EPFL
École polytechnique fédérale de Lausanne

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SuNMiL
Supramolecular NanoMaterials and Interfaces Laboratory

Idealized Grain Boundary Description
Lesson 9

MSE 304

Francesco Stellacci

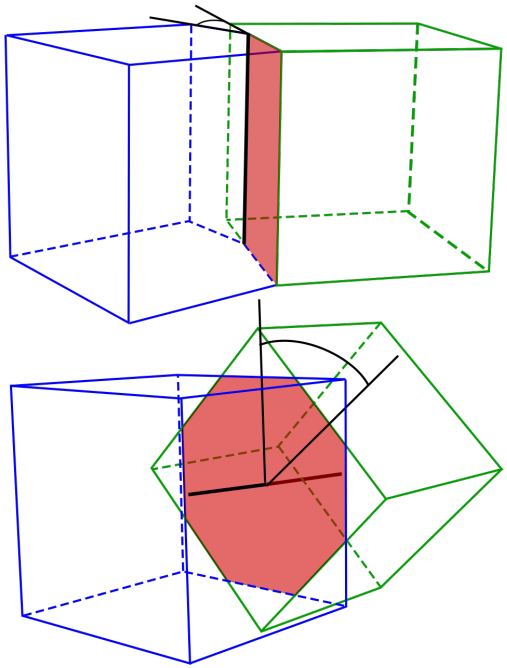
桑缪 썬밀 सानमिल ΣouNMιΛ سنمل CaHMПЛ

Key Topics in the Previous Class

Reading for this Class

What is a Grain Boundary?

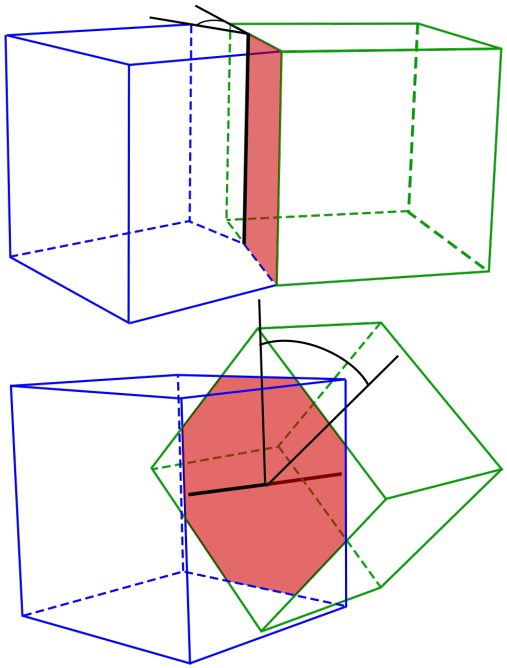
Idealized Grain Boundary Construction



Tilt Grain Boundary

Twist Grain Boundary

Idealized Grain Boundary Construction



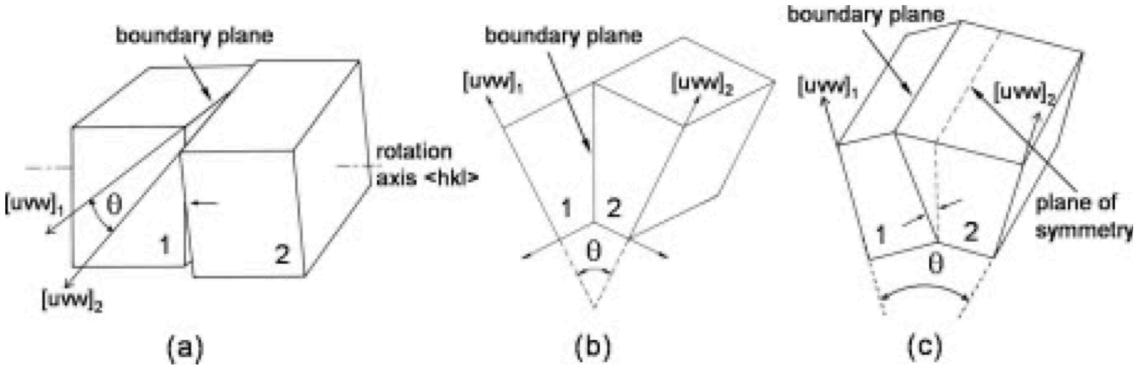
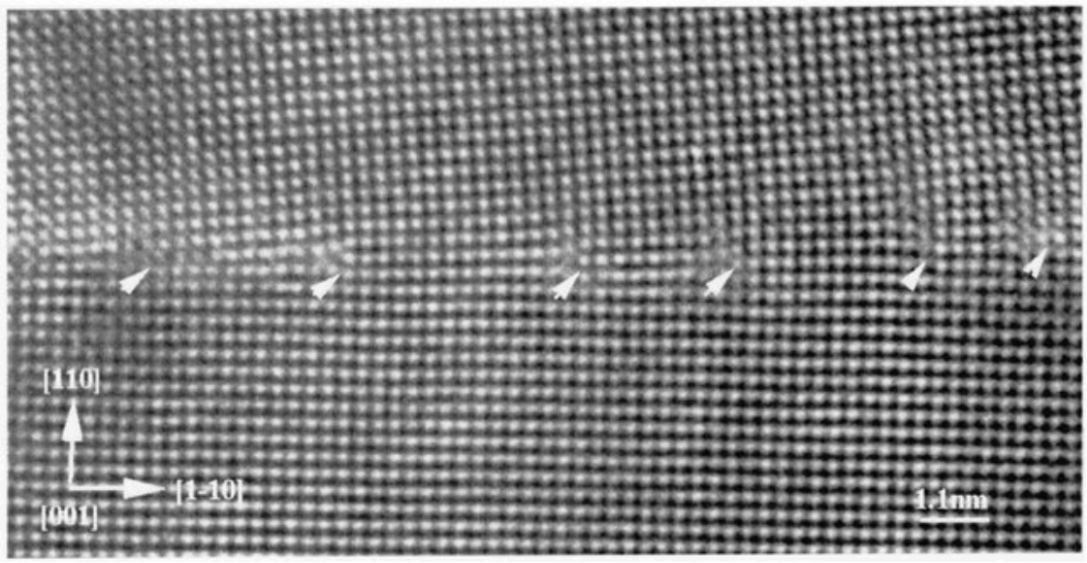


