EPFL
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SuNMiL
Supramolecular NanoMaterials and Interfaces Laboratory

# Idealized Grain Boundary Description
# Lesson 9

MSE 304

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# Key Topics in the Previous Class

$\gamma_{12} = \gamma_1 + \gamma_2 - W_{12} = \sum_i b_i + E_e$

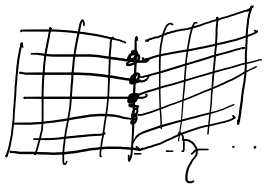
1 and 2 solids

$W_{12} \simeq \gamma_1 + \gamma_2$

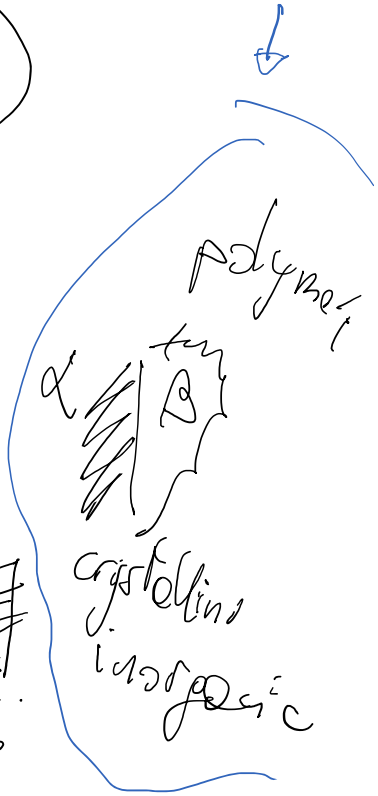
presence of dislocations

homogeneous grain boundary

low angle $\gamma_{12} = 2\gamma_1 - W_{12} = E_e$



2°



# Reading for this Class

Ch. 13 Howe book

# What is a Grain Boundary?

A G.B. is a solid - solid interfaces between 2 crystalline phases

→ α and β have different elements and different Bravais lattice

Special cases

→ the same B.L different elements

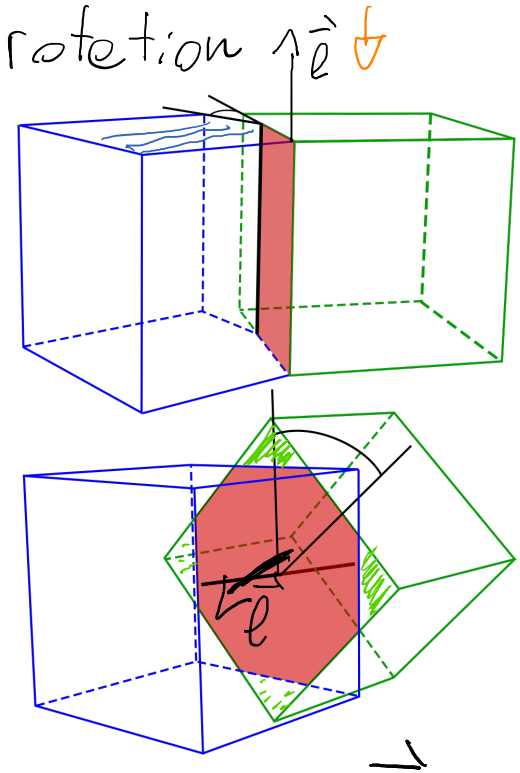
→ different B.L. same elements

→ same B.L same elements different composition

homophase

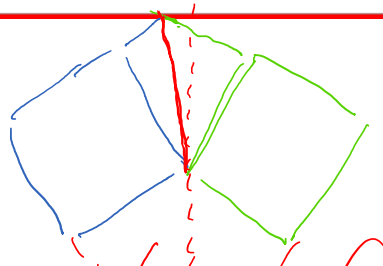
→ same crystalline phase, same composition, same interfacial plane

# Idealized Grain Boundary Construction





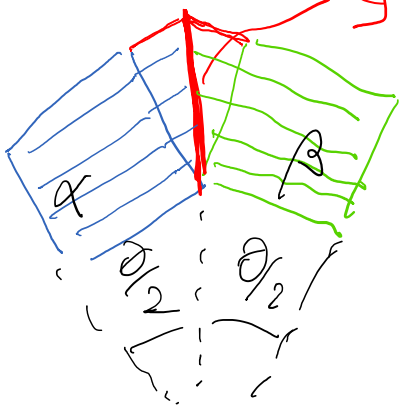
**Tilt Grain Boundary**



grain boundary plane

**Twist Grain Boundary**

from the top




$\vec{e} \wedge \vec{n} = \begin{cases} 0^\circ \text{ tilt} \\ \updownarrow \\ 90^\circ \text{ twist} \end{cases}$



