Solid-solid Interfaces

M. Ceriotti - MSE304

EPFL

Outline

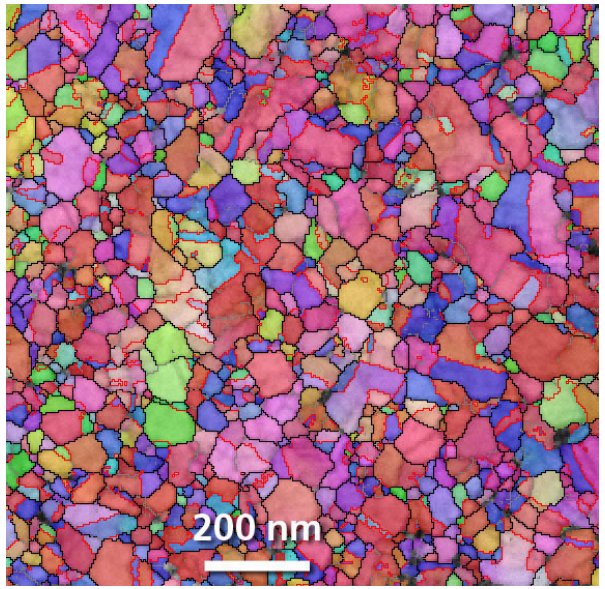
- Chapters 12 and 13 of your book
- Solid-solid interfaces (homophase, heterophase)
- Grain boundary energy
- Dislocation models, coincident site lattice models
- Defects at grain boundaries

Grain Boundaries & C.

- Most bulk materials are polycrystalline, composed of many grains with different orientation
  - Grain boundaries affect mechanical or electronic properties
  - The story gets even more complex when it comes to interfaces between different phases (heterophase interfaces)



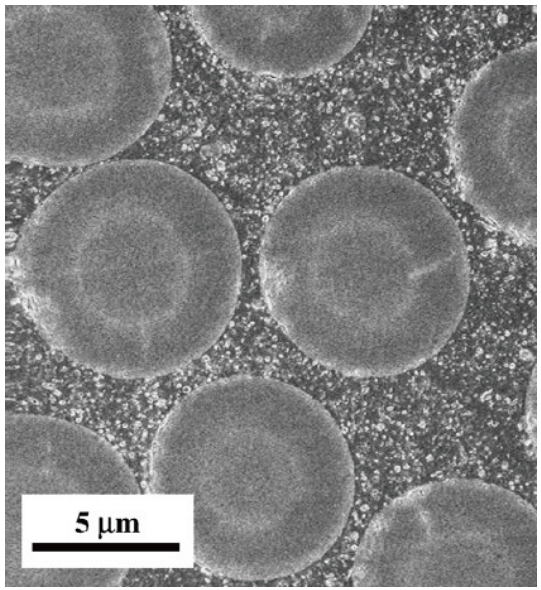


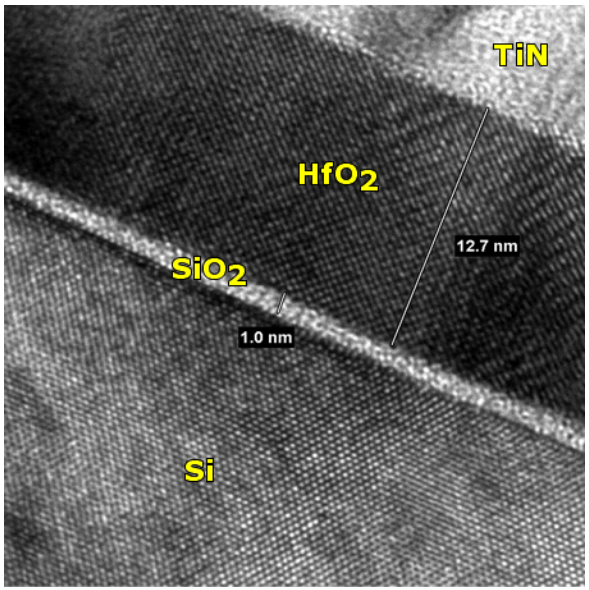


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Measuring the Grain Boundary Energy

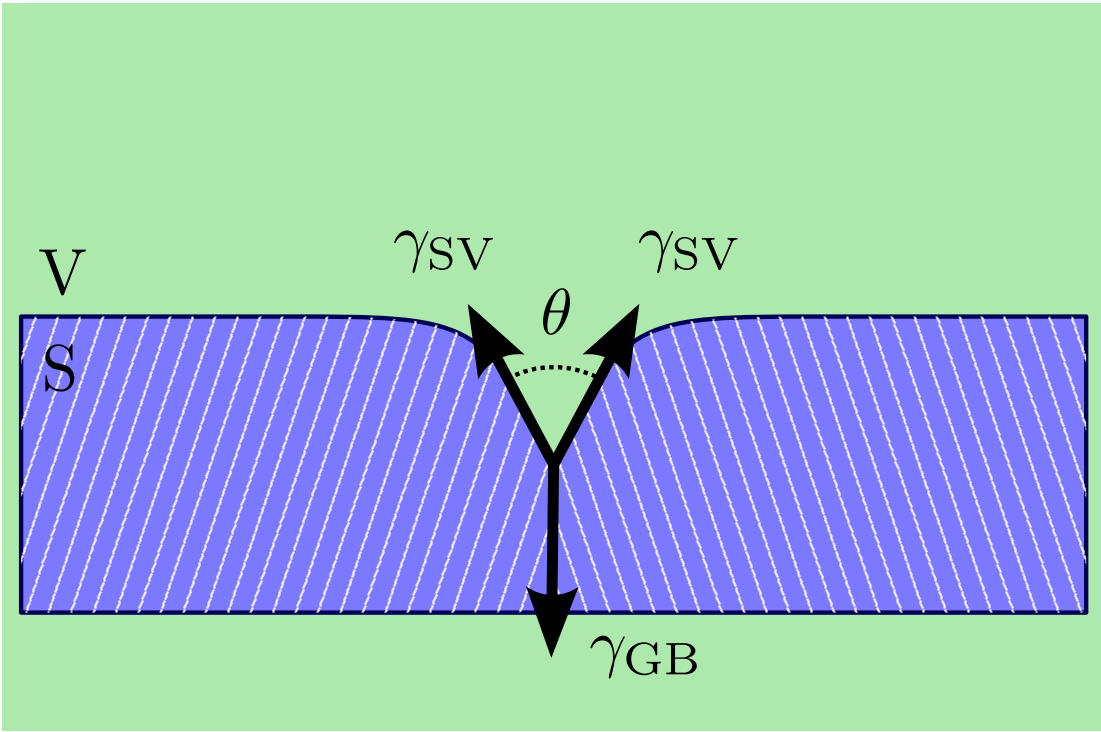
- One can associate a surface-energy term γ_{GB} to the presence of GBs

$$\gamma_{GB} = 2\gamma_{SV} - W_{GB}$$

  - The GB energy can be estimated by thermal grooving
  - Balance between surface energy γ_{SV} and γ_{GB} (typically $\gamma_{SV} \approx 3\gamma_{GB}$)

$$2\gamma_{SV} \cos\frac{\theta}{2} = \gamma_{GB}$$

- What happens if $\gamma_{GB} > 2\gamma_{SL}$?