Figure 1.2: Various types of grain boundaries: (a) twist grain boundary, (b) symmetrical tilt grain boundary, (c) asymmetrical tilt grain boundary [6]

Atomistic View of Tilt Grain Boundaries

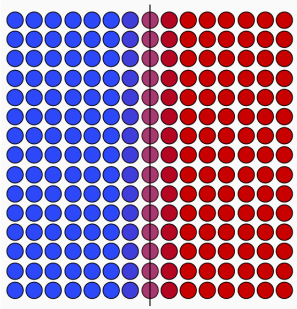


Figure

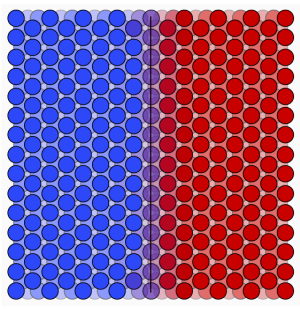
Caption

FIG. 1. HRTEM image of the 5° 001(110) symmetrical tilt grain boundary. Note that each GB dislocation has dissociated into two partial dislocations by a climb mechanism.

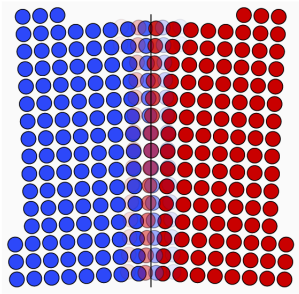
Atomistic View of Tilt Grain Boundaries



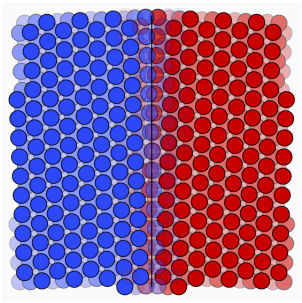
sc, $\mathbf{u} = \langle 001 \rangle$,
$\mathbf{n} = (100)$, $\theta = 0$



fcc, $\mathbf{u} = \langle 111 \rangle$,
$\mathbf{n} = (11\bar{2})$, $\theta = 0$



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



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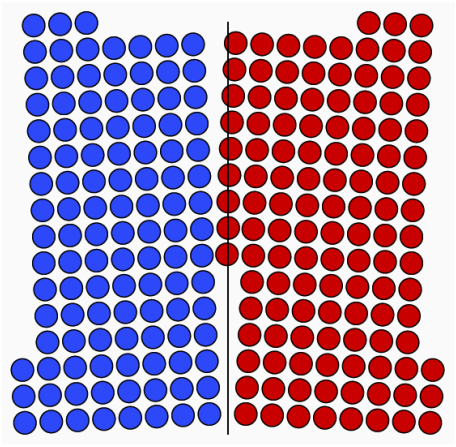
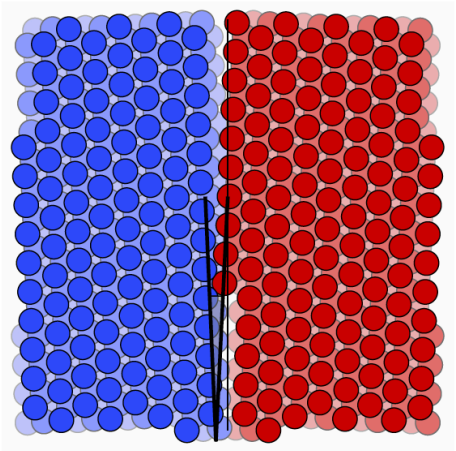
Atomistic View of Tilt Grain Boundaries



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



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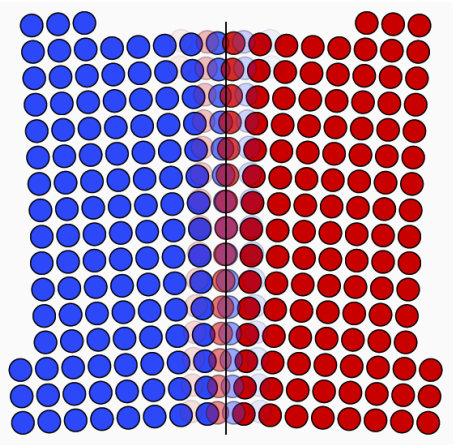
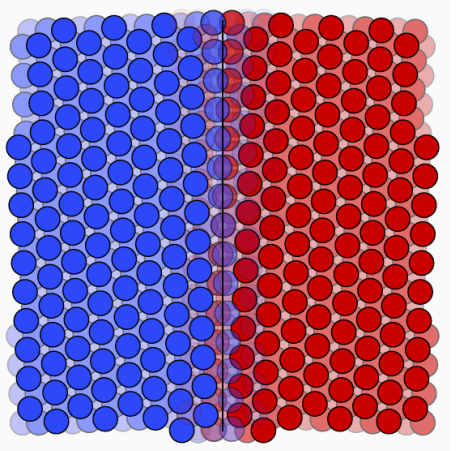


sc, $\mathbf{u} = \langle 001 \rangle$,
$\mathbf{n} = (100), \quad \theta = 5$



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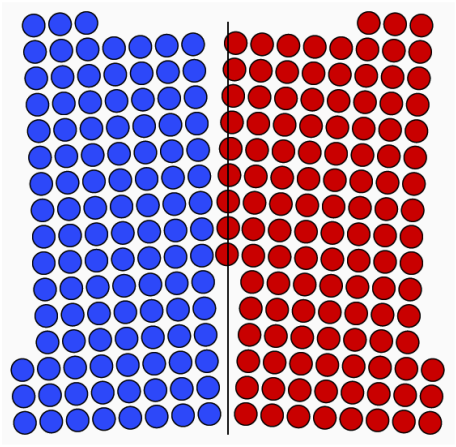
Atomistic View of Tilt Grain Boundaries



