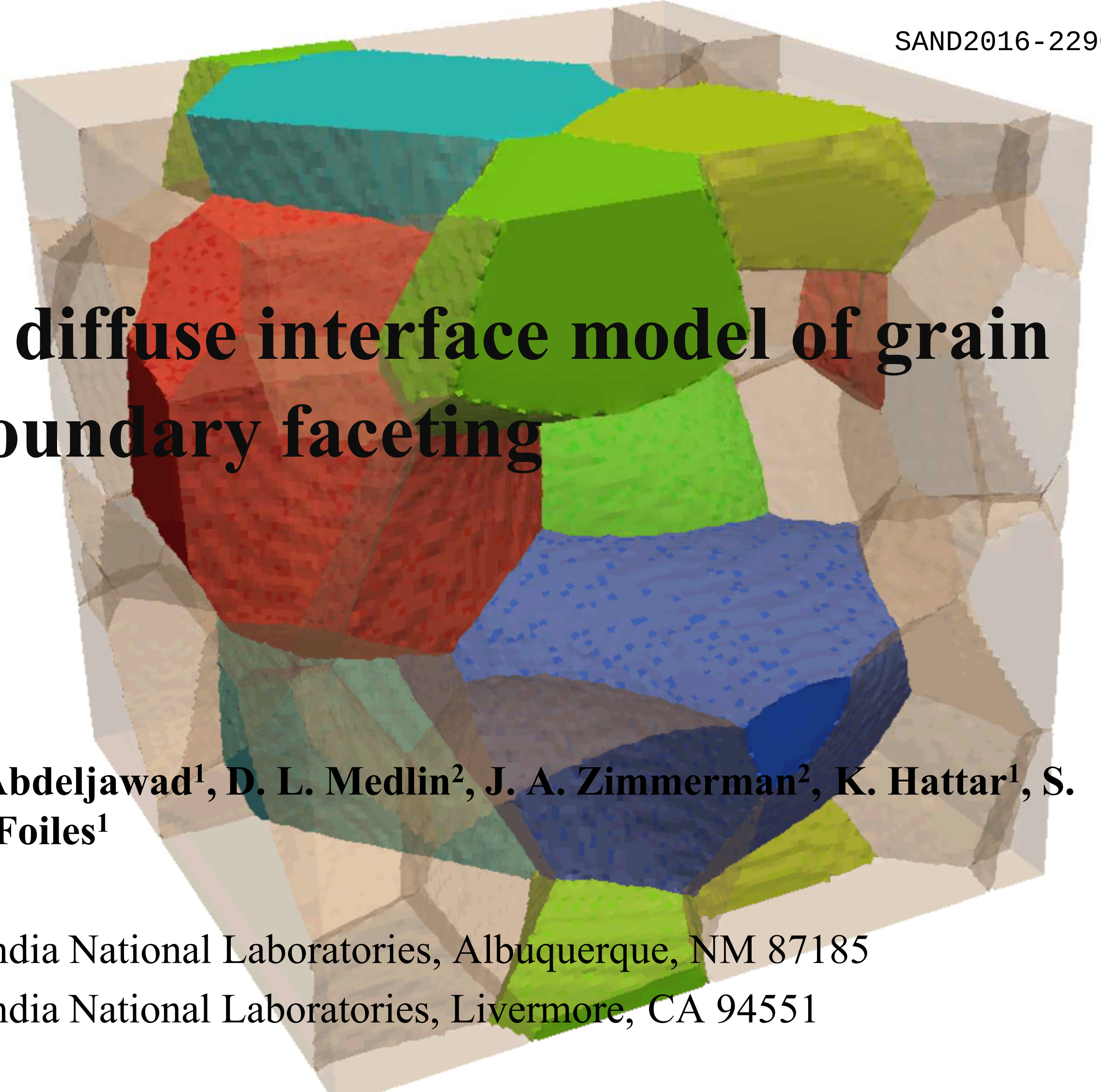

A diffuse interface model of grain boundary faceting

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Grain Boundary (GB) Faceting

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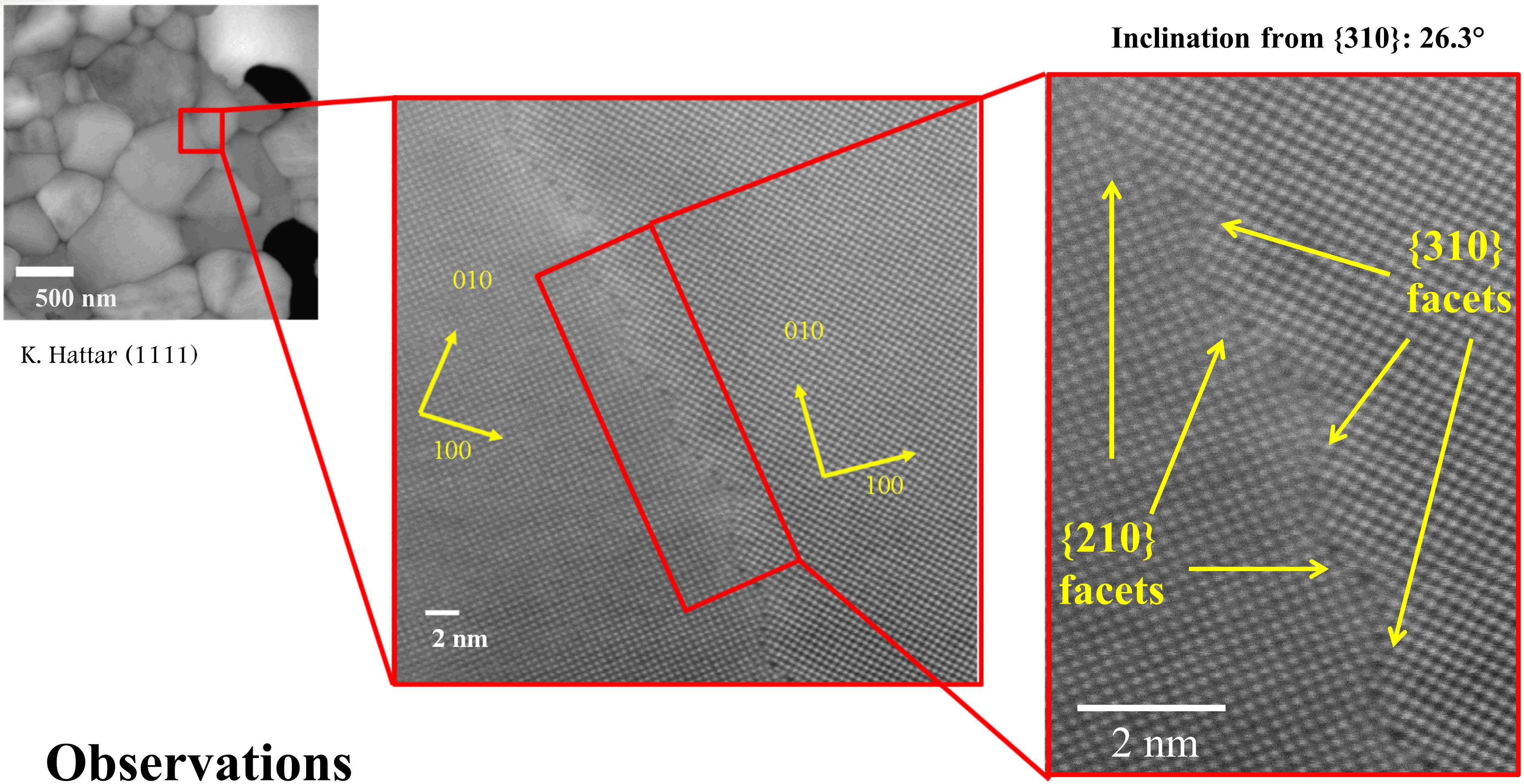
HAADF-STEM Σ5 <001> GB in Fe