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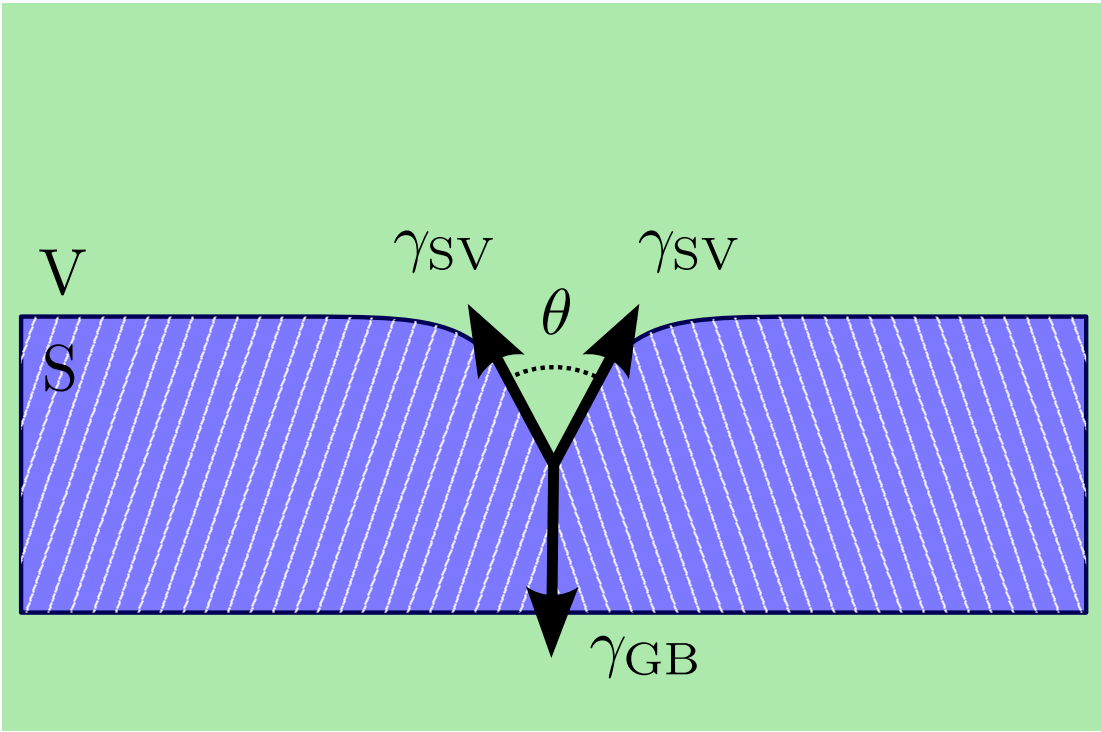
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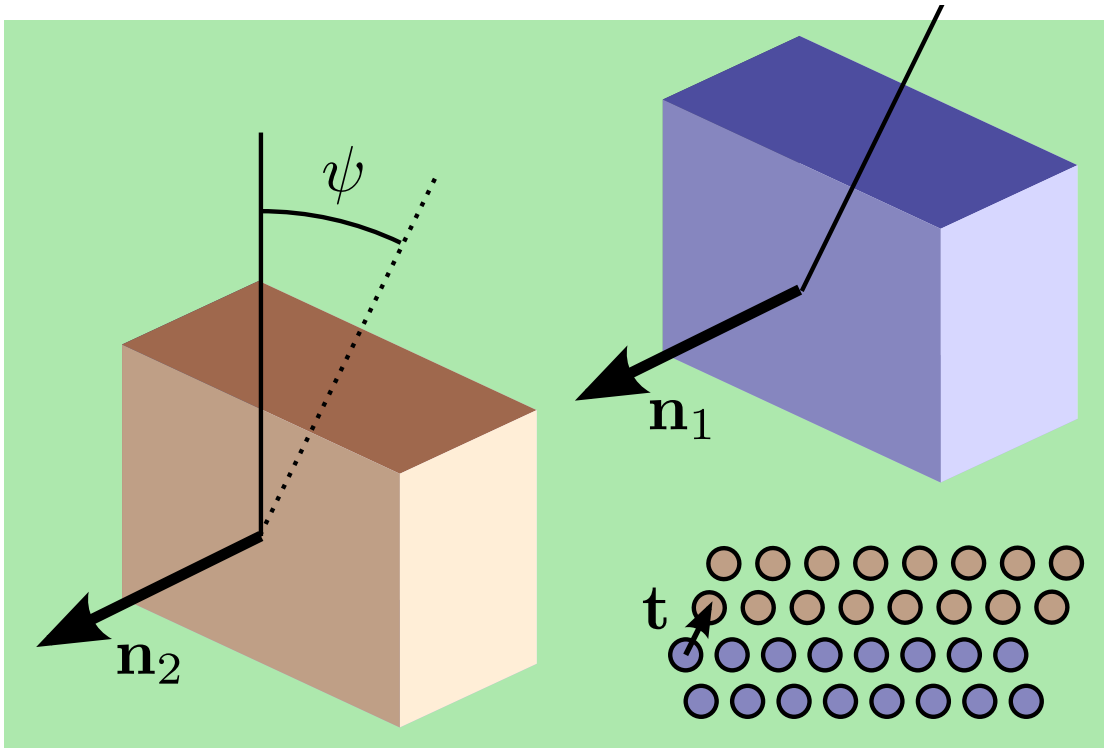
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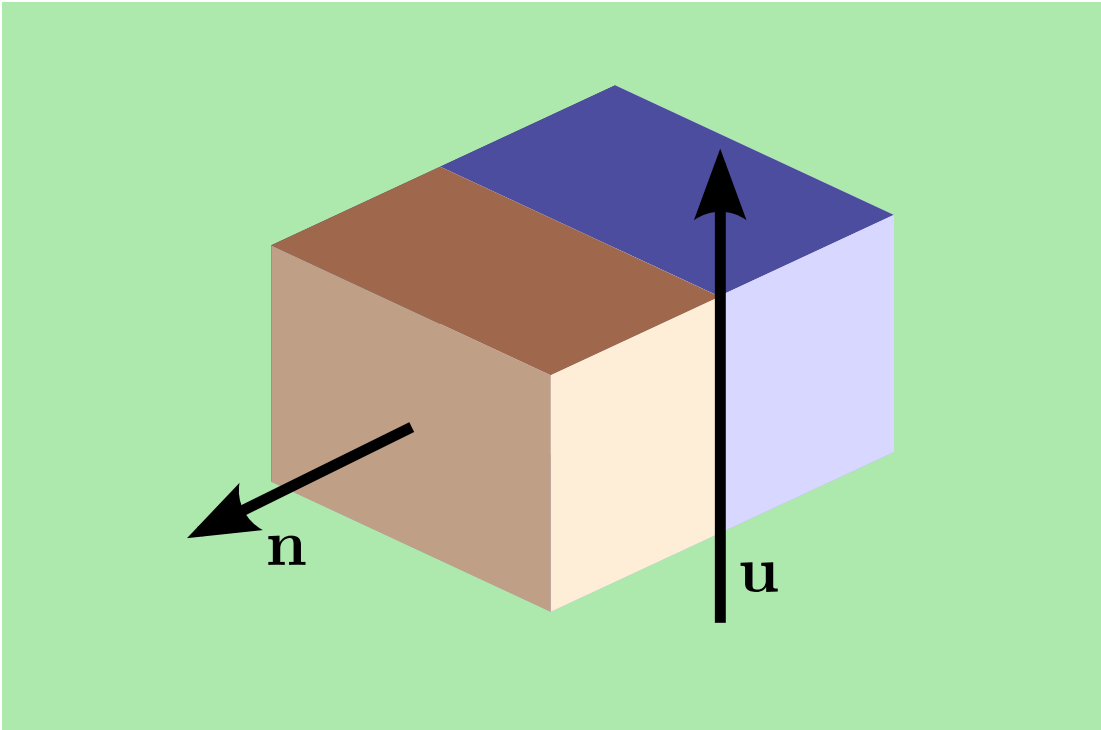
The Structure of Grain Boundaries

- How many parameters we need to describe the geometry of a GB?
  - Orientation of the two surfaces + relative tilt = 5 degrees of freedom
  - Atomic-scale register between the surfaces
- Simpler geometry - simmetric tilt boundaries



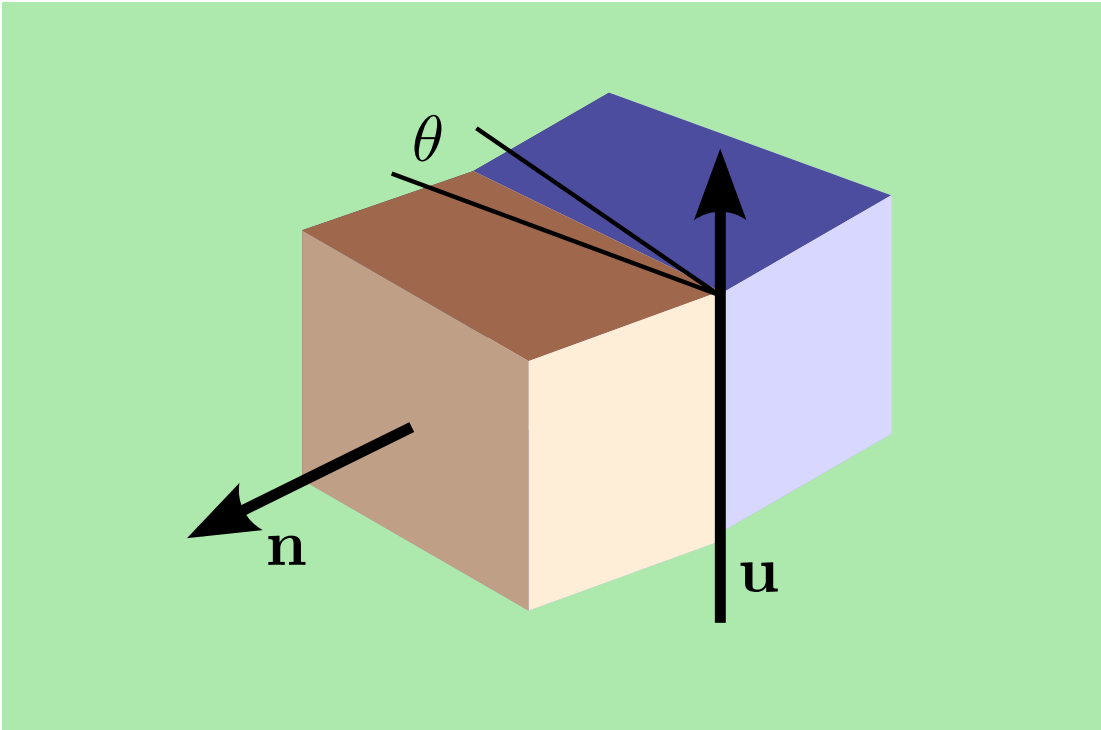
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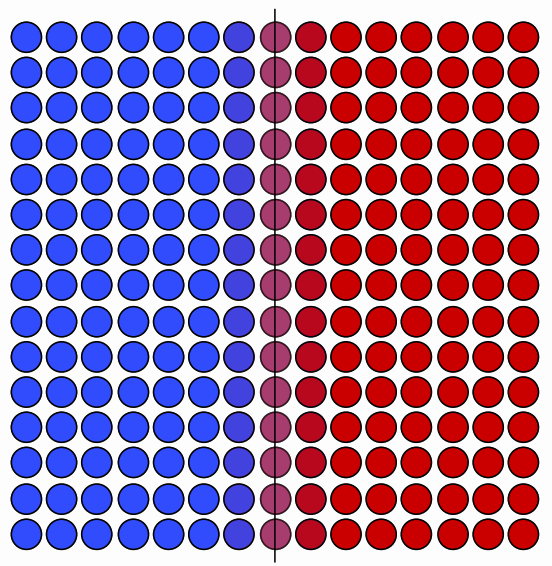
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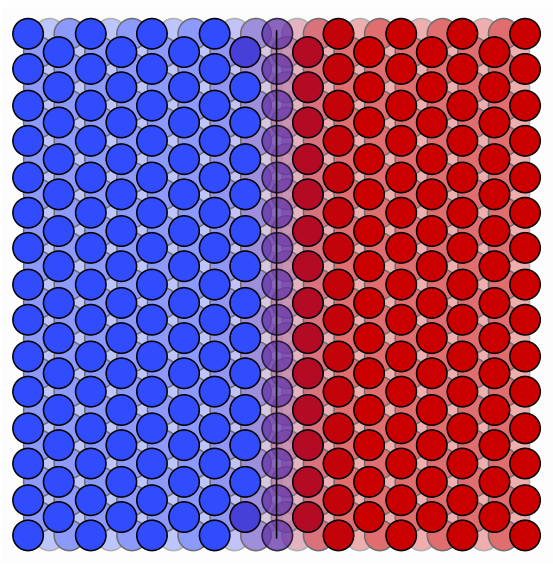


Symmetric Tilt Grain Boundaries

- Consider the interface between two identical surfaces, related by a rotation around an axis in the plane of the grain boundary
  - Dislocation model for the GB energy. Dislocation density, elastic energy of a dislocation, interaction between dislocations
  - At higher energy fine structure and cusps appear, corresponding to very regular arrays of dislocations



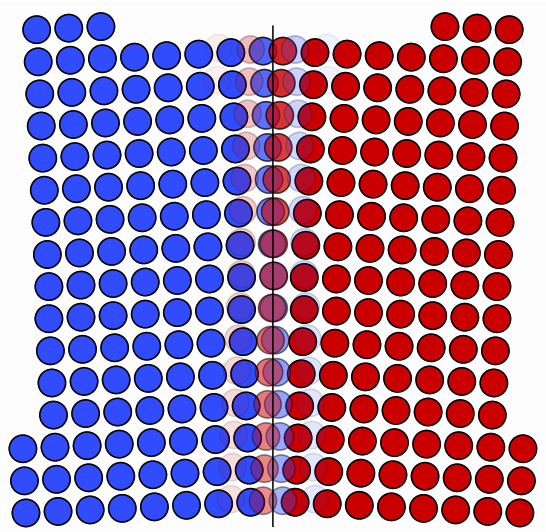
sc, $\mathbf{u} = \langle 001 \rangle$,
$\mathbf{n} = (100)$, $\theta = 0$