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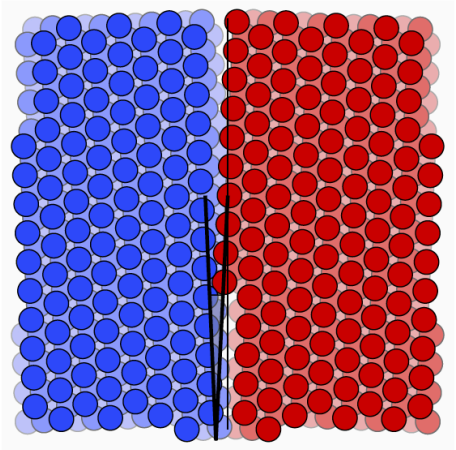
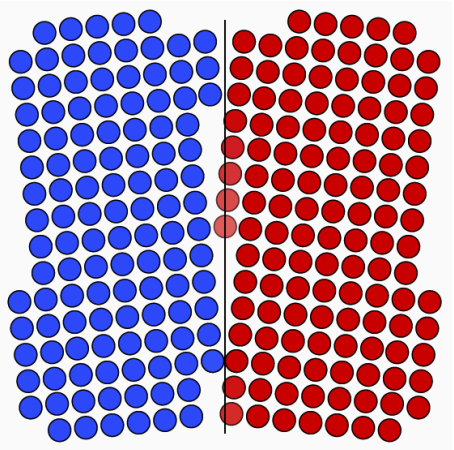
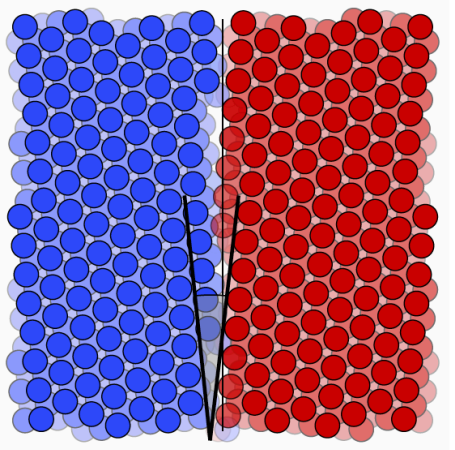


fcc, $\mathbf{u} = \langle 111 \rangle$,
$\mathbf{n} = (11\bar{2})$, $\quad \theta = 5$



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



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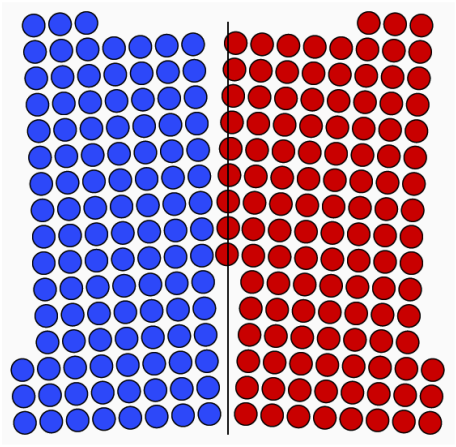
$\mathbf{n} = (11\bar{2})$, $\quad \theta = 12$

Atomistic View of Tilt Grain Boundaries



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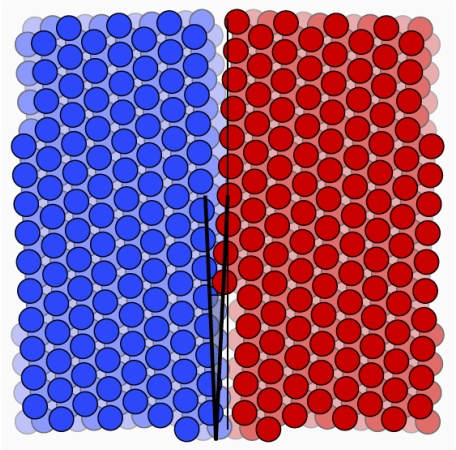

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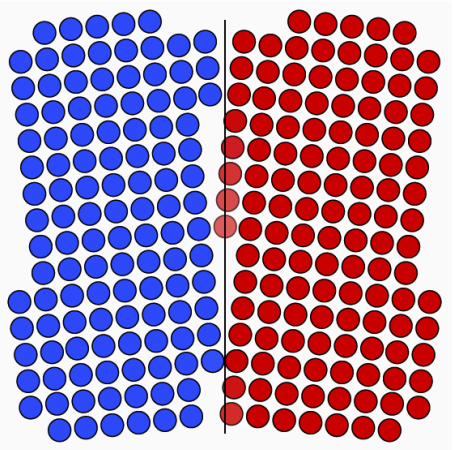

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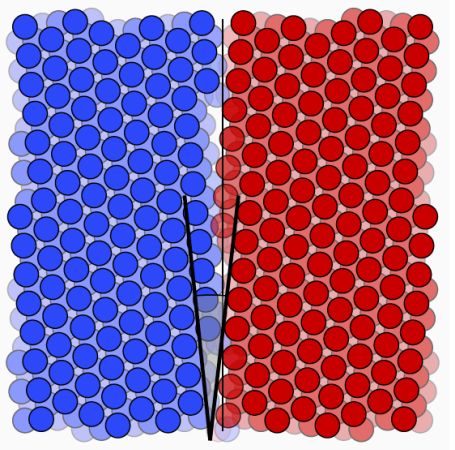
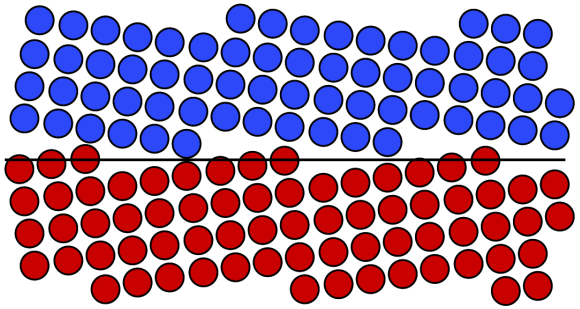
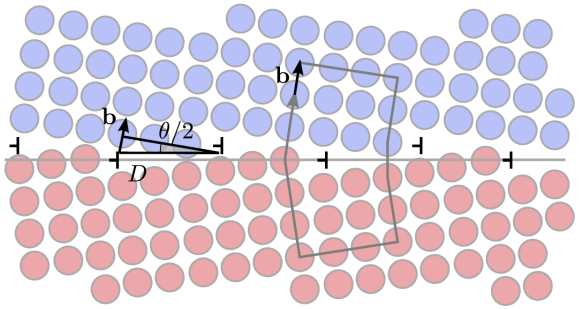


fcc, $\mathbf{u} = \langle 111 \rangle$,
$\mathbf{n} = (11\bar{2})$, $\quad \theta = 12$