D. L. Medlin (8341)

Observations

- Thermal faceting into "hill-and-valley" morphology
- Boundary is faceted on {210} and {310} inclinations

Key Questions

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- Thermodynamics of interface faceting (i.e., which GBs do facet?)
- Detailed examination via
    - Experimental characterization (HRSTEM)
    - Atomistic studies (DFT and MD)
    - Mesoscale framework (diffuse-interface model)
- Facet energetics and non-local interactions

Interface Thermodynamics

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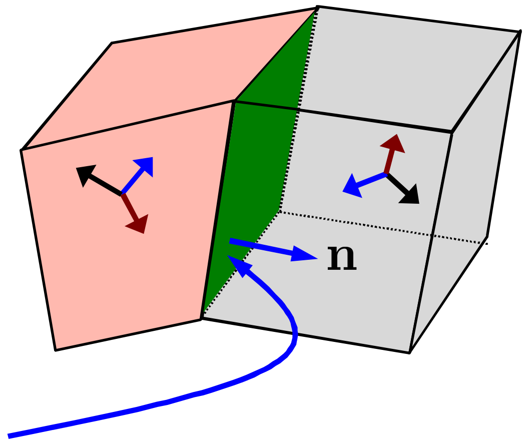
$$\gamma = \gamma_o + f(\{\theta_1, \theta_2\}, c, T, \{\phi_1 \Phi \phi_2\})$$

GB inclination
"GB plane normal"

GB misorientation
"crystallographic orientation of abutting grains"

Interface stiffness: $\gamma + \frac{\partial^2 \gamma}{\partial \theta^2}$

Interface stress: $\tau_{ij} = \delta_{ij}\gamma + \frac{\partial \gamma}{\partial \epsilon_{ij}}$



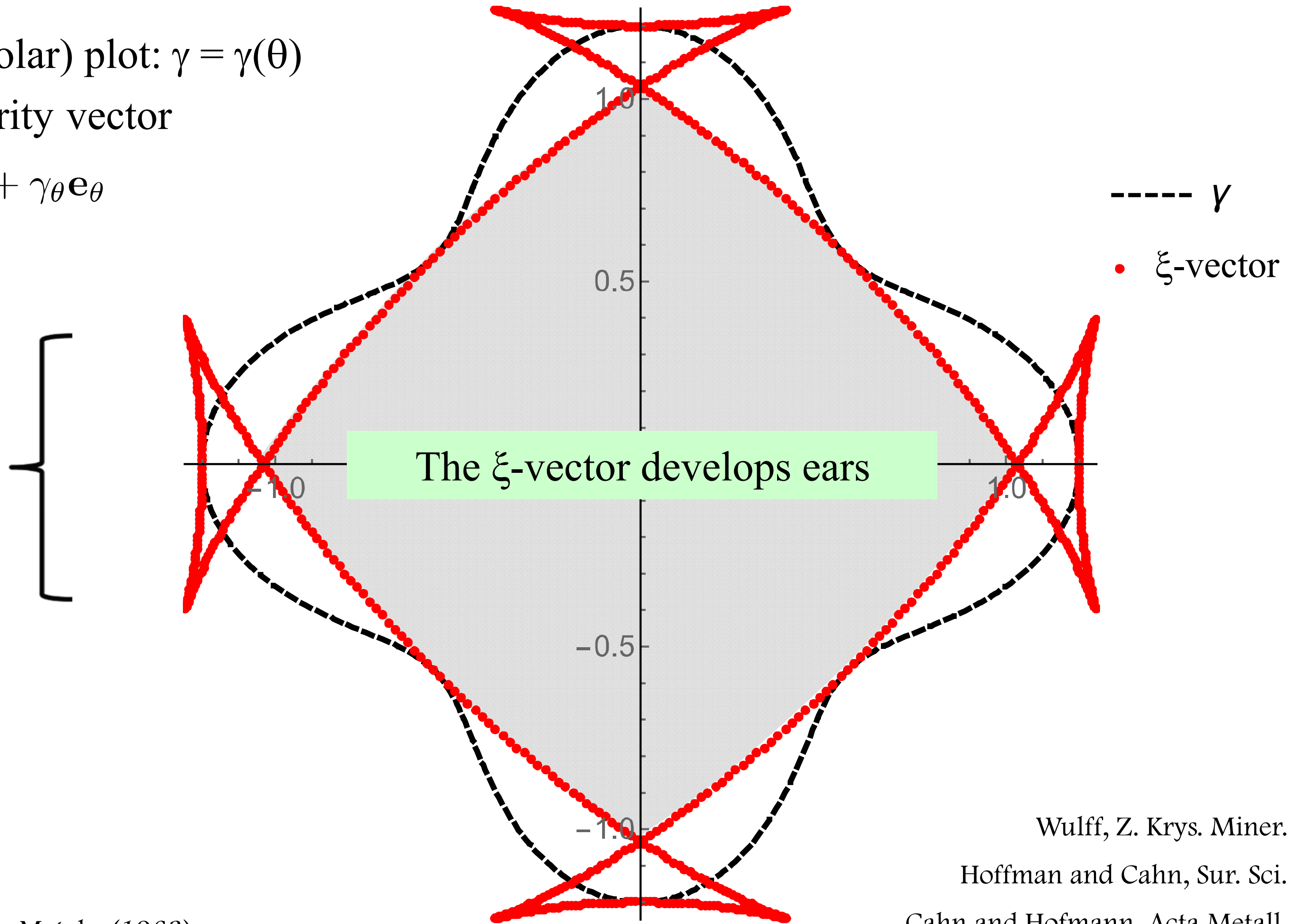
GB plane: **n** normal unit vector or $\{\theta_1, \theta_2\}$ inclination angles