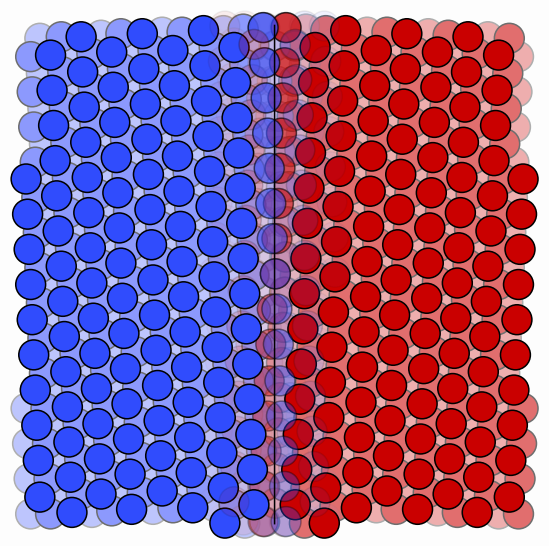
fcc, $\mathbf{u} = \langle 111 \rangle$,
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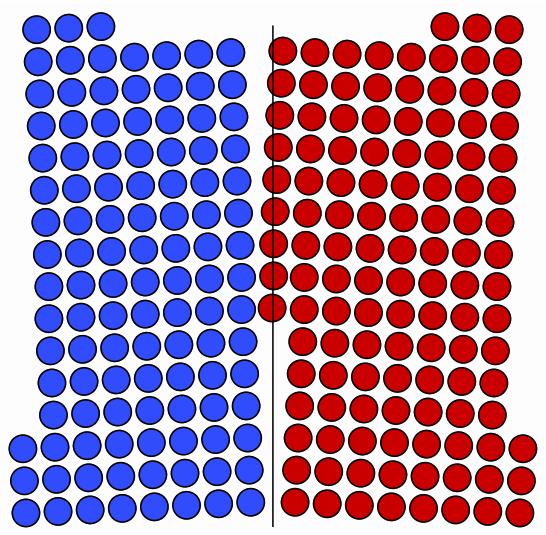
sc, $\mathbf{u} = \langle 001 \rangle$,
$\mathbf{n} = (100)$, $\theta = 5$



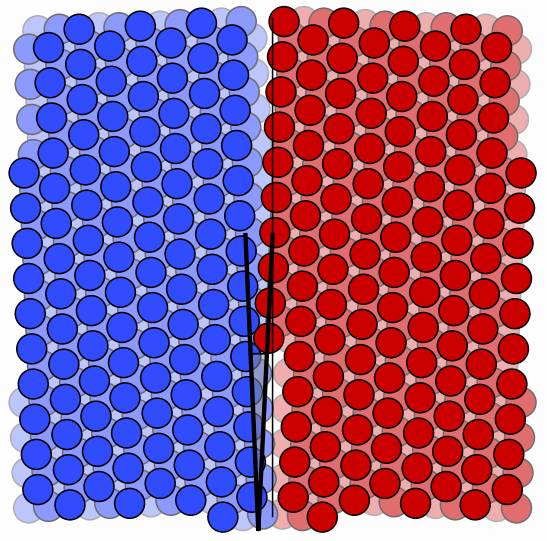
fcc, $\mathbf{u} = \langle 111 \rangle$,
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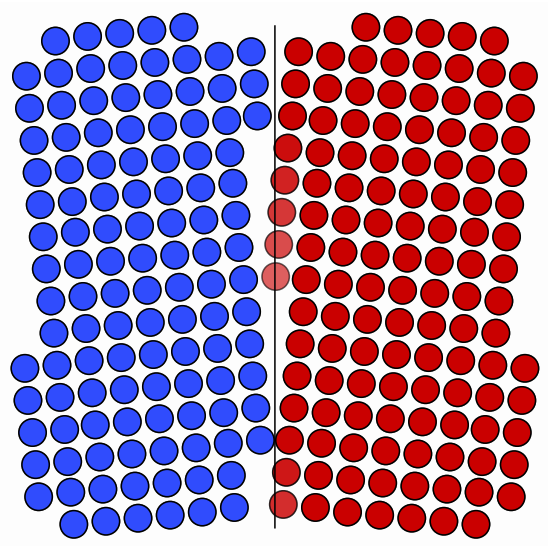
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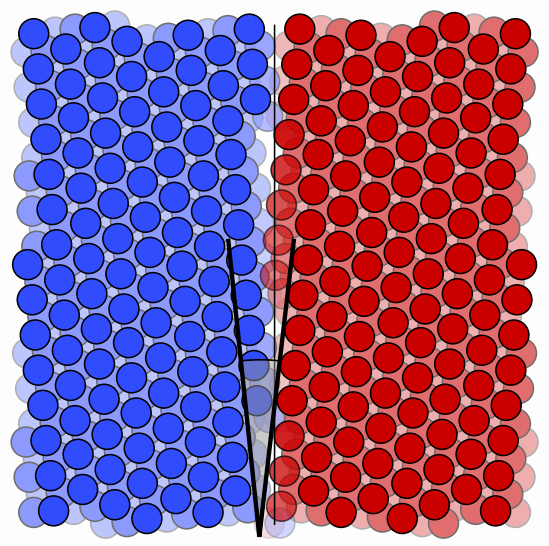
fcc, $\mathbf{u} = \langle 111 \rangle$,
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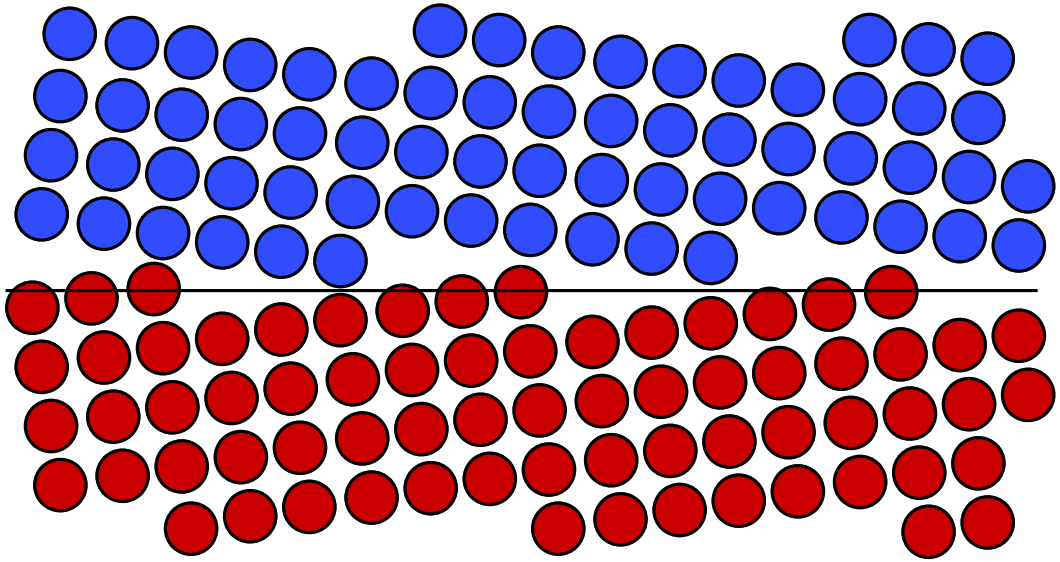
sc, $\mathbf{u} = \langle 001 \rangle$,
$\mathbf{n} = (100)$, $\theta = 12$



fcc, $\mathbf{u} = \langle 111 \rangle$,
$\mathbf{n} = (11\bar{2})$, $\theta = 12$

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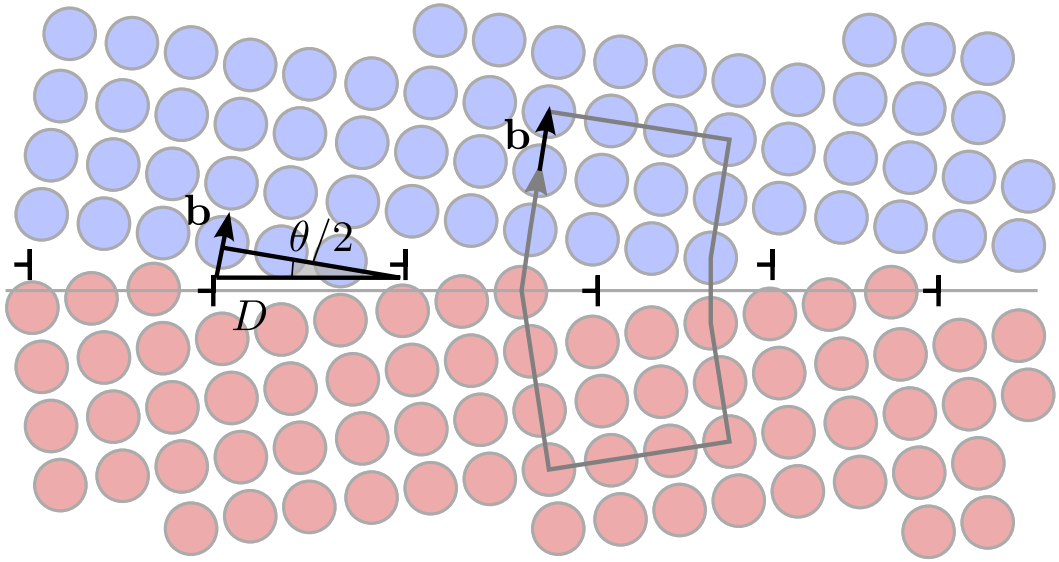
sc, $\mathbf{u} = \langle 001 \rangle$,
$\mathbf{n} = (100)$, $\theta = 18$

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$$\frac{b}{2} \approx D \sin\frac{\theta}{2} \quad \longrightarrow \frac{1}{D} \approx \frac{\theta}{b}$$

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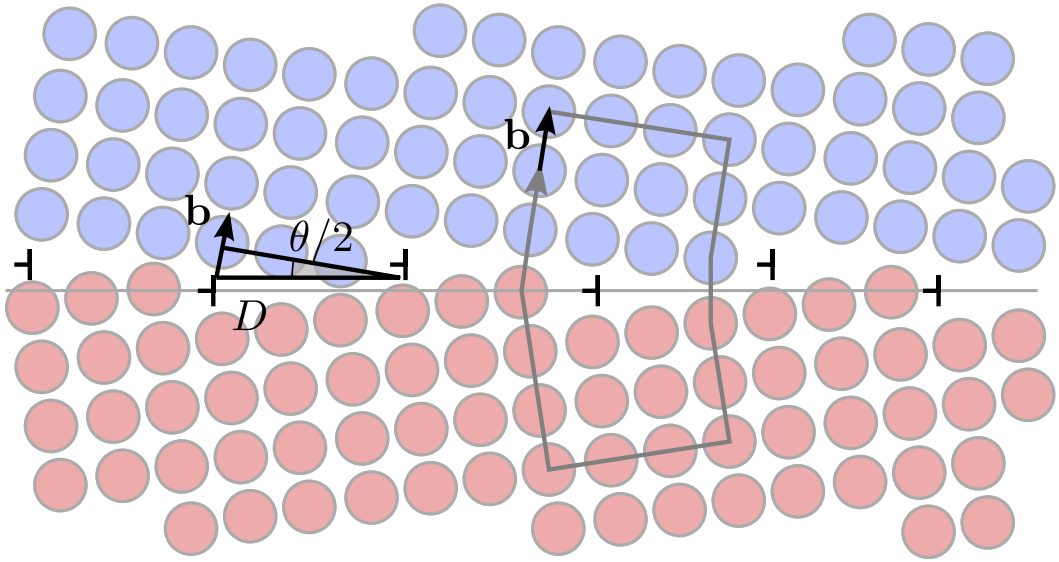
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$$\gamma_{GB} \approx E_{\perp}(D)\frac{1}{D} = \frac{\theta}{2}E_0(A_0 - \ln\theta)$$ Read-Shockley