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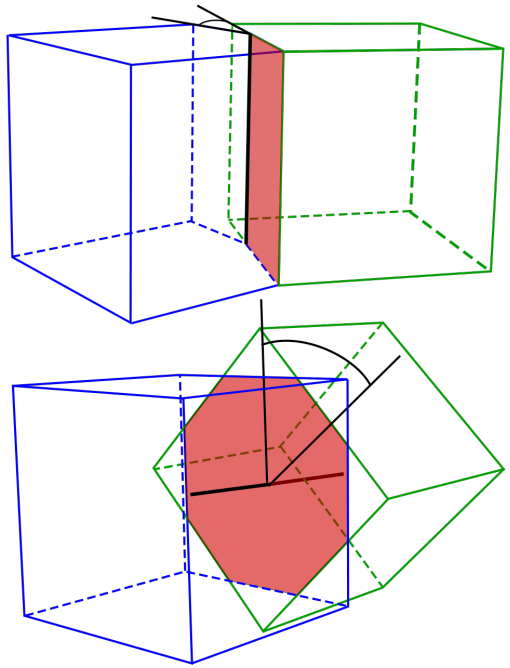
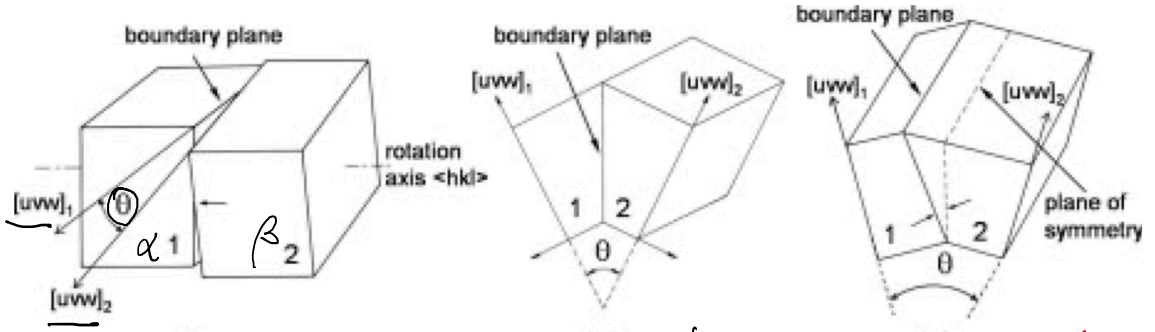
# Idealized Grain Boundary Construction



twist

tilt grain boundary



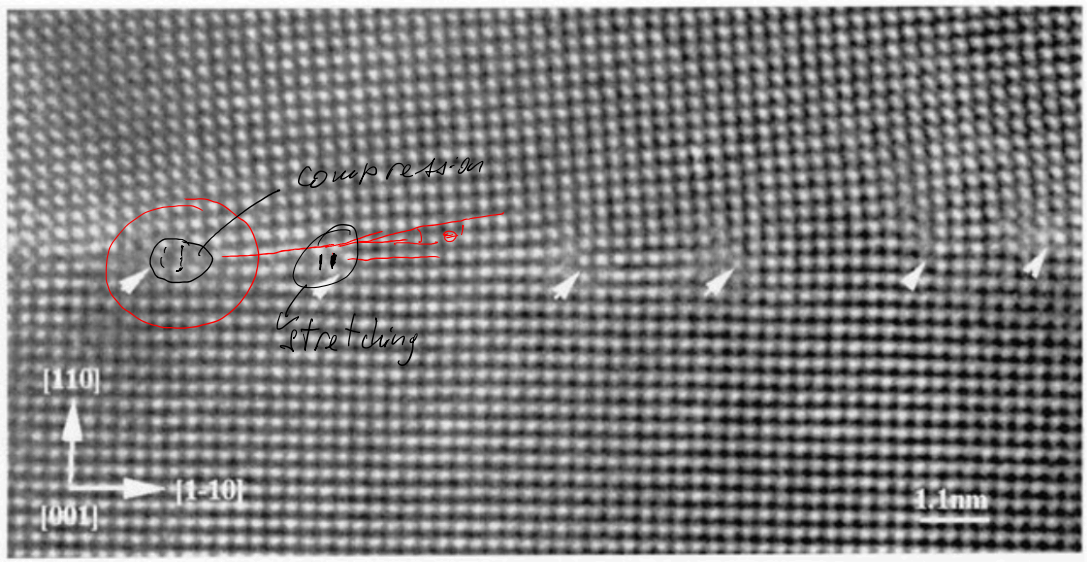

symmetric

asymmetric

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

the g. boundary is atomically flat
how the TLK [7 4 3]