Faceting: Graphically

- Wulff (polar) plot: $\gamma = \gamma(\theta)$
- ξ-capillarity vector

$$\xi = \gamma \mathbf{e_r} + \gamma_\theta \mathbf{e}_\theta$$

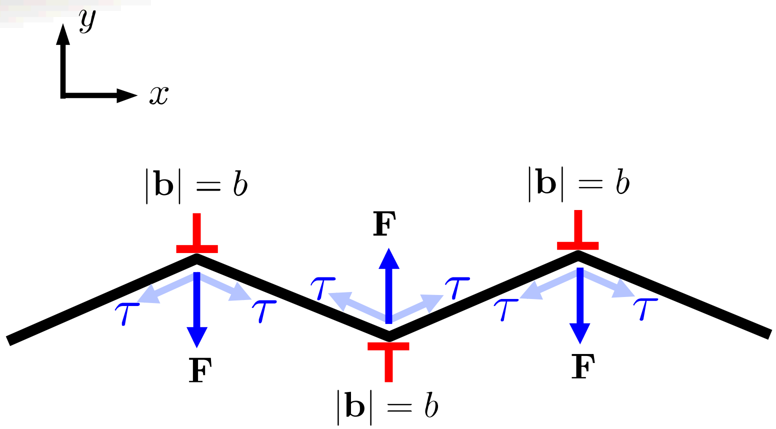
An ear in ξ-vector



F. Frank, Amer. Soc. Metals (1963)
N. Cabrera, Sur. Sci. (1964)

Wulff, Z. Krys. Miner. **34** (1901)
Hoffman and Cahn, Sur. Sci. **31** (1972)
Cahn and Hofmann, Acta Metall. **22** (1974)
Herring, Phys. Rev. **82** (1951)

Energetics of a Faceted GB



$\perp$ Dislocation with Burgers vector $\mathbf{b}$ due to mismatch in translation vectors of interfaces

Dimitrakopulos et al. Interface Sci. (1996)

τ : Interface stress. Discontinuity across junction leads to line forces

Hamilton et al. Phys. Rev. Lett. (2003)

- Interface anisotropy (high/low energy planes)
- Balance of interface stress (τ) at facet junctions leads to line forces **F = ±P**
- Dislocation content at facet junctions and their elastic interactions

$$\mathcal{F}_{tot} = f_{inter} + f_{local} + f_{nonlocal}$$

Anisotropic interface

Junction energy due to dislocation and interface stress

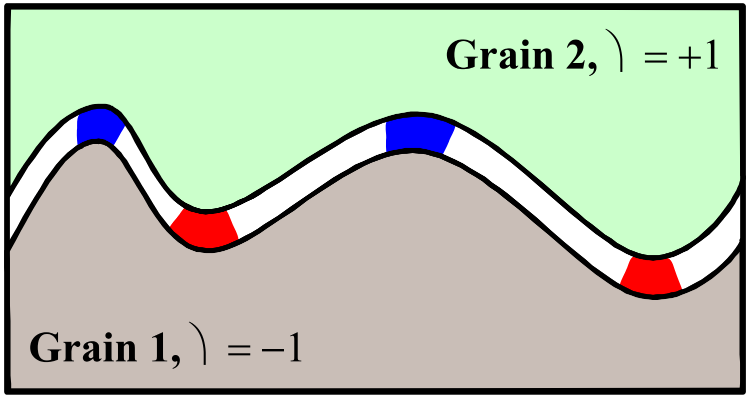
Non-local interactions between dislocations, and point forces

Phase Field Framework

- Structural Order Parameter
  - Mean curvature: $\mathcal{K} = \nabla \cdot \left(\frac{\nabla \phi}{|\nabla \phi|} \right) \sim \nabla^2 \phi$
  - Higher order expansion:

$$\gamma = a_o(\theta) + a_2(\theta)\mathcal{K}^2 + a_4(\theta)\mathcal{K}^4 + \cdots$$

Herring, Phys. Powd. Metall. (1951)



- Total Energy

$$\mathcal{F}_{tot} = \int d\mathbf{r} \left[A_H f(\phi) + \frac{\epsilon^2(\theta)}{2} |\nabla \phi|^2 + \Gamma_o \left(\nabla^2 \phi \right)^2 + \Gamma_1 \int_{|\mathbf{r}-\mathbf{r}'|>R_c} d\mathbf{r}' \frac{\nabla^2 \phi(\mathbf{r}) \ \nabla^2 \phi(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} \right]$$

Bulk

Anisotropic GB (Wulff, ξ-vector)

Local facet junction energy

facet junction-junction interactions

- Dynamics

$$\frac{\partial \phi}{\partial t} = -L \left(\frac{\delta \mathcal{F}_{tot}}{\delta \phi} \right)$$

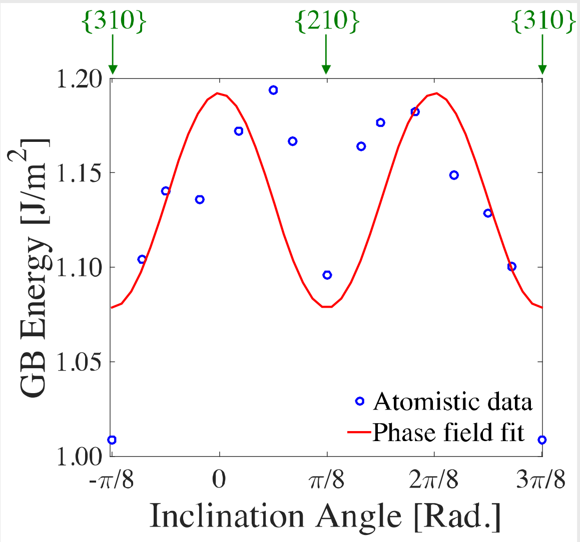
Einstein's razor: "Everything should be made as simple as possible, but no simpler"

A. Einstein

Abdeljawad et al. (Under review for J. App. Phys.)

Model Parameters: Atomistics

- The case for Σ5 <001> tilt GB in BCC Fe



Proposed fit

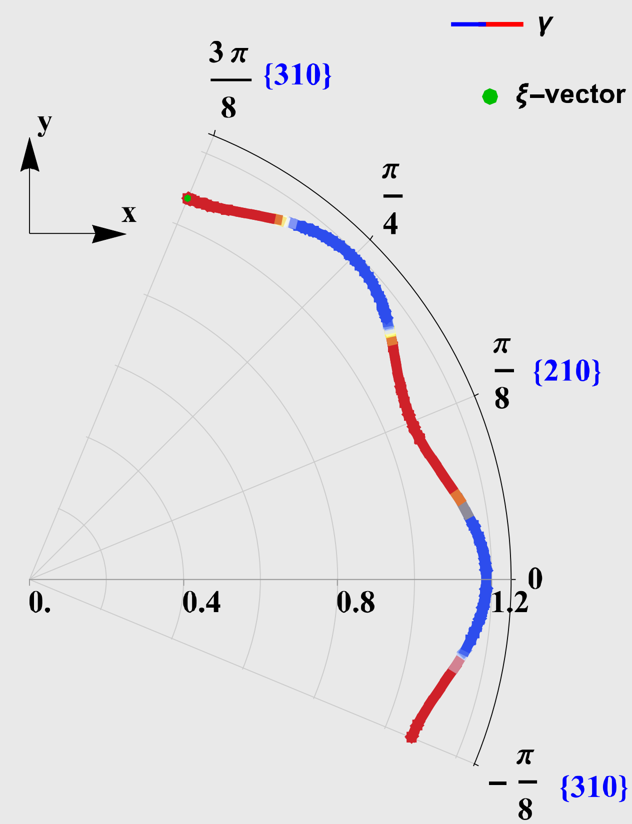
$$\epsilon(\theta) = \lambda\,[1 + \delta\cos(8\theta)]$$