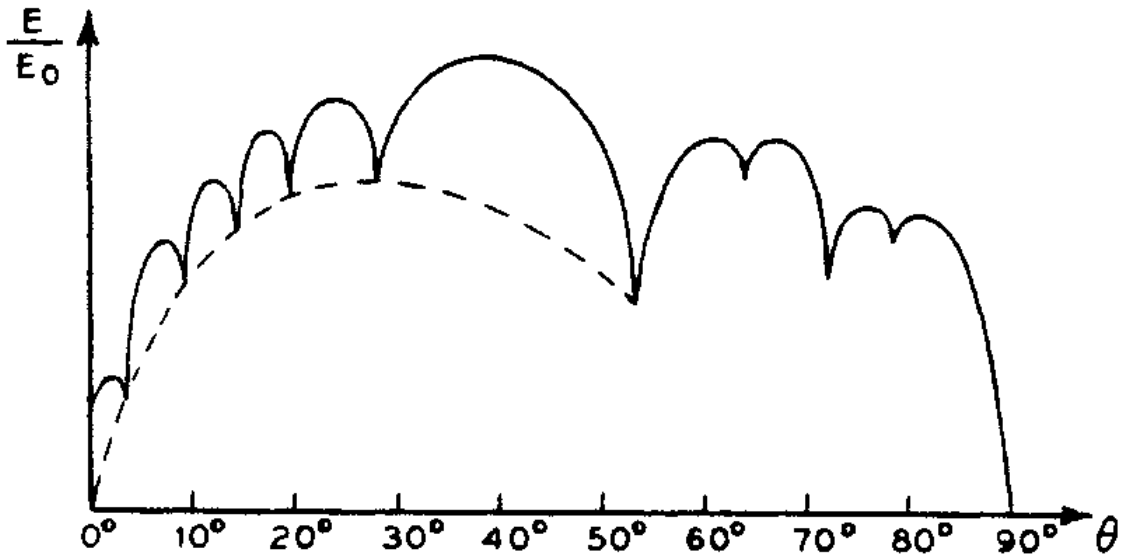
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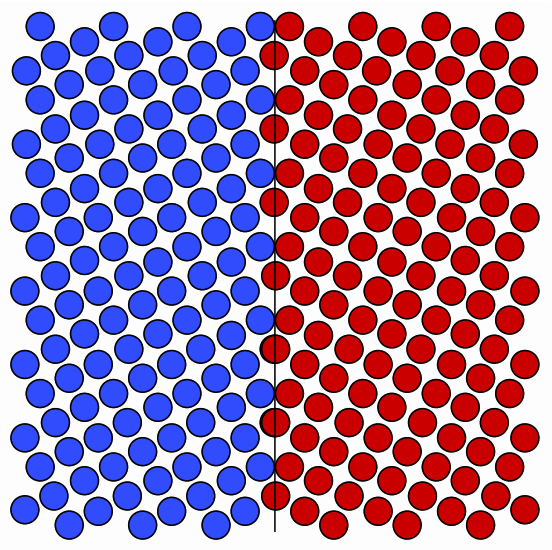
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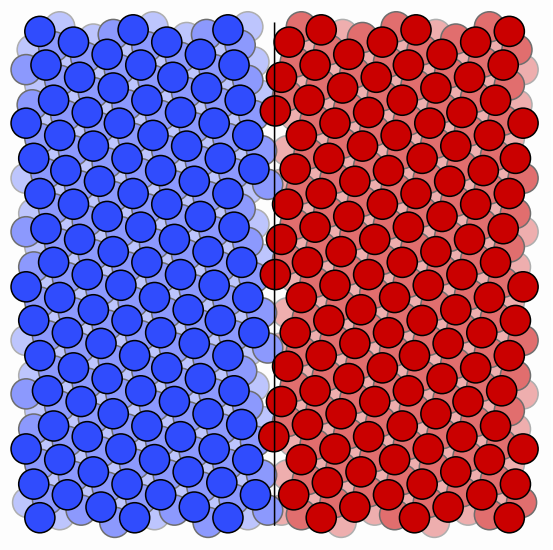


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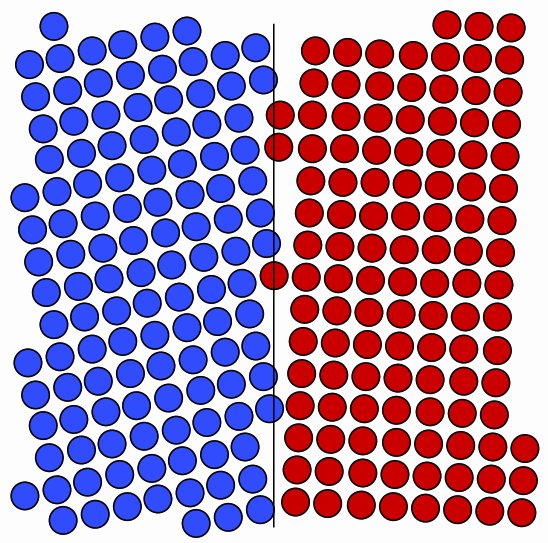
sc, $\mathbf{u} = \langle 001 \rangle$,
$\mathbf{n} = (100)$, $\theta = 53°$



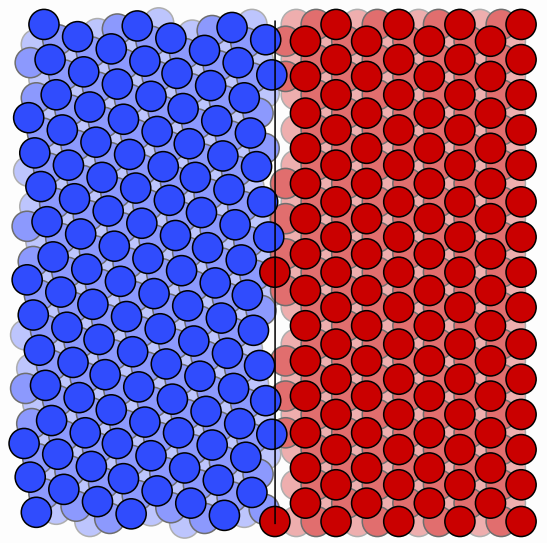
fcc, $\mathbf{u} = \langle 111 \rangle$,
$\mathbf{n} = (11\bar{2})$, $\theta = 22°$

Other Types of Grain Boundaries

- The tilt plane in a pure-tilt GB can be offset by a rotation ϕ relative to a low-index plane.
  - Asymmetric tilt GB, can be described by including an array of perpendicular edge dislocations
- The two sides of the GB can be *twisted* around **n**



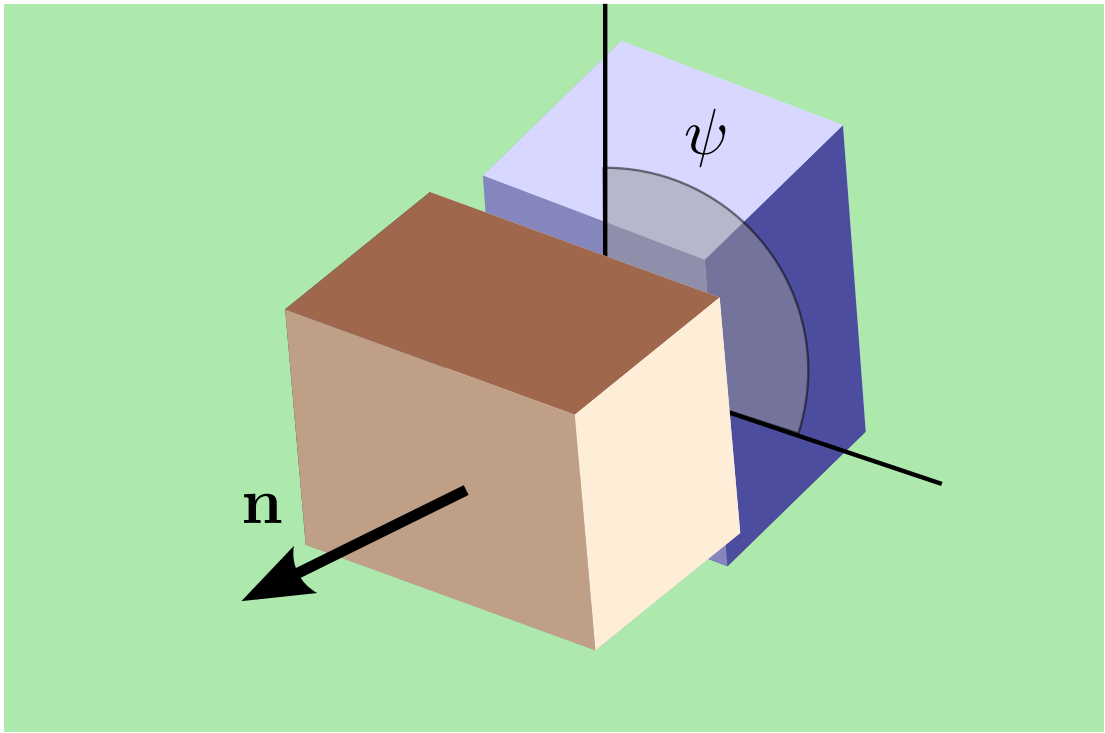
sc, $\mathbf{u} = \langle 001 \rangle$,
$\mathbf{n} = (100)$, $\phi = 5°$, $\theta = 10°$



fcc, $\mathbf{u} = \langle 111 \rangle$,
$\mathbf{n} = (11\bar{2})$, $\phi = 5°$, $\theta = 10°$

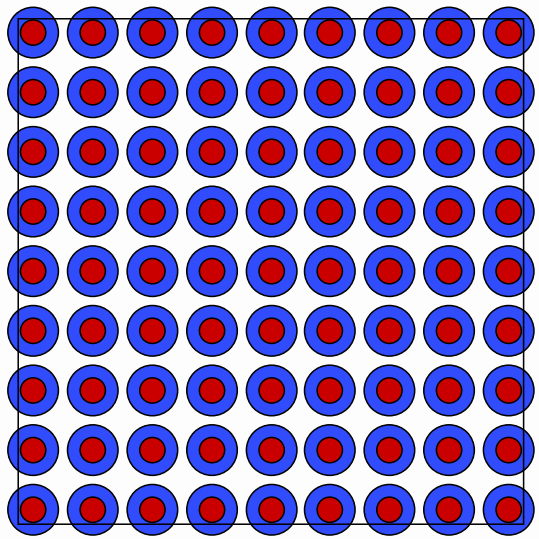
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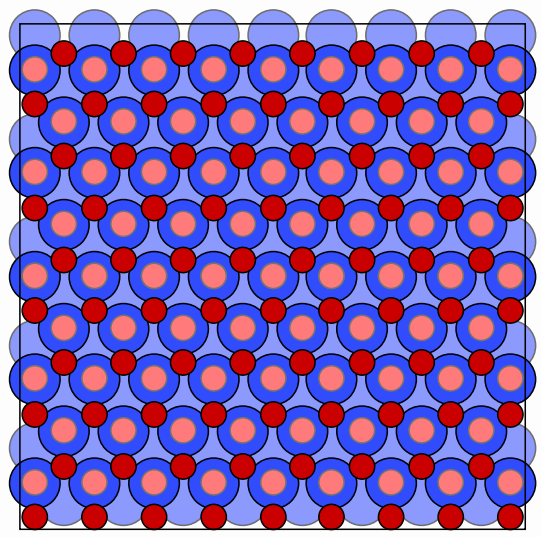