# Atomistic View of Tilt Grain Boundaries



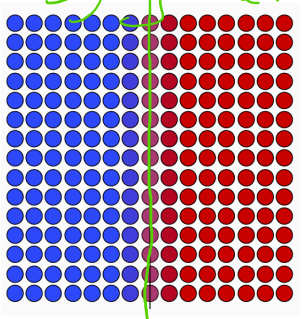

## Figure

Caption

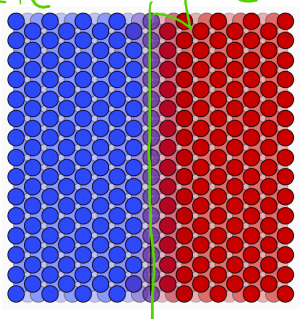
FIG. 1. HRTEM image of the 5° 001(110) symmetrical tilt grain boundary. Note that each GB dislocation has dissociated into two partial dislocations by a climb mechanism.

# Atomistic View of Tilt Grain Boundaries

1) generate a grain boundary plane



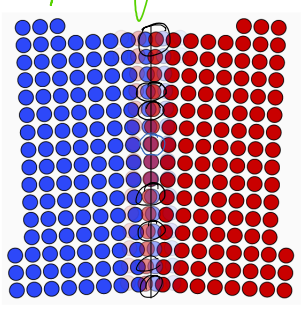
*sc*, $\mathbf{u} = \langle 001 \rangle$,
$\mathbf{n} = (100)$, $\theta = 0$



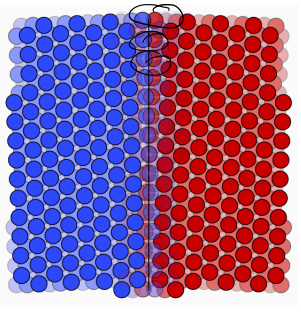
*fcc*, $\mathbf{u} = \langle 111 \rangle$,
$\mathbf{n} = (11\bar{2})$, $\theta = 0$