Fit to atomistics

λ = 1.1
δ = 0.05

Model Parameters

λ: Nominal GB energy
δ: Strength of anisotropy
Γ_o: Junction energy
Γ_1: Non-local interactions



Linear Stability

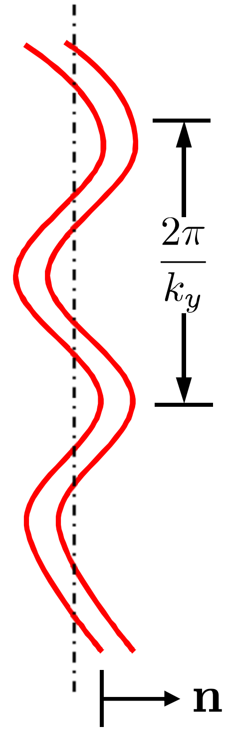
Γ_o: Junction energy
Γ_1: Junction interactions

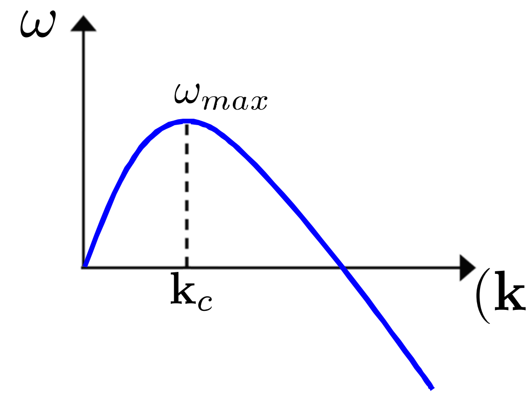
- Linearize integro-differential Eq.
- Assume Fourier modes $\phi = \hat{\delta}_\phi \exp\left[i\mathbf{k}\cdot\mathbf{x} + \omega(\mathbf{k})t\right]$
- Dispersion relation $\omega(\mathbf{k}, \Gamma_o, \Gamma_1; \lambda, \delta)$

$$\omega(\mathbf{k}, \Gamma_o, \Gamma_1; \lambda, \delta)$$

$\omega > 0$: Growing (unstable)

$\omega < 0$: Decaying (stable)





$$\omega(\mathbf{k}) = 4A_H - \lambda^2(1+\delta)\left[\left(1+\delta - \frac{4\pi\Gamma_1}{\lambda^2(1+\delta)R_c}\right)k_x^2 + \left(1 - 63\delta - \frac{4\pi\Gamma_1}{\lambda^2(1+\delta)R_c}\right)k_y^2 + \frac{2\Gamma_o}{\lambda^2(1+\delta)}\left(k_x^2 + k_y^2\right)^2\right]$$

Abdeljawad et al. (Under review for J. App. Phys.)

Linear Stability (cont.)

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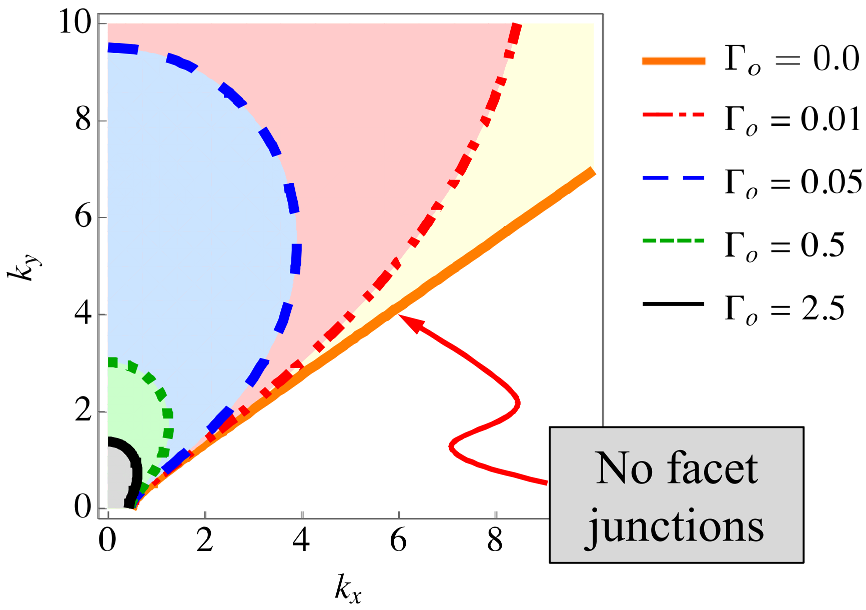
Facet junction energy with no interactions ($\Gamma_1 = 0$)

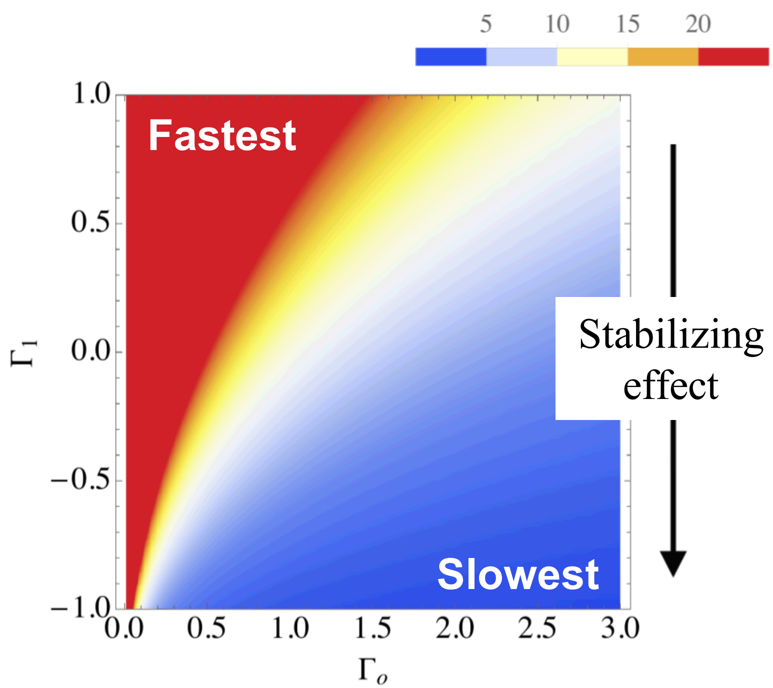
Γ_o: Junction energy
Γ_1: Junction interactions