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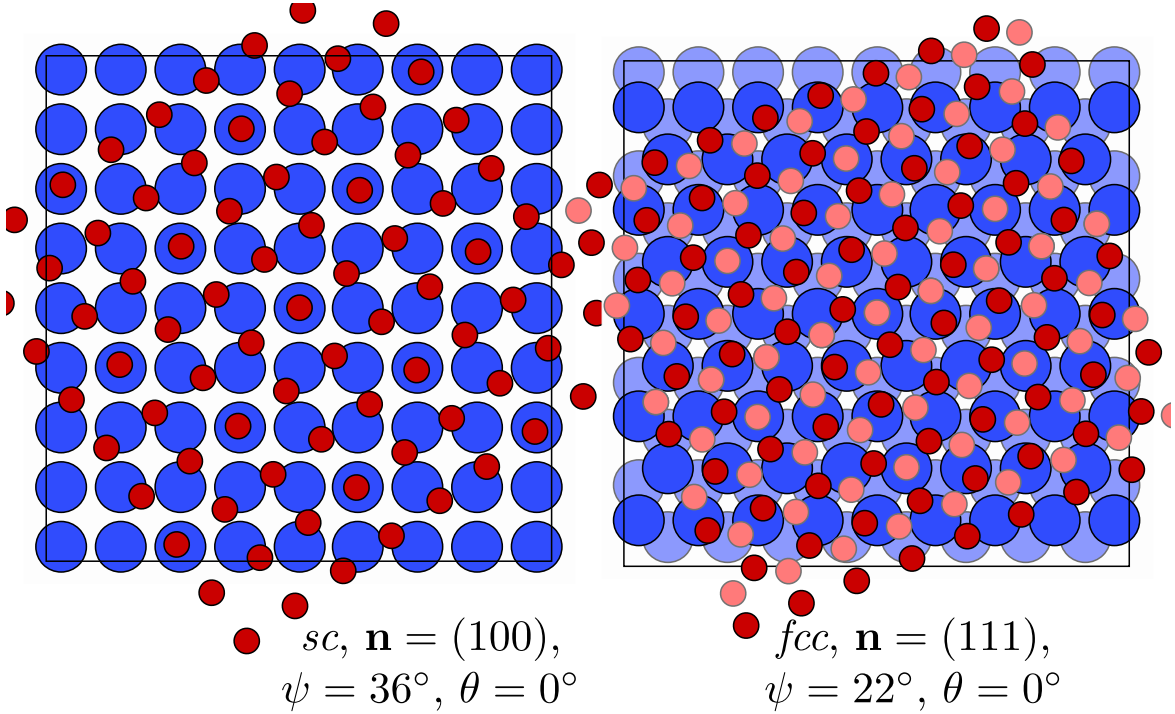
sc, $\mathbf{n} = (100)$,
$\psi = 0°$, $\theta = 0°$



fcc, $\mathbf{n} = (111)$,
$\psi = 0°$, $\theta = 0°$

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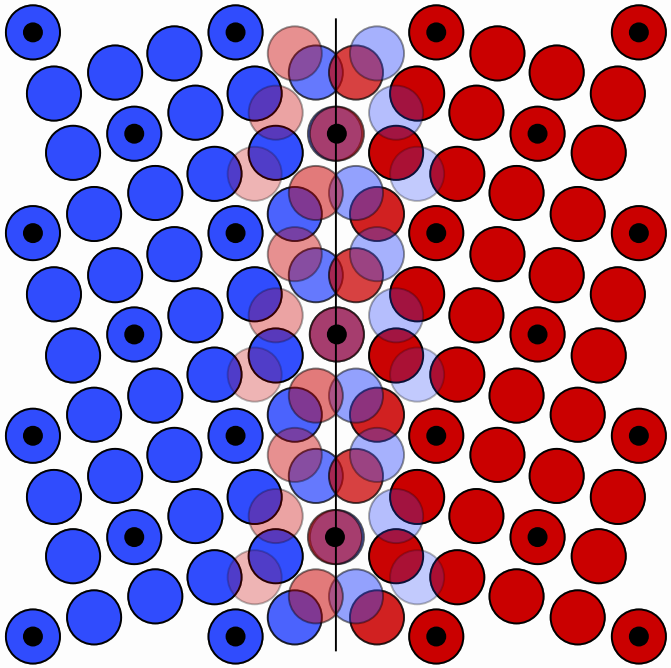


sc, $\mathbf{n} = (100)$, $\psi = 36°$, $\theta = 0°$

fcc, $\mathbf{n} = (111)$, $\psi = 22°$, $\theta = 0°$

Naming & Energetics of High-Angle GB

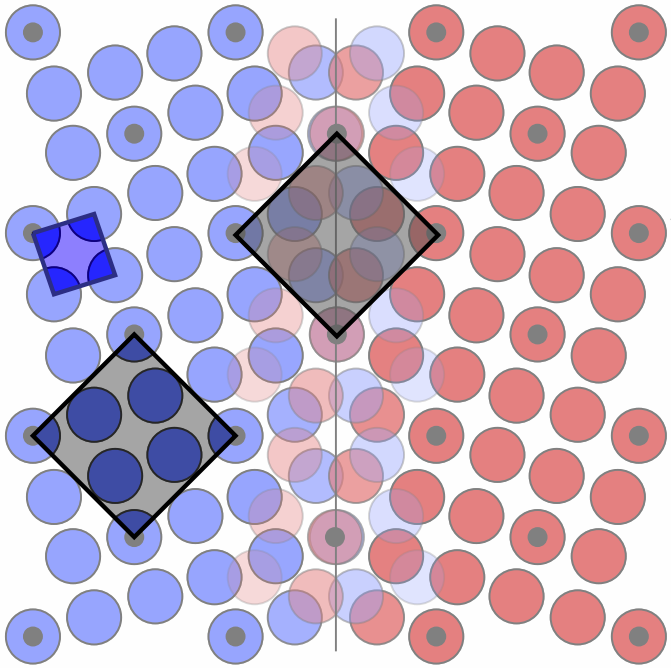
- Many theories try to estimate the energy of GBs -- best thing is to run an atomistic calculation!
- Coincident Site Lattice formalism classifies high-angle GB with a regular arrangement of defects
  - CSL = lattice formed by coincident sites grain lattices
  - Naming scheme:$\Sigma = Na$, where N is the ratio between the size of the CSL cell and that of the primitive cell
  - Misorientation can be included by *secondary* dislocations



sc, $\mathbf{n} = (100)$,
$\mathbf{u} = \langle 001 \rangle$, $\theta = 36.9°$

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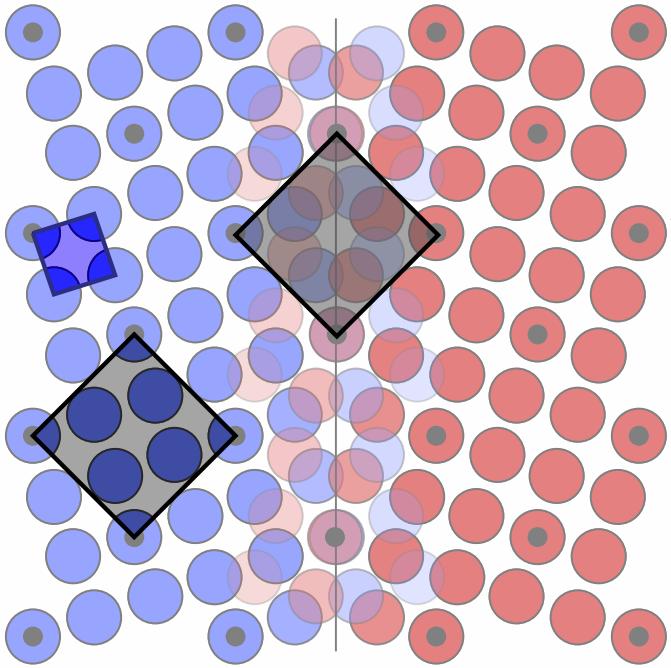
Atoms per unit cell: 1
Atoms per CSL cell: 5

$\boxed{\Sigma = 5}$

sc, $\mathbf{n} = (100)$,
$\mathbf{u} = \langle 001 \rangle$, $\theta = 36.9°$

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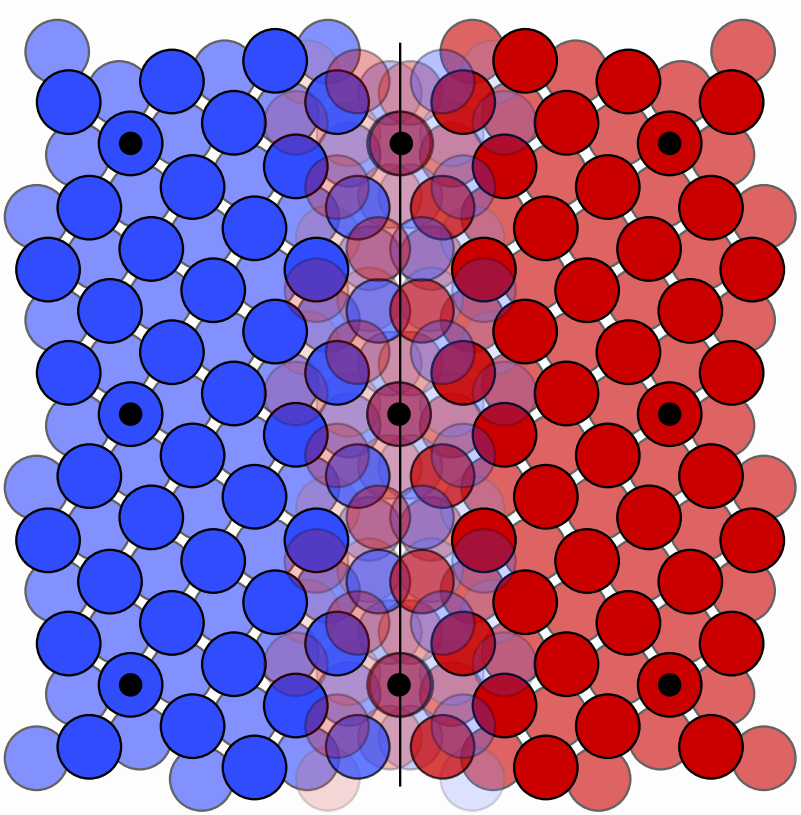