Dislocations in Symmetric Tilt Grain Boundaries



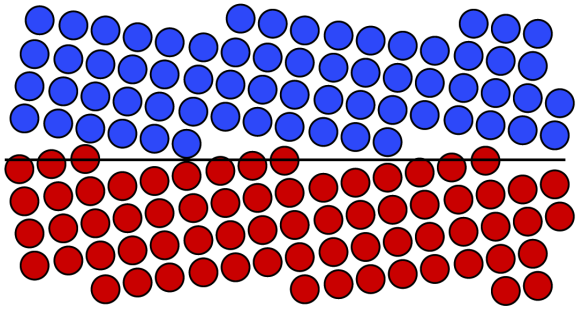
sc, $\mathbf{u} = \langle 001 \rangle$,
$\mathbf{n} = (100)$, $\theta = 18$



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

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

Dislocations in Symmetric Tilt Grain Boundaries



sc, $\mathbf{u} = \langle 001 \rangle$,
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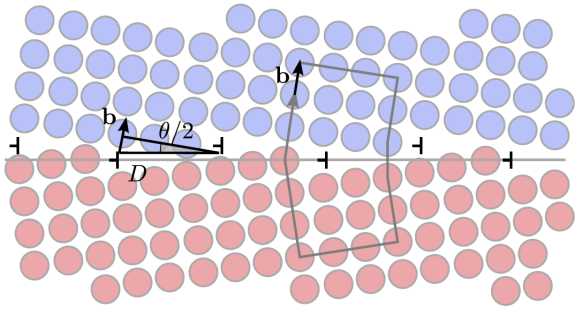

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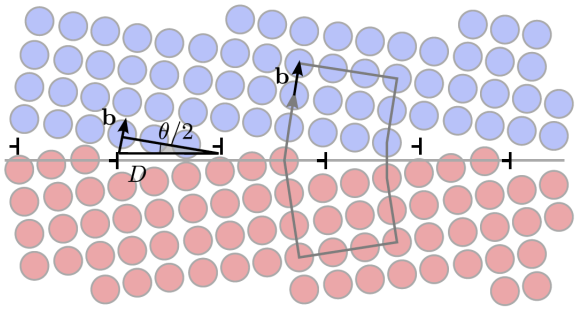
Dislocations in Symmetric Tilt Grain Boundaries



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

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

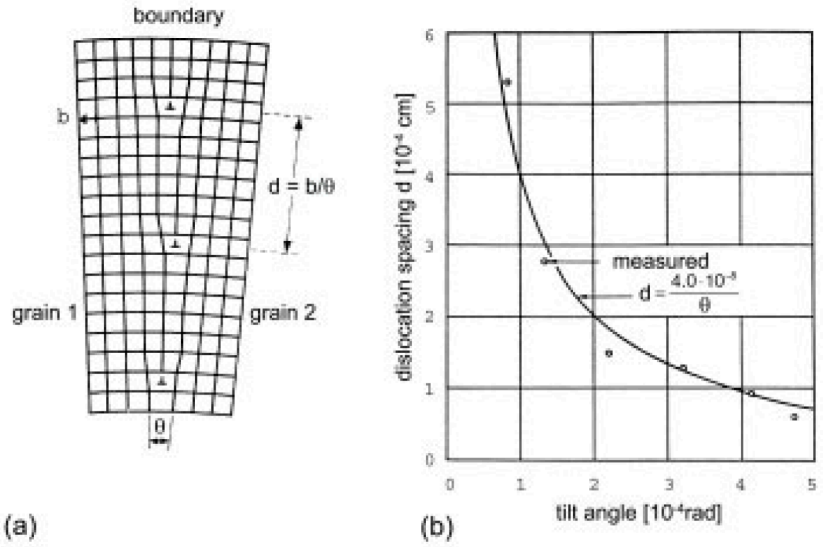
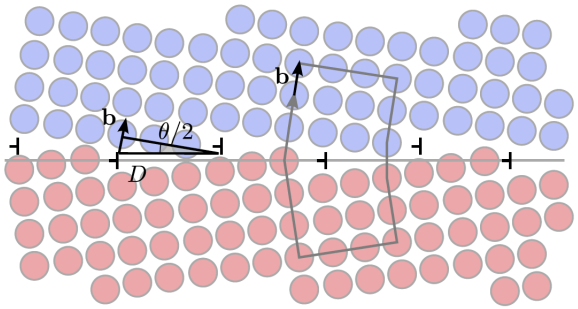


Figure 1.4: (a) Dislocation configuration of a symmetrical tilt <100> SAGB simple cubic crystal. (b) Measured and calculated dislocation spacing in a symmet SAGB in Germanium [6]

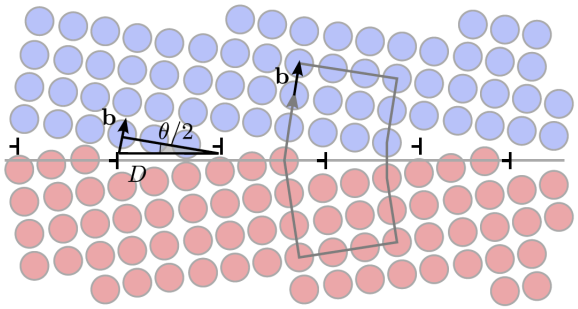
Dislocations in Symmetric Tilt Grain Boundaries



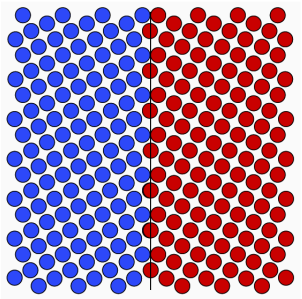
sc, $\mathbf{u} = \langle 001 \rangle$,
$\mathbf{n} = (100)$, $\theta = 18$