Shaded regions correspond to unstable perturbations



Maximum growth rate

$\omega_{max}(\mathbf{k}_c, \Gamma_o, \Gamma_1; \lambda, \delta)$

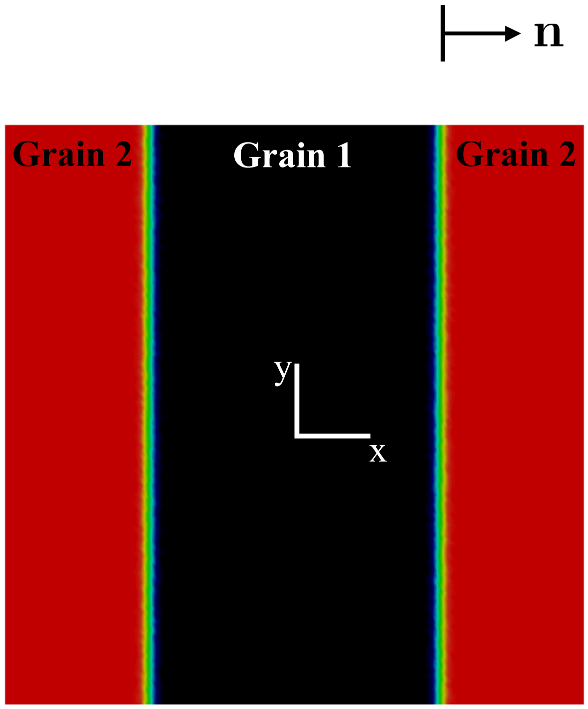


- Regions of instability decrease in size as facet junction energy increases
- Faceted GBs with large spacing between junctions

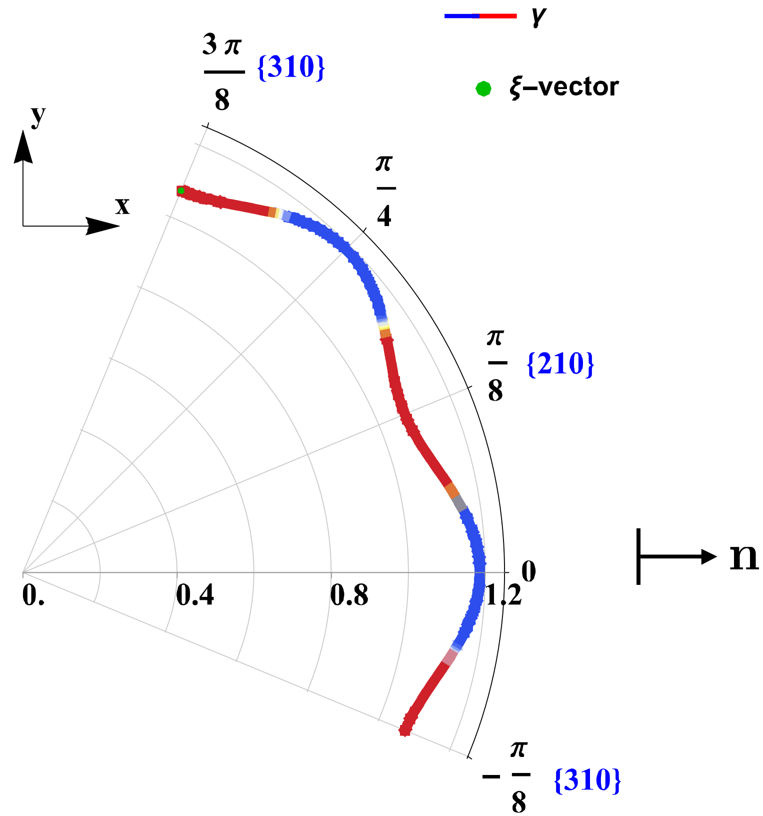
Abdeljawad et al. (Under review for J. App. Phys.)

Results: A Two Grain Structure

- Vary the facet junction energy (Γ_o) with no junction interactions ($\Gamma_1 = 0$)
- Vary junction interactions (Γ_1) for a fixed junction energy