↓
atom that overlap imperfectly

2) perform the rotation



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



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

S.C. simple cubic

f.c.c. face centered cubic

$\theta = 5°$

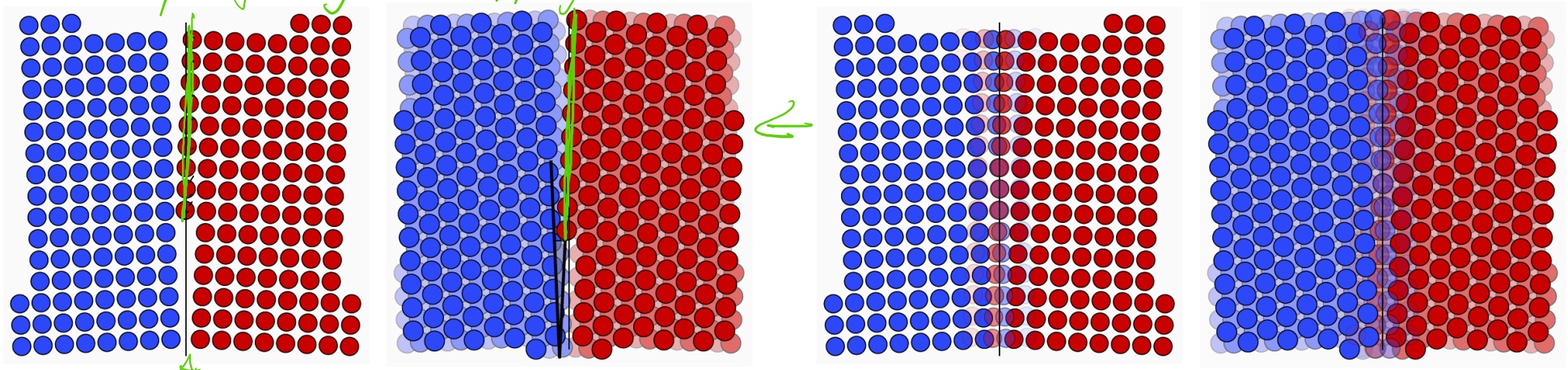
$\vec{n}$ ⊥ to the grain boundary plane

$\vec{u} \equiv \vec{l}$ rotation axis

# Atomistic View of Tilt Grain Boundaries

3) remove 1 of the 2 imperfectly overlapping atoms

2) step 2



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

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

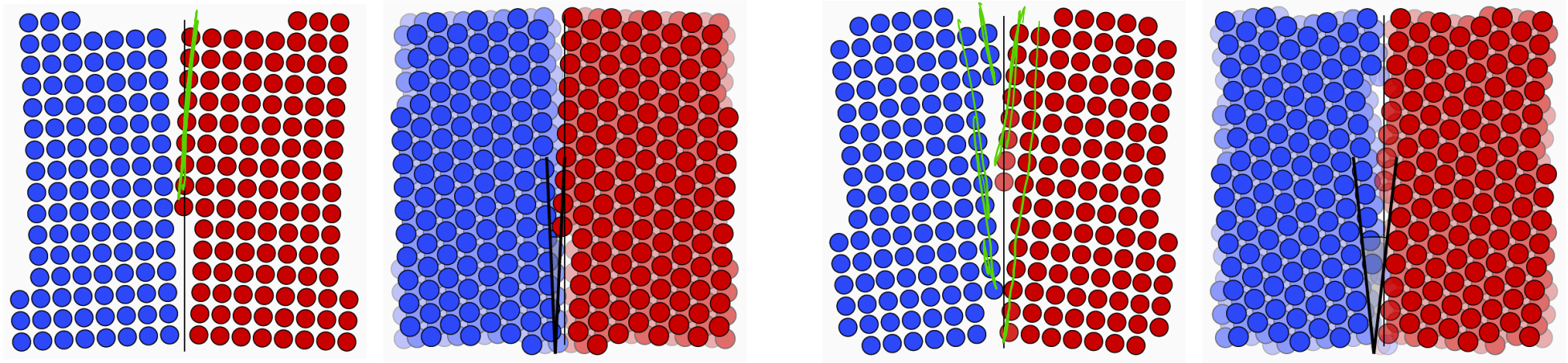
*sc*, $\mathbf{u} = \langle 001 \rangle$, $\mathbf{n} = (100)$, $\theta = 5$

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

dislocations appear

# Atomistic View of Tilt Grain Boundaries

$\theta = 5°$ $\theta = 12°$



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

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

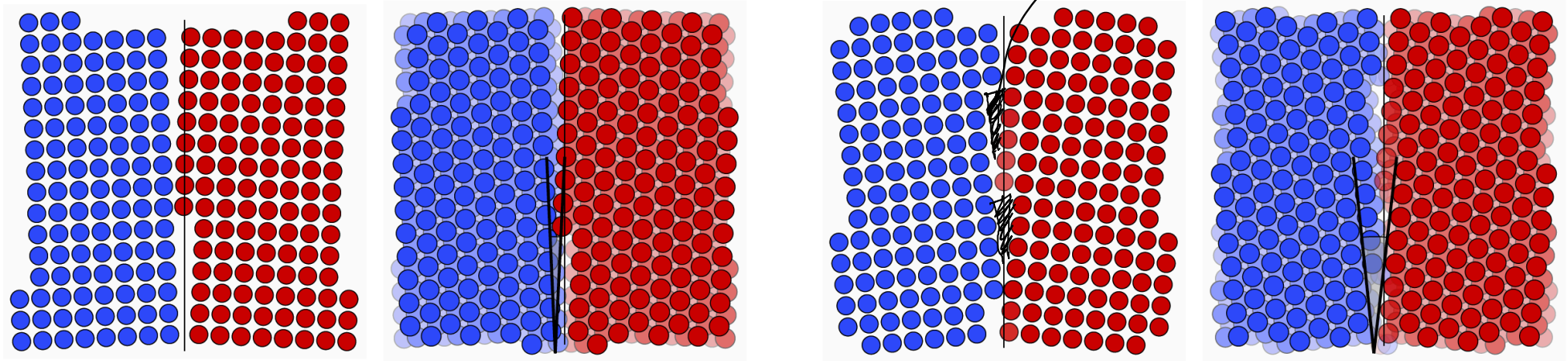
*sc*, $\mathbf{u} = \langle 001 \rangle$, $\mathbf{n} = (100)$, $\theta = 12$

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

# of dislocations depends on $\theta$

dislocations are evenly spaced!