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

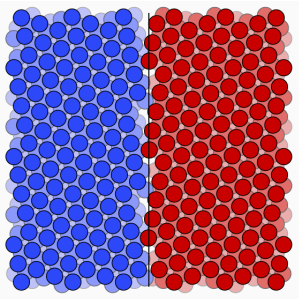
Dislocations in Symmetric Tilt Grain Boundaries



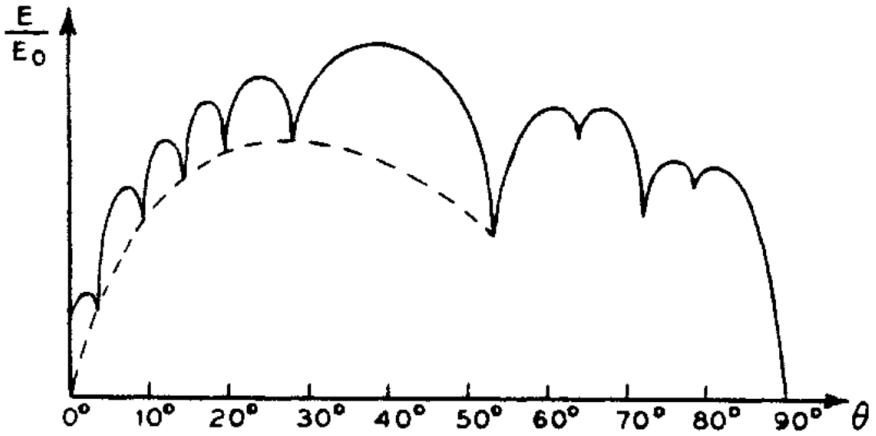
sc, $\mathbf{u} = \langle 001 \rangle$,
$\mathbf{n} = (100)$, $\theta = 18$



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



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



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Asymmetric Tilt Grain Boundaries

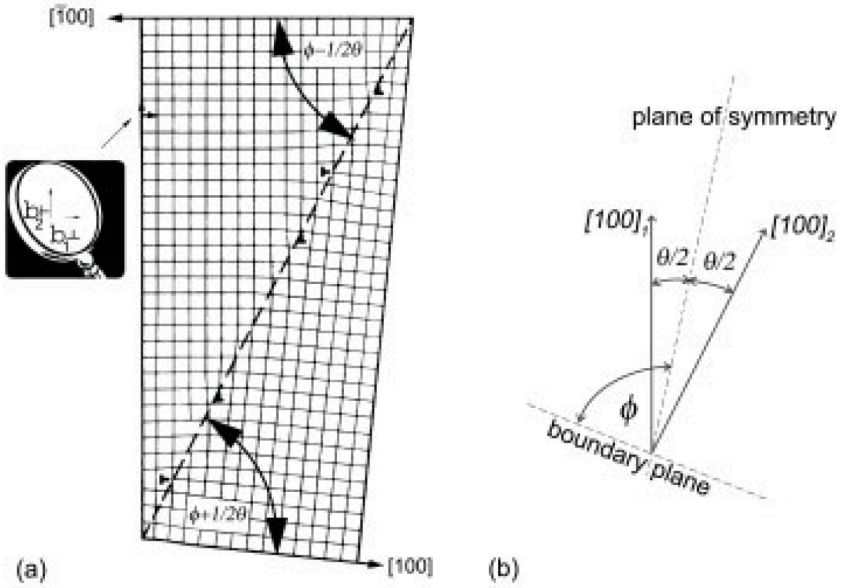
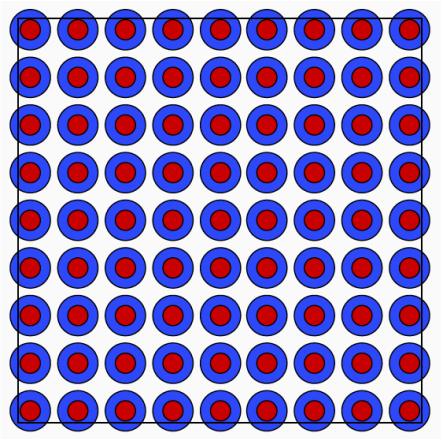
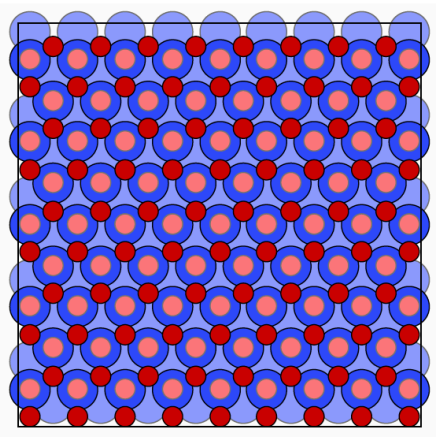


Figure 1.5: (a) Lattice dislocation arrangement [6] and (b) rotation angle θ and inclination ϕ of an asymmetric tilt SAGB [14]

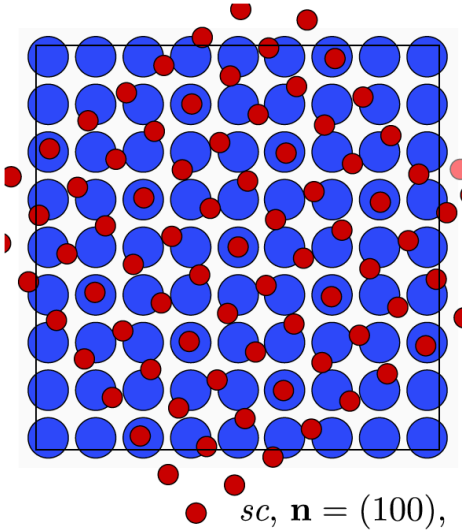
Twist Grain Boundaries



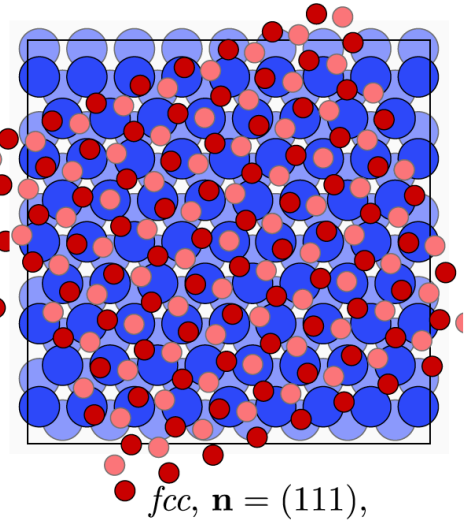
sc, $\mathbf{n} = (100)$,
$\psi = 0°$, $\theta = 0°$