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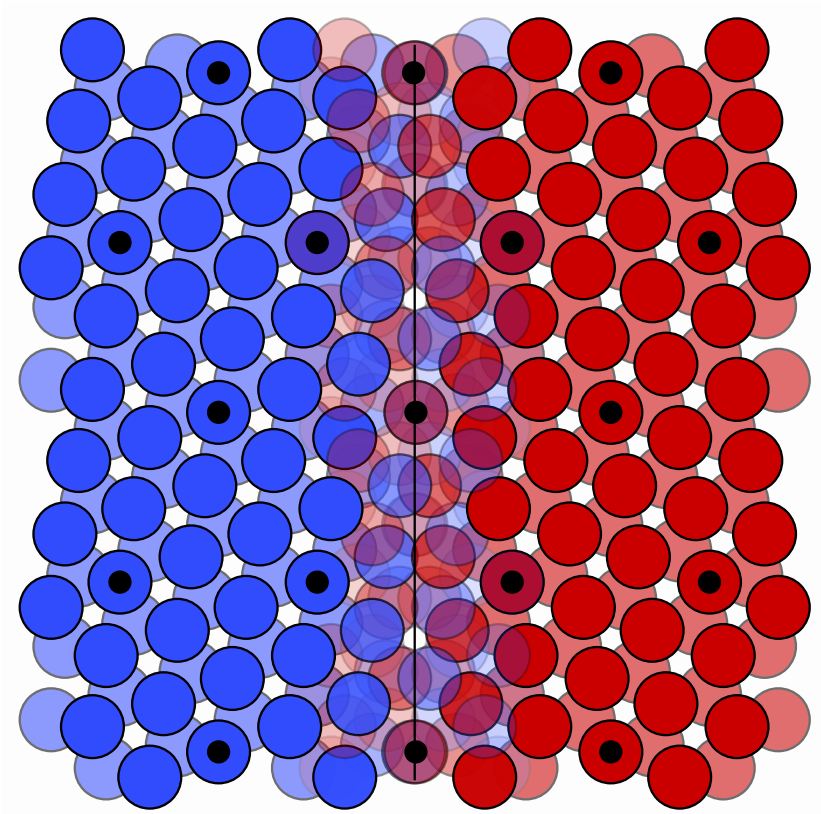
sc, $\mathbf{n} = (100)$,
$\mathbf{u} = \langle 001 \rangle$, $\theta = 36.9°$

Name the Grain Boundary!



fcc, $\mathbf{n} = (100)$,
$\mathbf{u} = \langle 001 \rangle$, $\theta = 22.6°$

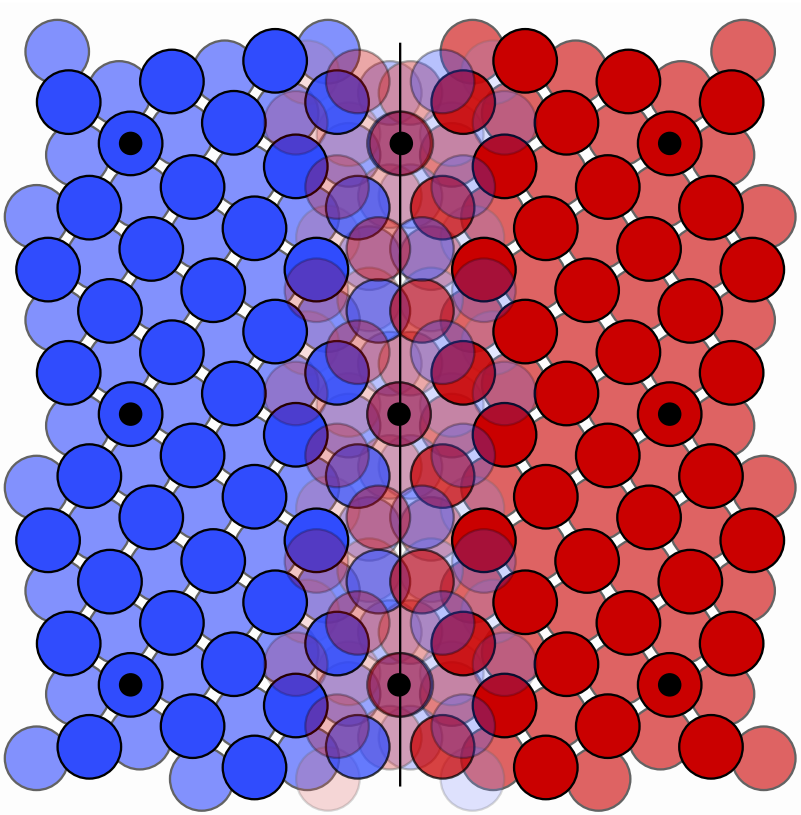
[redacted]



fcc, $\mathbf{n} = (1\bar{1}0)$,
$\mathbf{u} = \langle 111 \rangle$, $\theta = 38.21°$

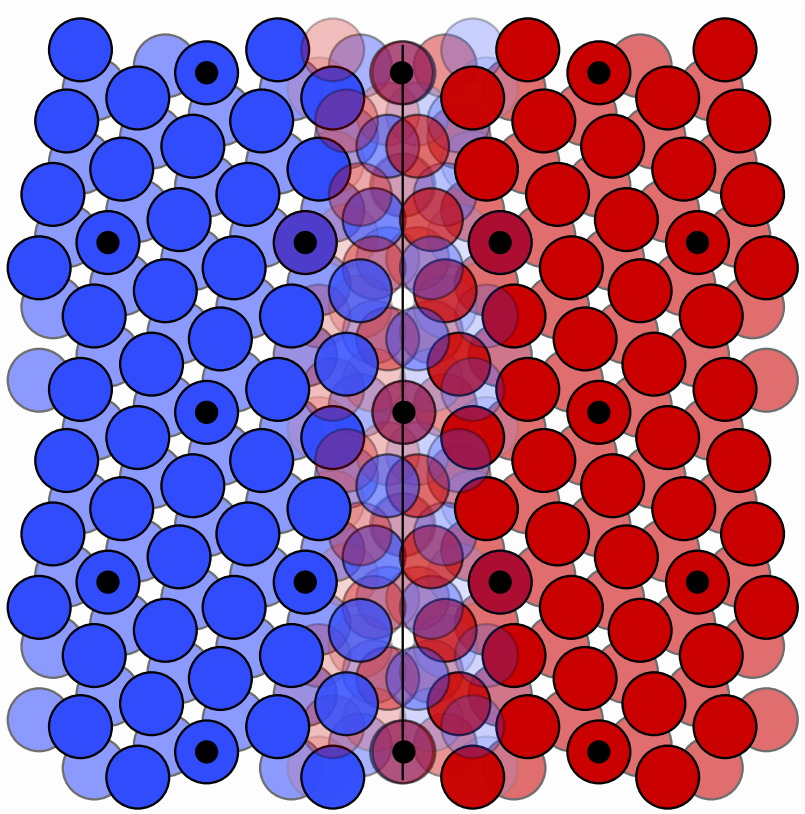
[redacted]

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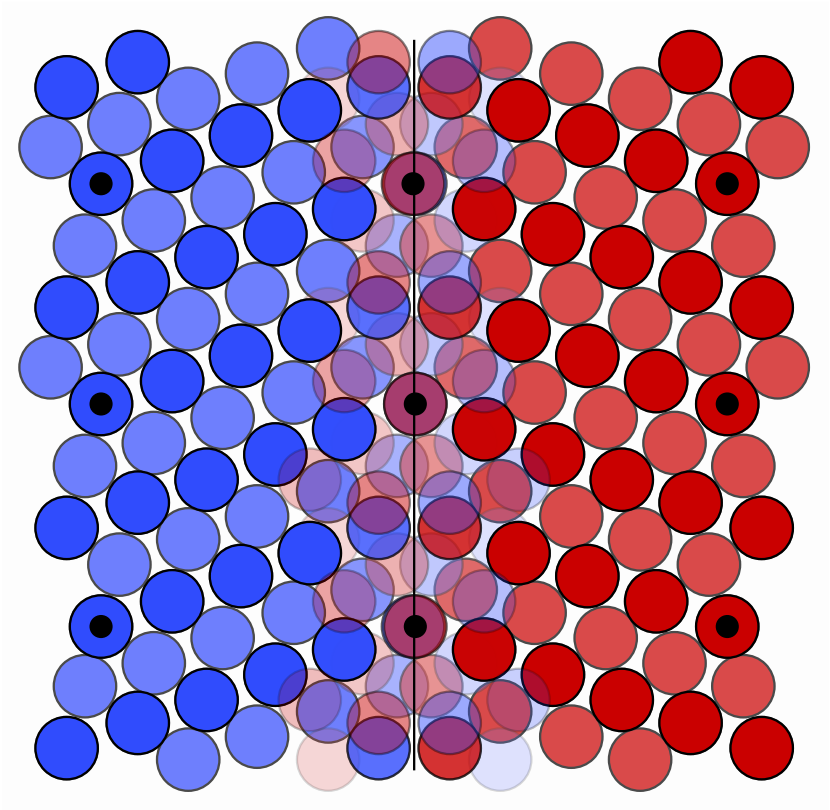
$\boxed{\Sigma = 13a}$



fcc, $\mathbf{n} = (1\bar{1}0)$,
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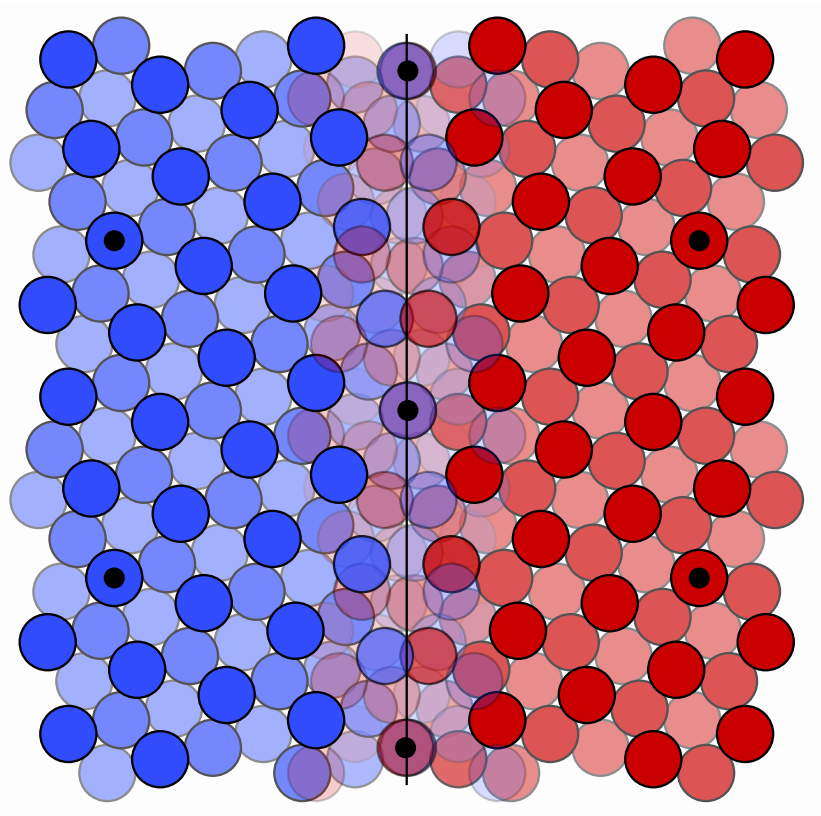
$\boxed{\Sigma = 7}$

Name the Grain Boundary!



fcc, $\mathbf{n} = (1\bar{1}0)$,
$\mathbf{u} = \langle 110 \rangle$, $\theta = 38.9°$