# Atomistic View of Tilt Grain Boundaries




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

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

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

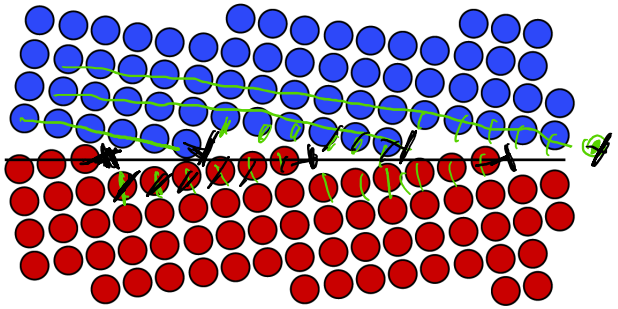
$fcc$, $\mathbf{u} = \langle 111 \rangle$, $\mathbf{n} = (11\bar{2})$, $\theta = 12$

E.S. ⇒ large stretching of bonds

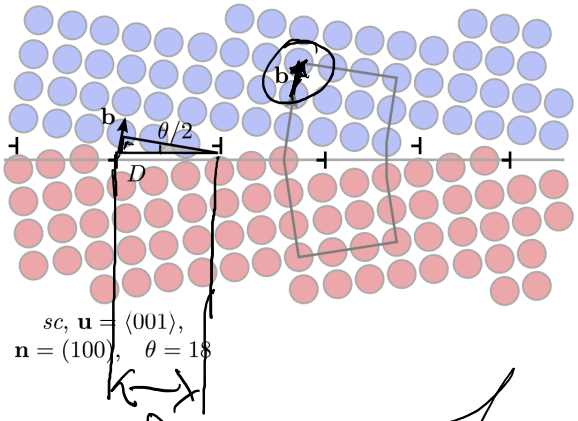
# Dislocations in Symmetric Tilt Grain Boundaries

$\theta = 18°$

D the distance between 2 neighbouring dislocations



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




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

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

low $\theta$

$\frac{1}{D}$ is the density of dislocations



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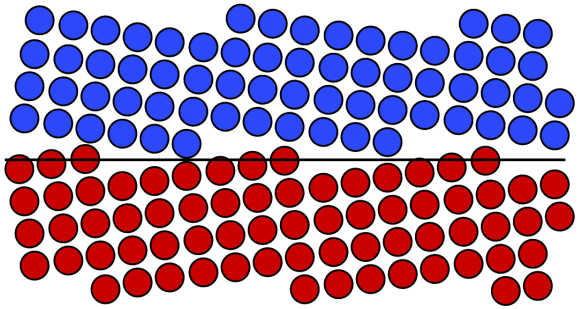
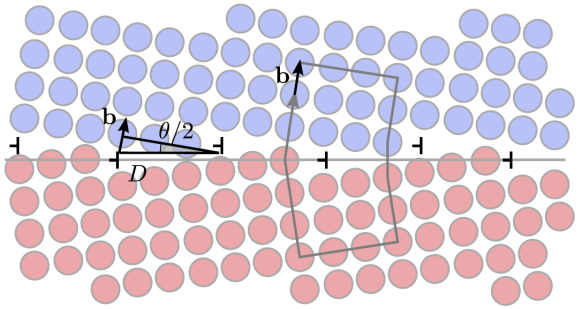
# Dislocations in Symmetric Tilt Grain Boundaries

what is the energy of this dislocation?



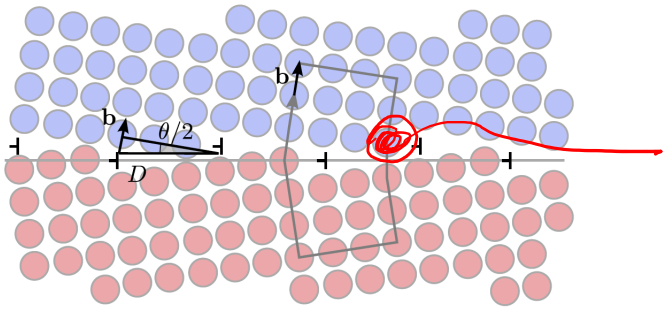
*sc*, $\mathbf{u} = \langle 001 \rangle$,
$\mathbf{n} = (100)$, $\theta = 18$