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



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



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

Twist Grain Boundaries

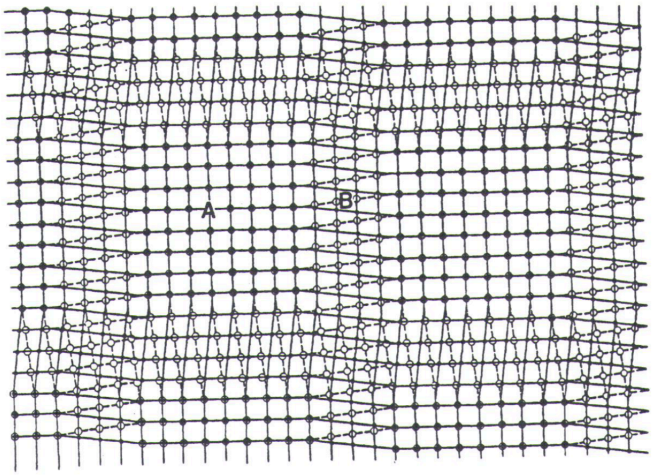
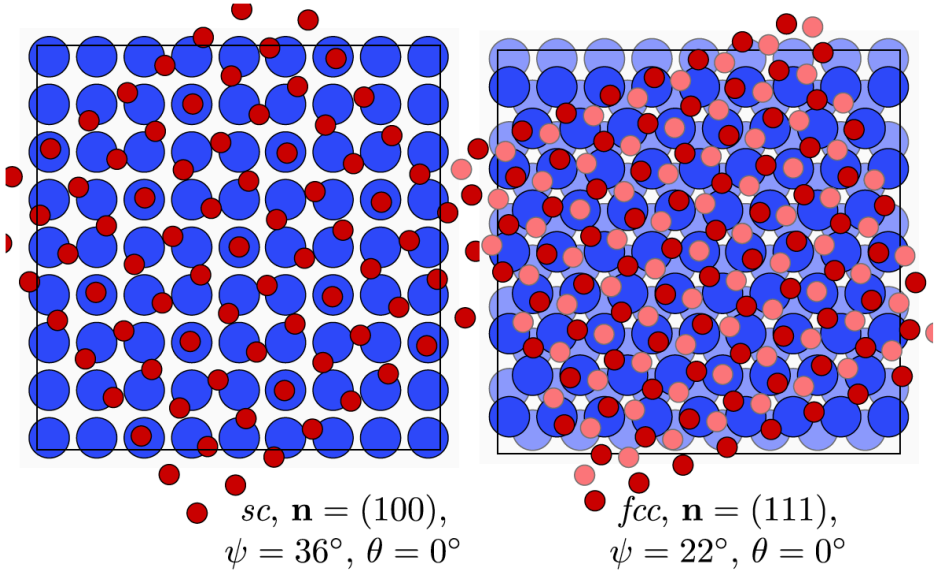


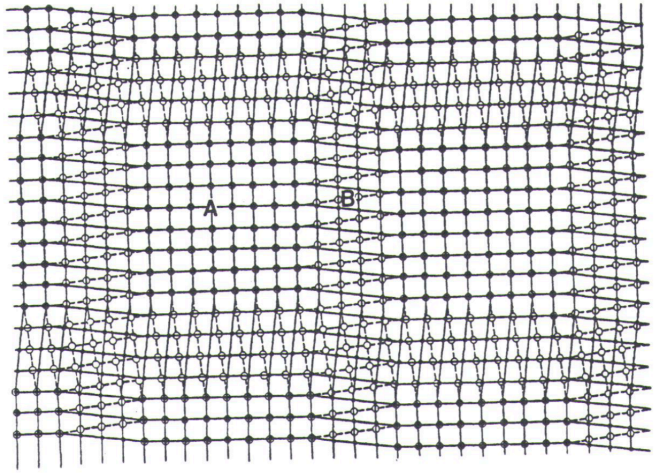
Figure 13.10. A pure (relaxed) twist boundary between two simple cubic crystals. The boundary is in the plane of the figure and the two grains have a small rotation about the cube axis normal to the boundary. The open circles represent atoms just above the plane of the boundary in one grain and the solid circles atoms just below in the opposite grain. Atoms at the interface have been relaxed to produce regions of good atomic matching (*A*) separated by regions of poor matching (*B*), which are the screw dislocations. From [25].