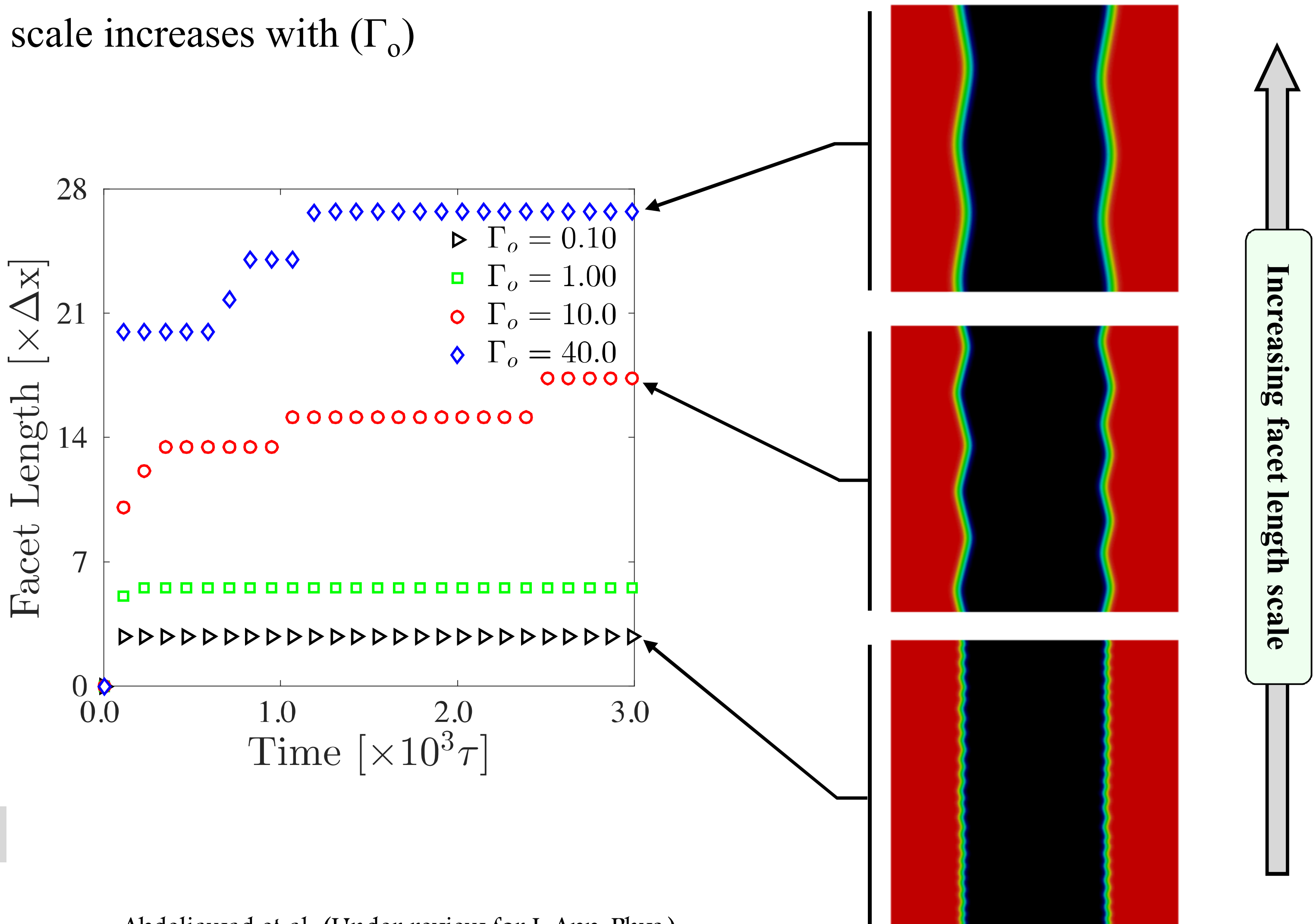


Critical quench



Results: Facet Junction Energy Γ_o

- A two-grain slab geometry
  - Facet length scale increases with (Γ_o)

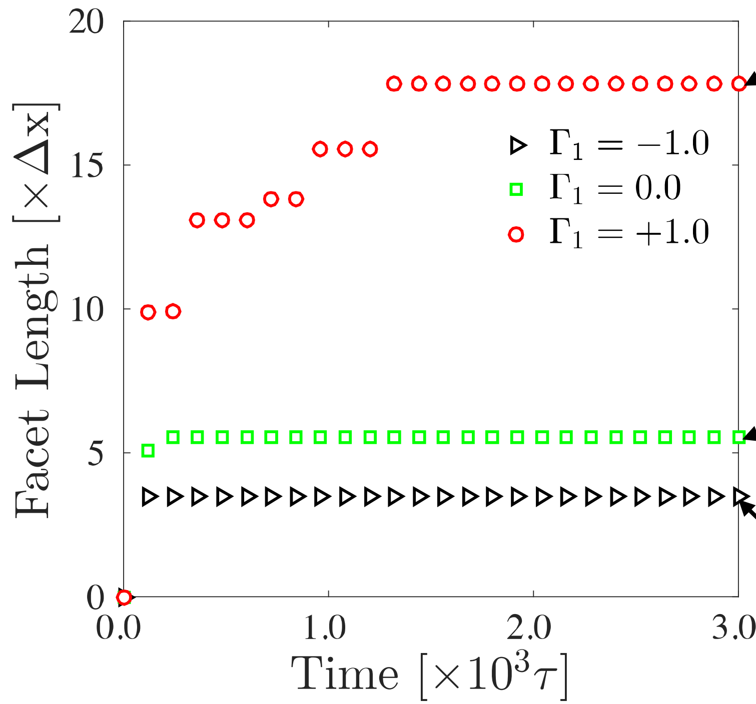


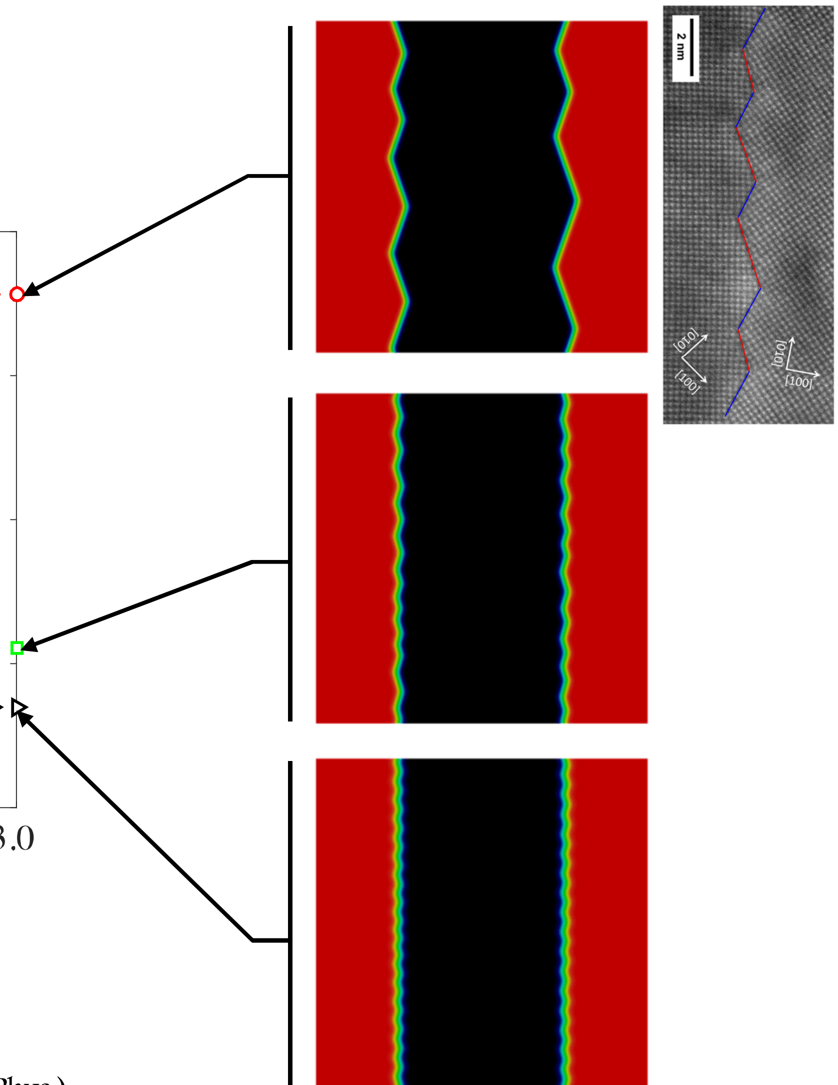
Γ_o: Junction energy

Abdeljawad et al. (Under review for J. App. Phys.)

Results: Junction Interactions Γ_1

- A two-grain slab geometry
  - Negative (Γ_1) plays a stabilizing role





Γ_1: Junction interactions

Abdeljawad et al. (Under review for J. App. Phys.)