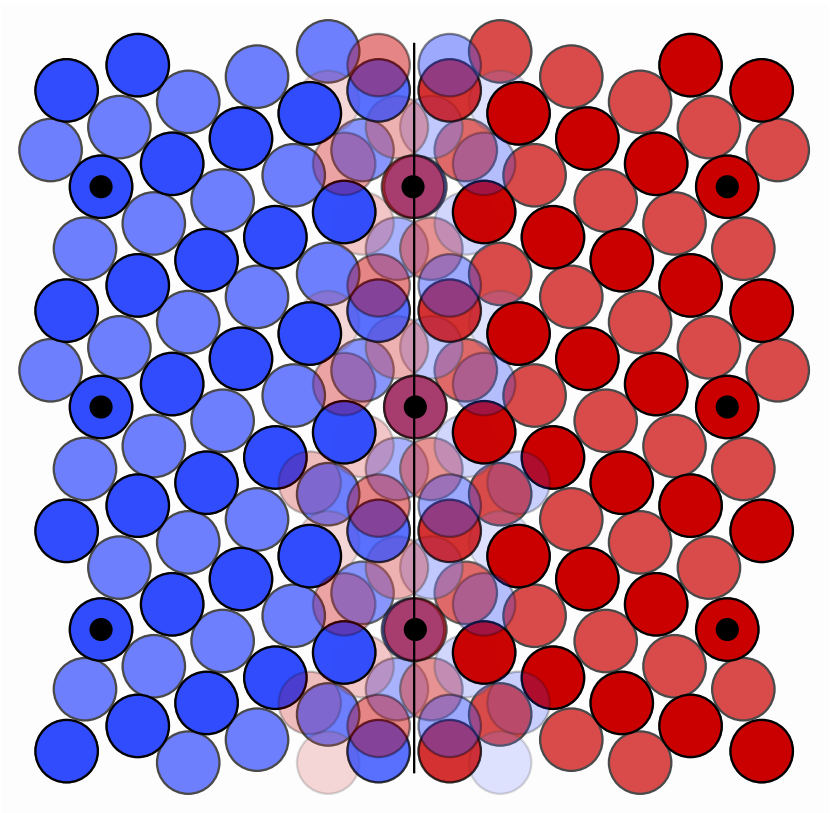
[redacted]



sc, $\mathbf{n} = (1\bar{1}0)$,
$\mathbf{u} = \langle 111 \rangle$, $\theta = 27.8°$

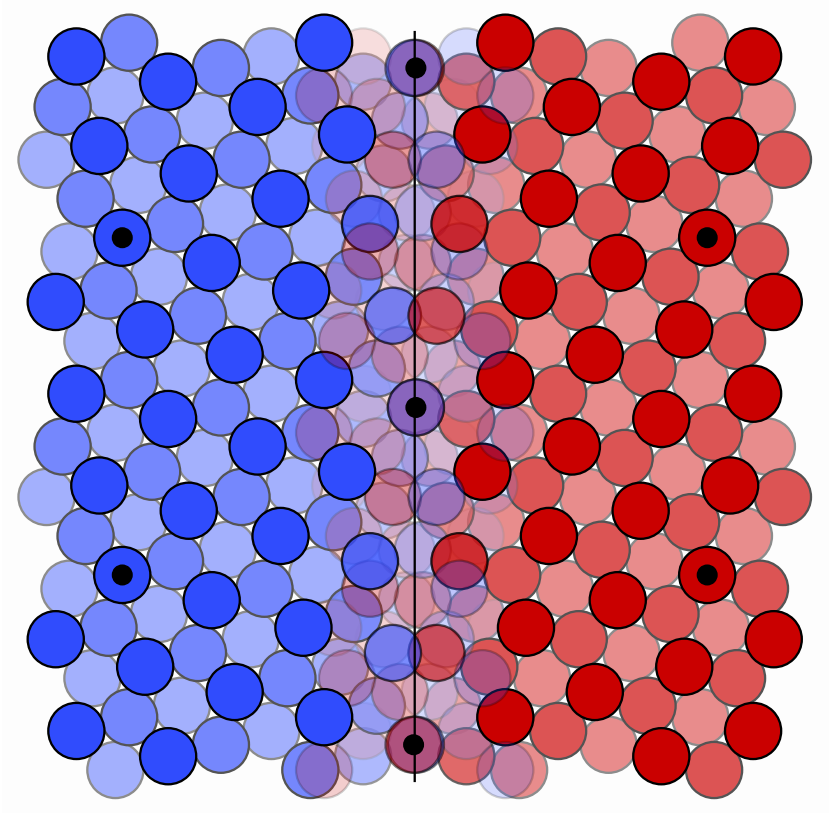
[redacted]

Name the Grain Boundary!



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$\boxed{\Sigma = 9}$

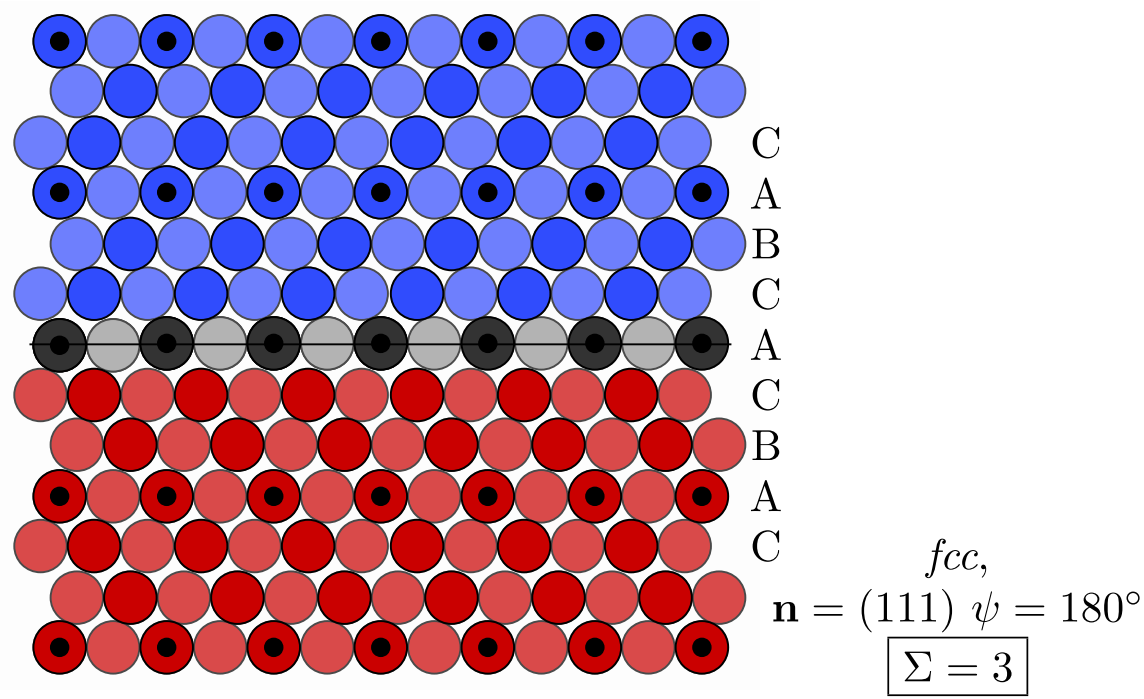


sc, $\mathbf{n} = (1\bar{1}0)$,
$\mathbf{u} = \langle 111 \rangle$, $\theta = 27.8°$

$\boxed{\Sigma = 13b}$

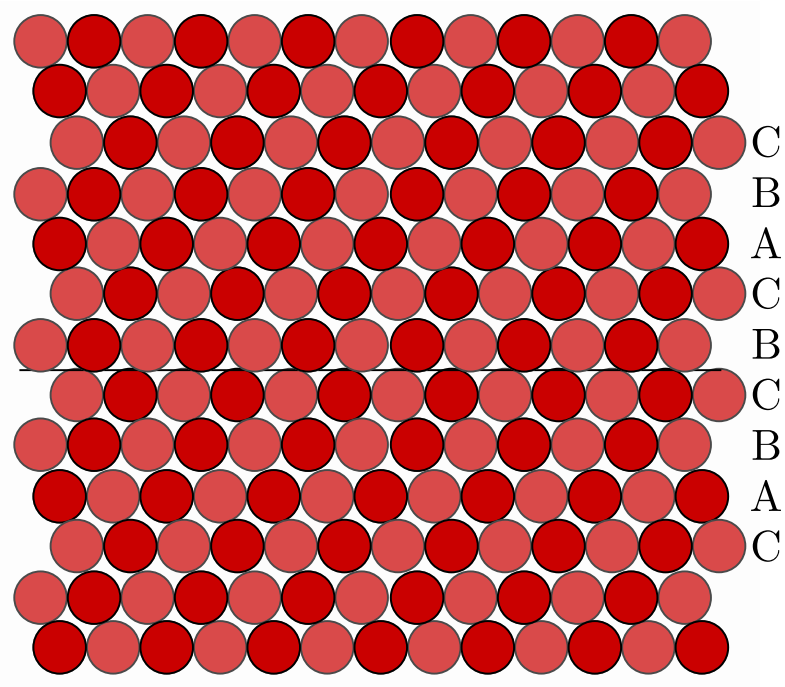
Twins and Stacking Faults

- Close-packed *fcc* have very low-energy **twin** grain boundaries, that correspond to reversal of the ABCABC stacking order
- Twins are closely related to **stacking faults**, ABCBCAB or ABCBABC
  - Stacking faults can be thought as a pair of twins, and in fact $\gamma_{sF} \approx 2\gamma_t$



Twins and Stacking Faults

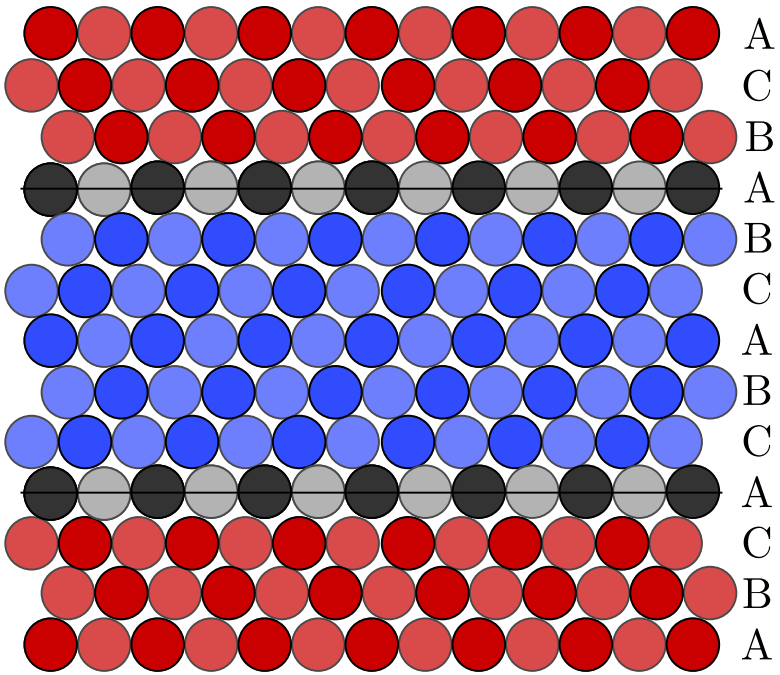
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fcc,
$\mathbf{n} = (111)$