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

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

Twist Grain Boundaries



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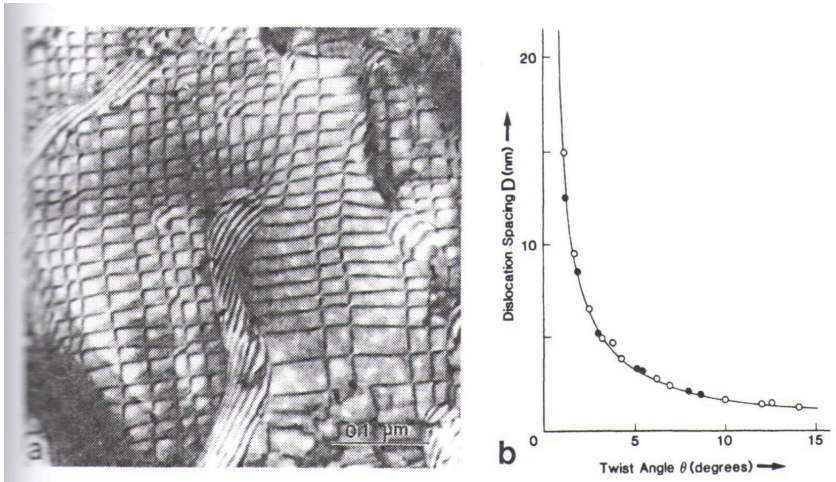
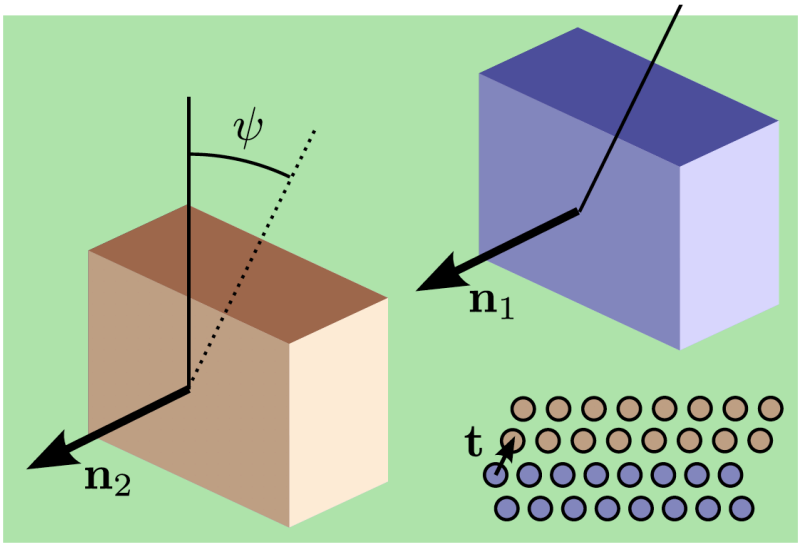


Figure 13.12. (a) Bright field TEM image of a cross-grid of screw dislocations in a pure twist boundary ($\theta = 1°$) in gold. From [34] copyright Taylor & Francis Ltd. (b) Comparison of experimental and calculated spacings of dislocations for (001) twist boundaries in gold. From [33]. The filled circles are the results of Schober and Balluffi [34] and the open circles are from the results of Tan et al. [35].

Generic Grain Boundaries



Generic Grain Boundaries

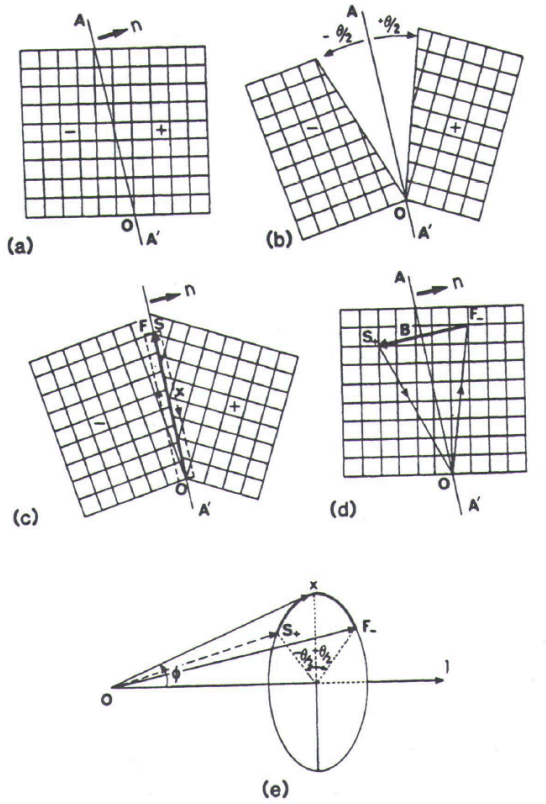


Figure 13.15. Illustration of the derivation of the net Burgers vector **B** crossing a vector **x** in a planar grain boundary *AA′* with unit normal **n**, where lattice + is rotated with respect to lattice − by an angle θ in a right-handed sense about an axis **l** directed into the plane of the page through the point *O*. From [33].

$$|\mathbf{B}| = |\mathbf{x}| 2 \sin(\theta/2) \sin \Phi \tag{13.10}$$

with a direction along $(\mathbf{x} \times \mathbf{l})$. Furthermore, because

$$|\mathbf{x} \times \mathbf{l}| = |\mathbf{x}| \sin \Phi, \tag{13.11}$$

then

$$\mathbf{B} = (\mathbf{x} \times \mathbf{l}) 2 \sin(\theta/2), \tag{13.12a}$$

which, for small θ, yields

$$\mathbf{B} = (\mathbf{x} \times \mathbf{l})\theta. \tag{13.12b}$$

$$n_1\mathbf{b}_1 + n_2\mathbf{b}_2 + n_3\mathbf{b}_3 = 2 \sin(\theta/2)(\mathbf{x} \times \mathbf{l}), \tag{13.14}$$

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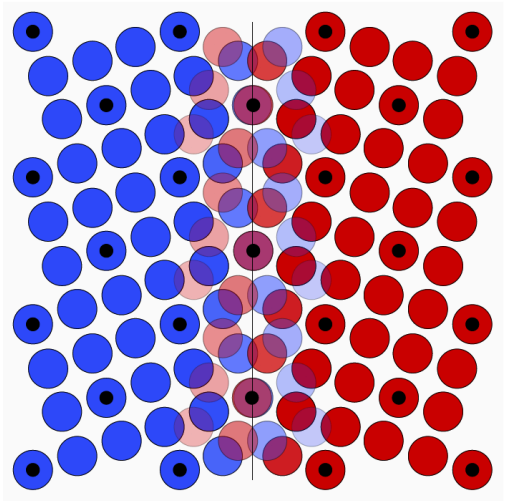
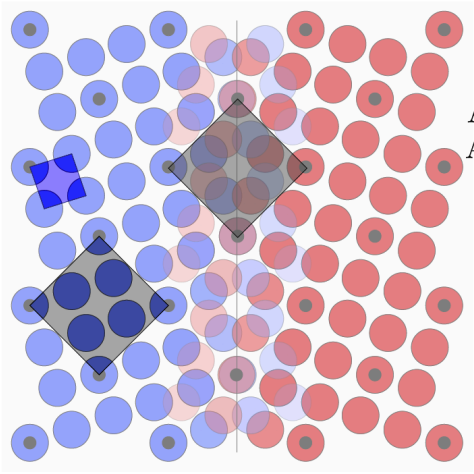
O-Lattice Description of a Generic Grain Boundary