Conclusion

- A mesoscale framework that examines
  - GB anisotropy (non-convexity in the GB free energy)
  - Facet junction energy due to defect content
  - Non-local junction-junction interactions
- Faceting and subsequent coarsening driven by junction energetics
- Capable of examining any GB given the GB energy vs. inclination diagram

Thank you

Results: Facet Junction Energy Γ_o

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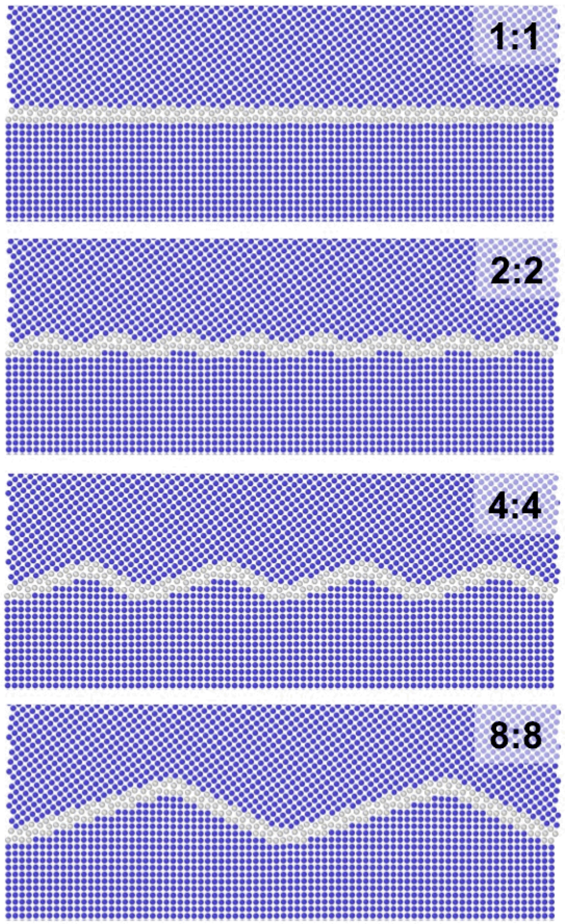
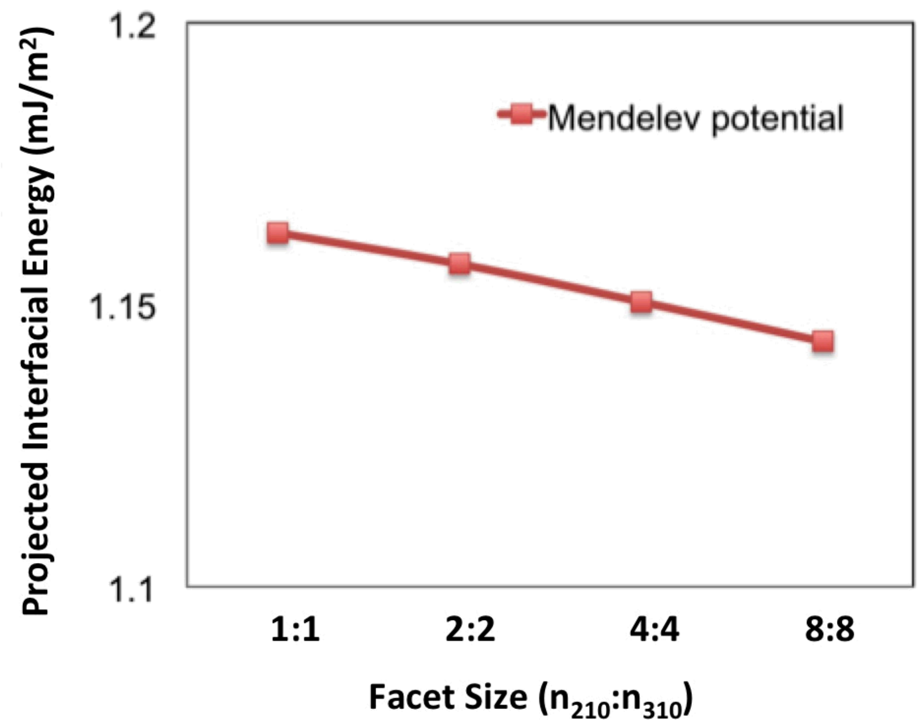
- Atomistic Simulations
  - Fix misorientation (Σ5) and inclination (26.565° from {310} plane)
  - Vary number of facet junctions for a given system size

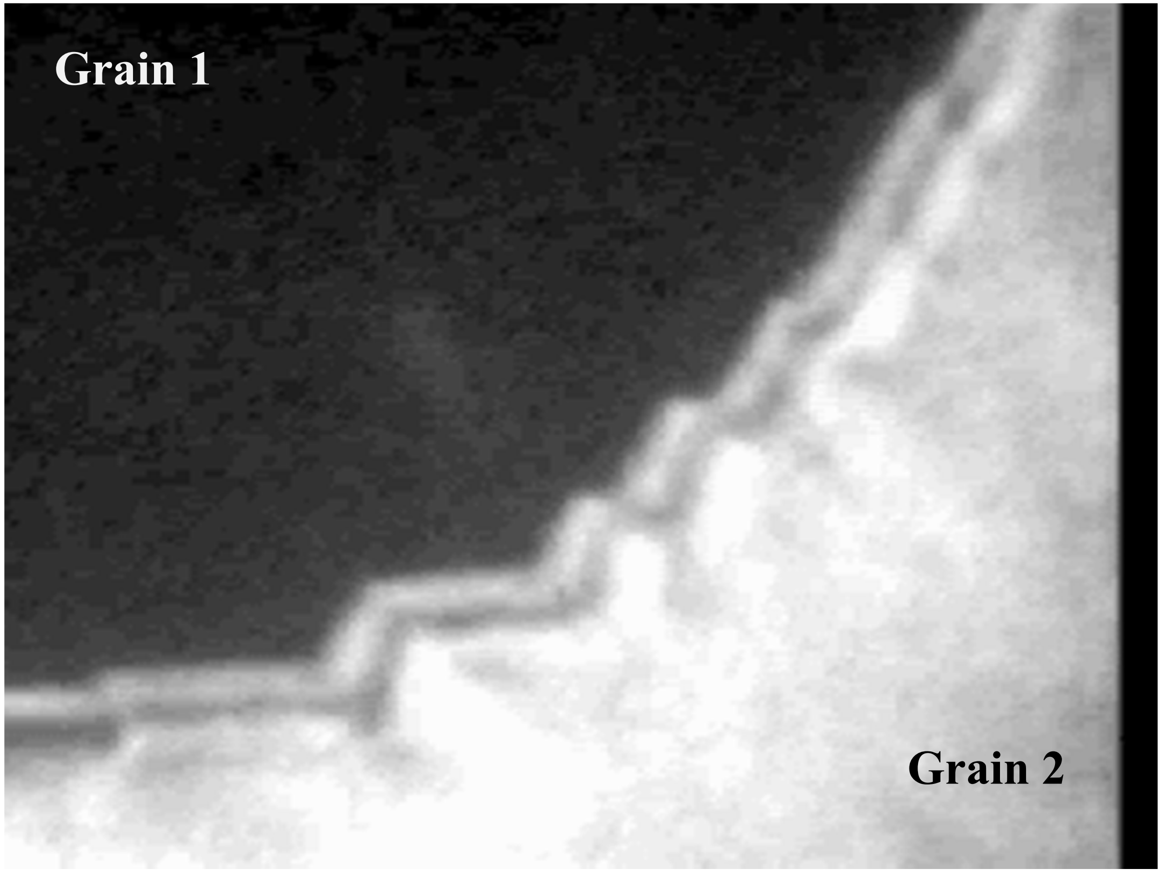




Energy is reduced with facet coarsening

Medlin et al. (Manuscript to be submitted to Acta Mater.)