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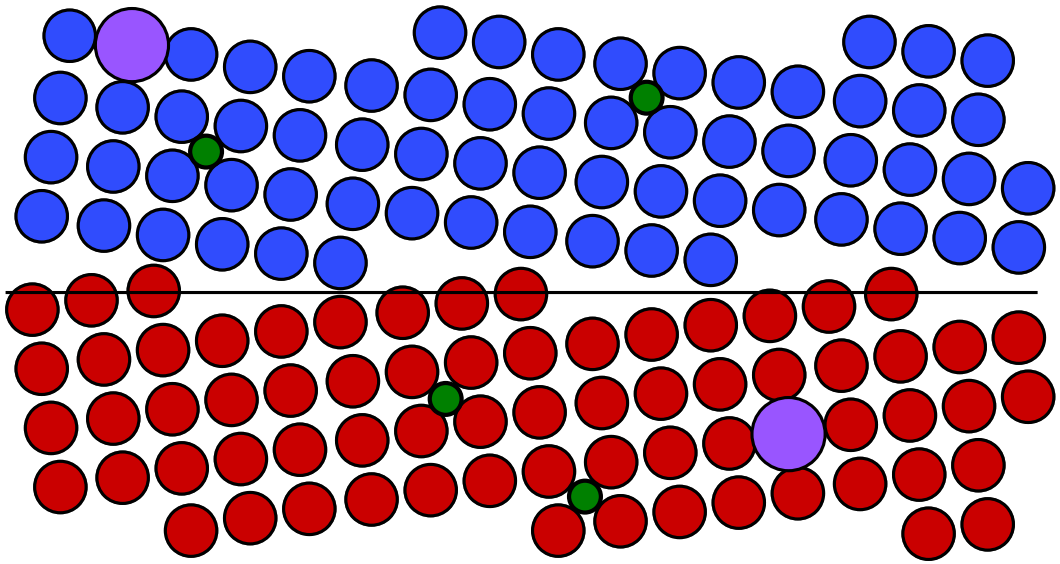
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Grain Boundary Engineering

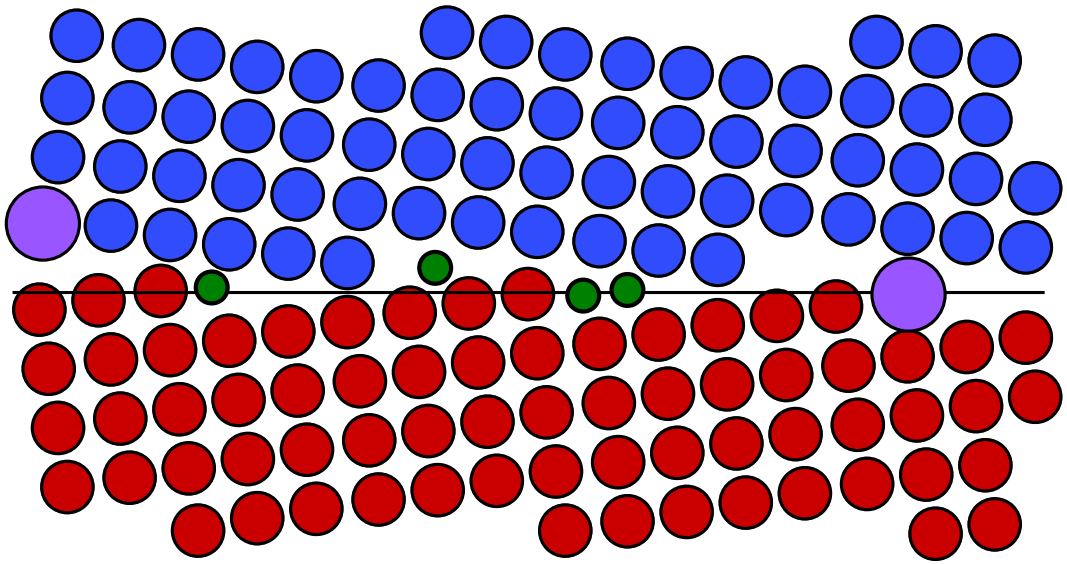
- The type, stability, and mechanical properties of grain boundaries can be tuned by the presence of impurities
- Interstitial or substitutional impurities can segregate at grain boundaries because they can better accommodate lattice mismatch
- Gibbs absorption equation holds: $\frac{\partial \gamma}{\partial c} \approx -\Gamma / c$. Segregating atoms lower γ_{GB}



sc, $\mathbf{u} = \langle 001 \rangle$,
$\mathbf{n} = (100)$, $\theta = 18°$

Grain Boundary Engineering

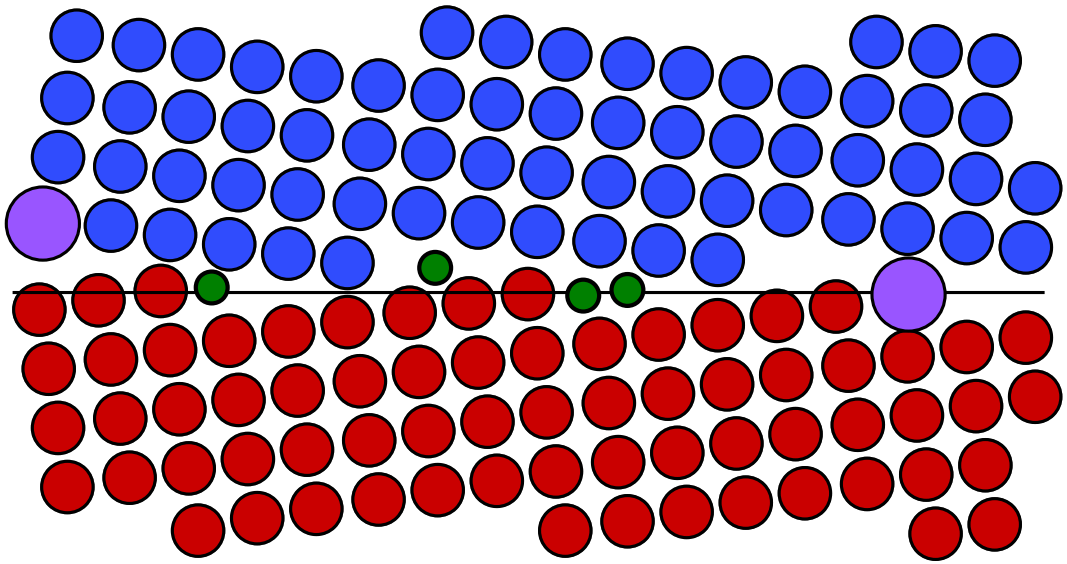
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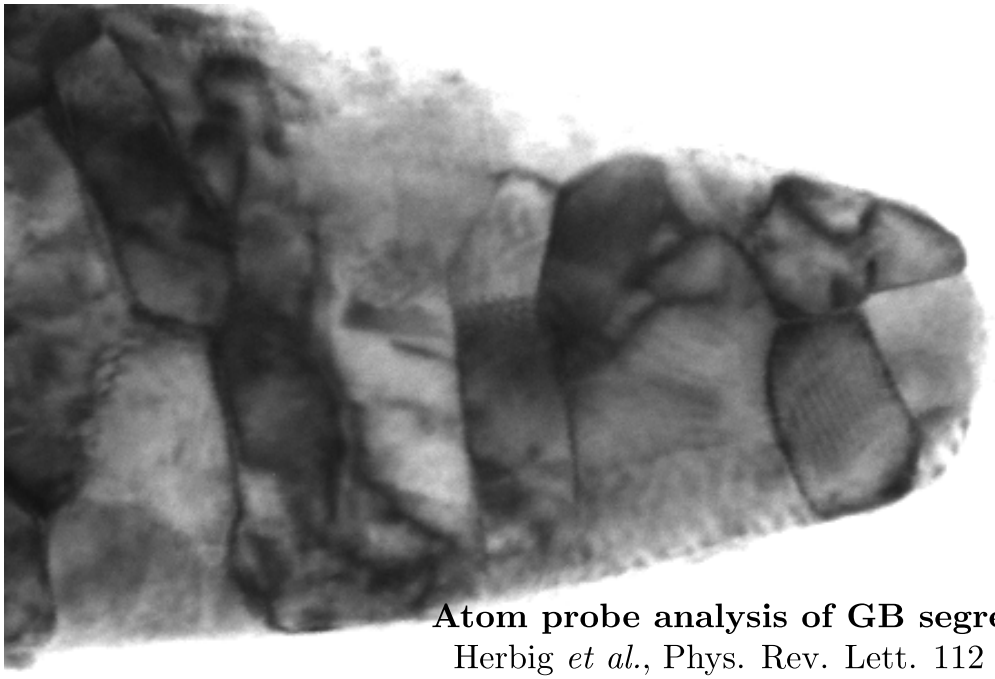
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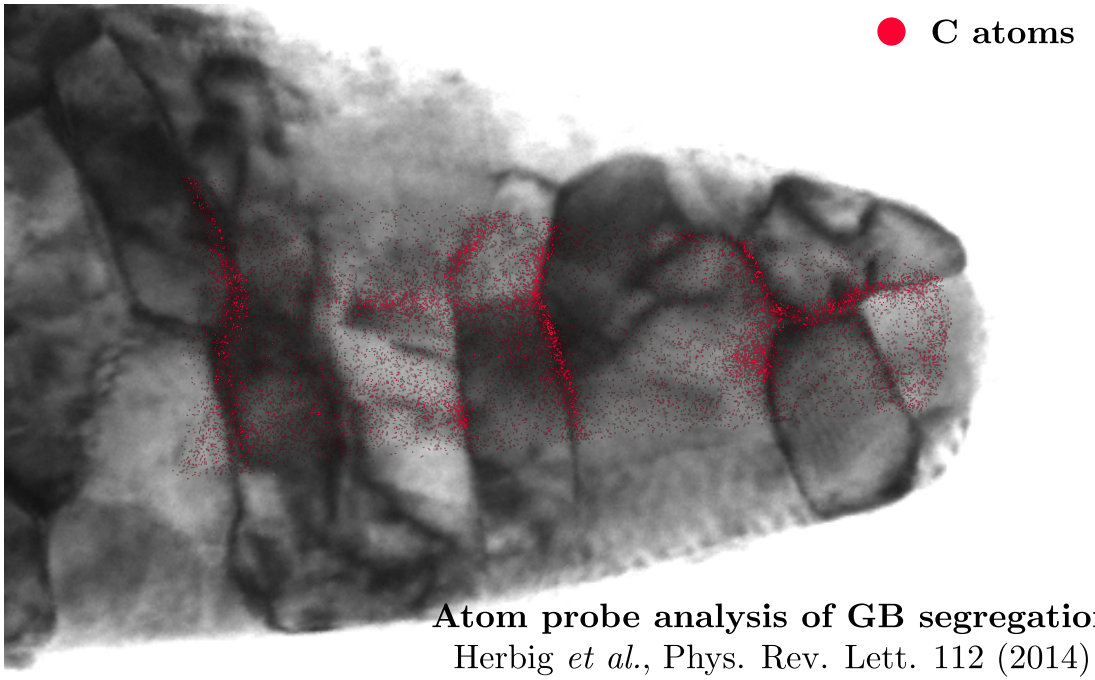
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Atom probe analysis of GB segregation
Herbig *et al.*, Phys. Rev. Lett. 112 (2014)
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