O-Lattice Description of a Generic Grain Boundary

Coincidence Lattice Description of a Generic Grain Boundaries



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

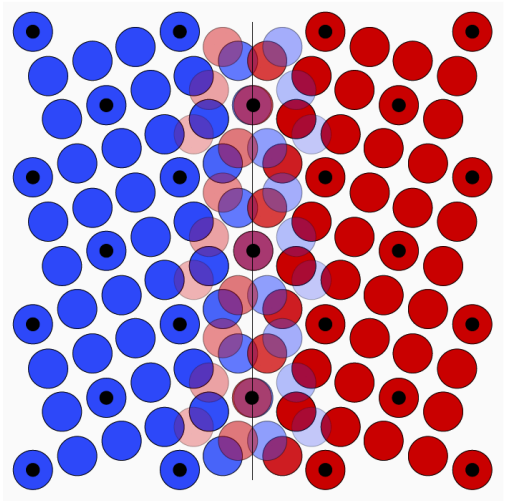


Atoms per unit cell: 1
Atoms per CSL cell: 5

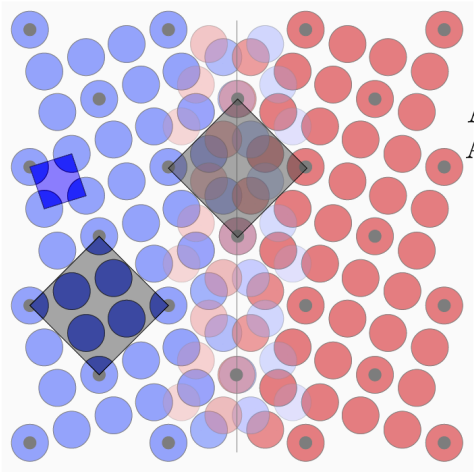
$\boxed{\Sigma = 5}$

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

Coincidence Lattice Description of a Generic Grain Boundaries



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

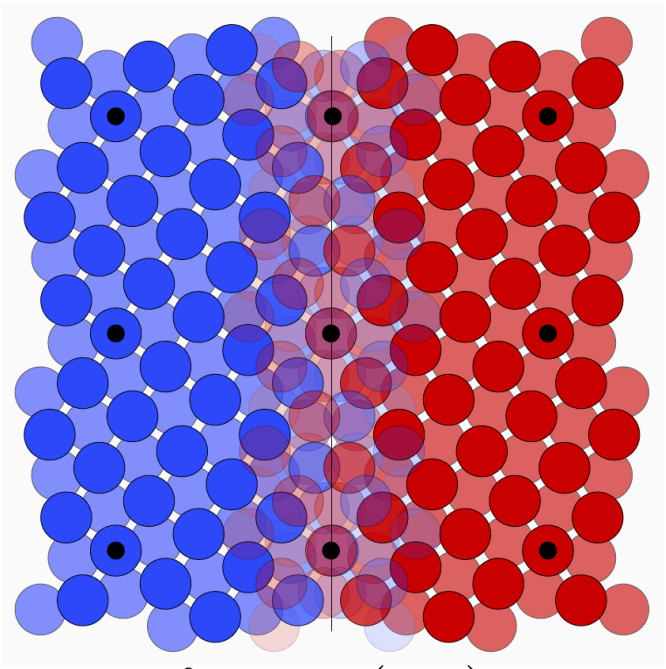


Atoms per unit cell: 1
Atoms per CSL cell: 5

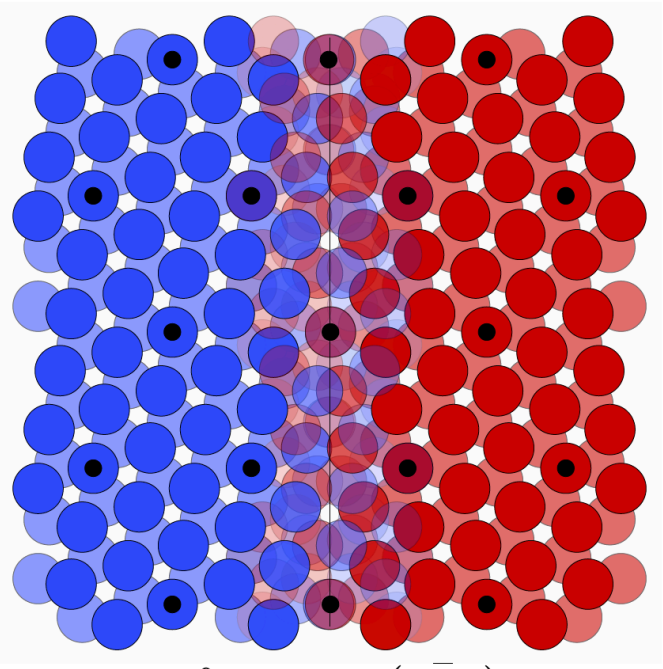
$\boxed{\Sigma = 5}$

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

Coincidence Lattice Description of a Generic Grain Boundaries

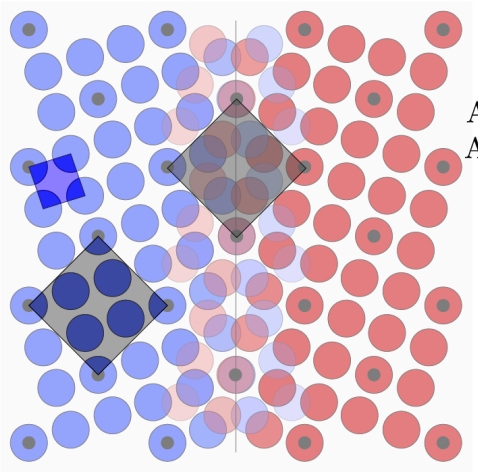


fcc, $\mathbf{n} = (100)$,
$\mathbf{u} = \langle 001 \rangle$, $\theta = 22.6°$
$\boxed{\Sigma = 13a}$



fcc, $\mathbf{n} = (1\bar{1}0)$,
$\mathbf{u} = \langle 111 \rangle$, $\theta = 38.21°$
$\boxed{\Sigma = 7}$

Energy Considerations



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

$$\boxed{\Sigma = 5}$$

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

Limitations of the Descriptions

Conclusions