Interface Faceting: Examples



50 nm

D. L. Medlin and G. Lucadamo (2000)

- Au films annealed at 500 °C
- Σ3 GB
- $\{11\bar{2}\}$ facets and subsequent facet coarsening

There Is More To It Than This

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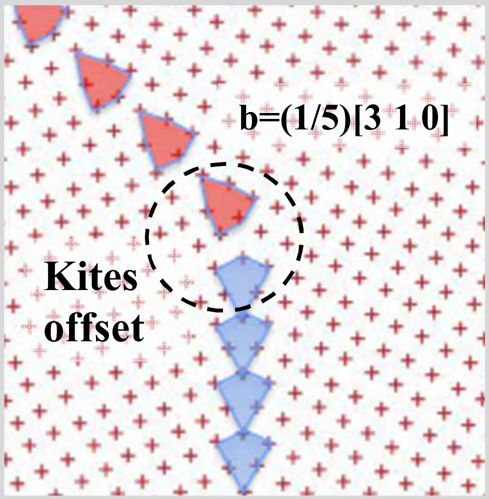
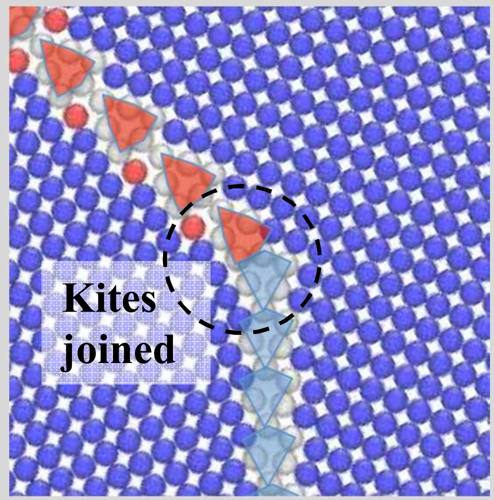
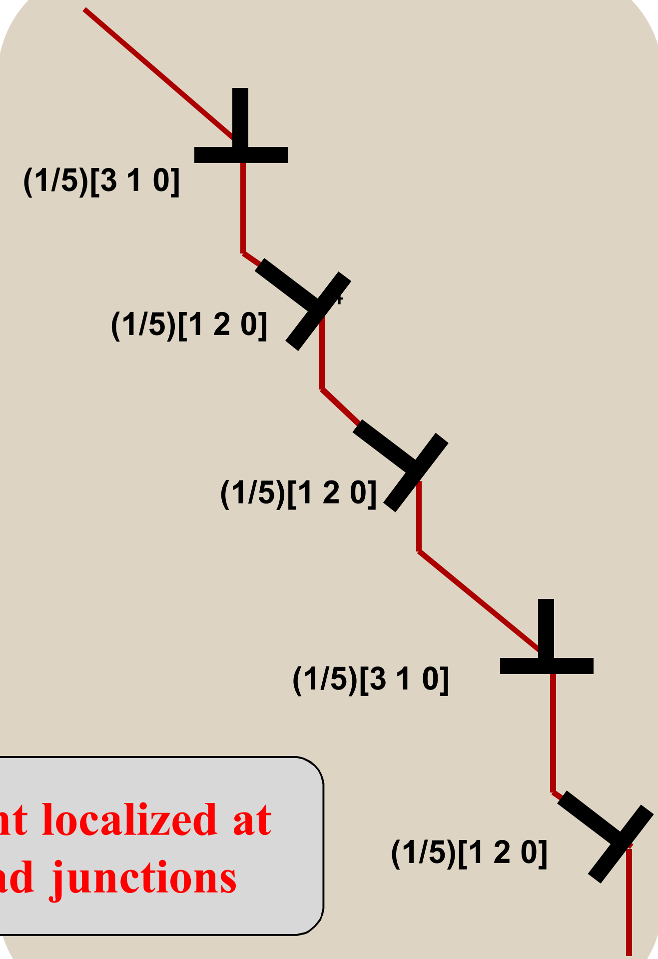
Experimental Junctions b=(1/5)(120) and (1/5)(310)



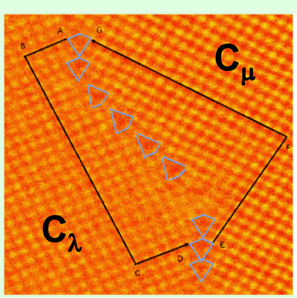
Relaxed Periodic Atomistic Structure



Defect Distribution



Interface circuit mapping



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.

Defect content localized at head-to-head junctions

Medlin et al. (Manuscript to be submitted to Acta Mater.)

Faceting: Mathematically

- Sharp interface law for GBs

$$\mathcal{V}_n = M_{gb}\left(\gamma_{gb} + \frac{\partial^2 \gamma_{gb}}{\partial \theta^2}\right)\mathcal{K}$$

Herring, Phys. Powd. Metall. (1951)

Mullins, J. App. Phys. 27 (1956)

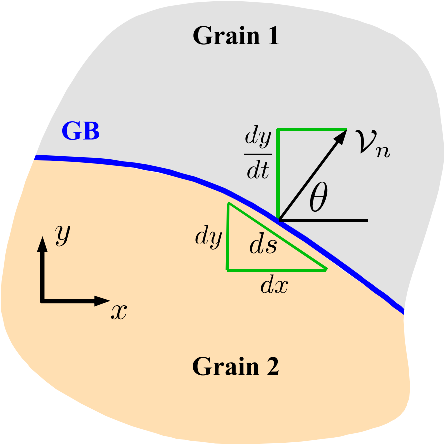
$\mathcal{V}_n$	: Normal velocity
M_{gb}	: GB mobility
γ_{gb}	: GB energy
$\mathcal{K}$	: Mean curvature

- Linearized

$$\frac{\partial y}{\partial t} = M_{gb}\left(\gamma_{gb} + \frac{\partial^2 \gamma_{gb}}{\partial \theta^2}\right)_o \frac{\partial^2 y}{\partial x^2}$$

When $\gamma_{gb} + \partial^2 \gamma_{gb}/\partial \theta^2 < 0$

Locally backward parabolic PDE



Thermodynamic instability of an initially planar surface with negative surface stiffness leads to faceting (hill and valley) structure

W. Mullins, Amer. Soc. Metals (1963)