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

under coordinated

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

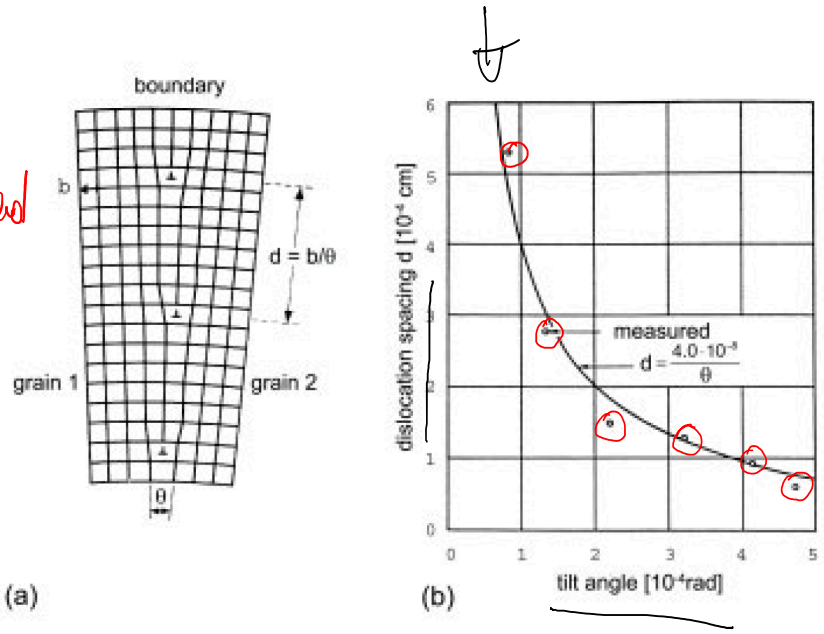



**Figure 1.4**: (a) Dislocation configuration of a symmetrical tilt <100> SAGB simple cubic crystal. (b) Measured and calculated dislocation spacing in a symmet SAGB in Germanium [6]

1) calculate the energy associated to the termination of a dislocation
2) calculate the elastic energy associated to a dislocation



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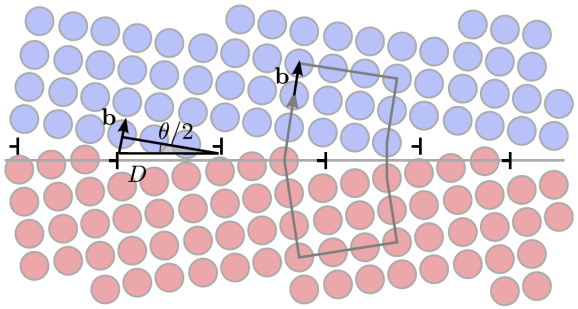
# Dislocations in Symmetric Tilt Grain Boundaries




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

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

$$\gamma_{gb} = \gamma_\alpha + \gamma_\beta - W_{12} =$$

$$= 2\gamma_\alpha - W_{12} = E_\perp \cdot \left(\frac{1}{D}\right) =$$

$$= E_\perp \left(\frac{\theta}{b}\right) =$$

$$= E_0 \theta \left(A_0 - \ln\theta\right)$$

$E_\perp$ → bonding
↳ elastic part

$$E_0 = \frac{\mu b}{4\pi(1-\nu)}$$

$\mu$ shear modulus
$\nu$ poisson ration

$$A_0 = 1 + \ln\left(\frac{b}{2\pi r_0}\right)$$

$r_0$ core energy of a dislocation



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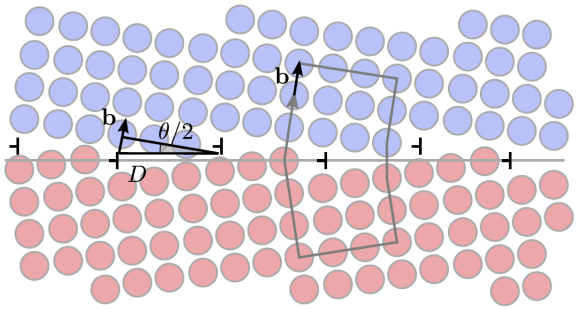
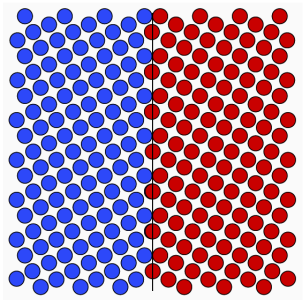
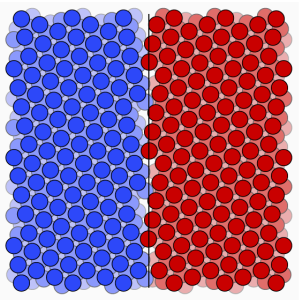
# Dislocations in Symmetric Tilt Grain Boundaries



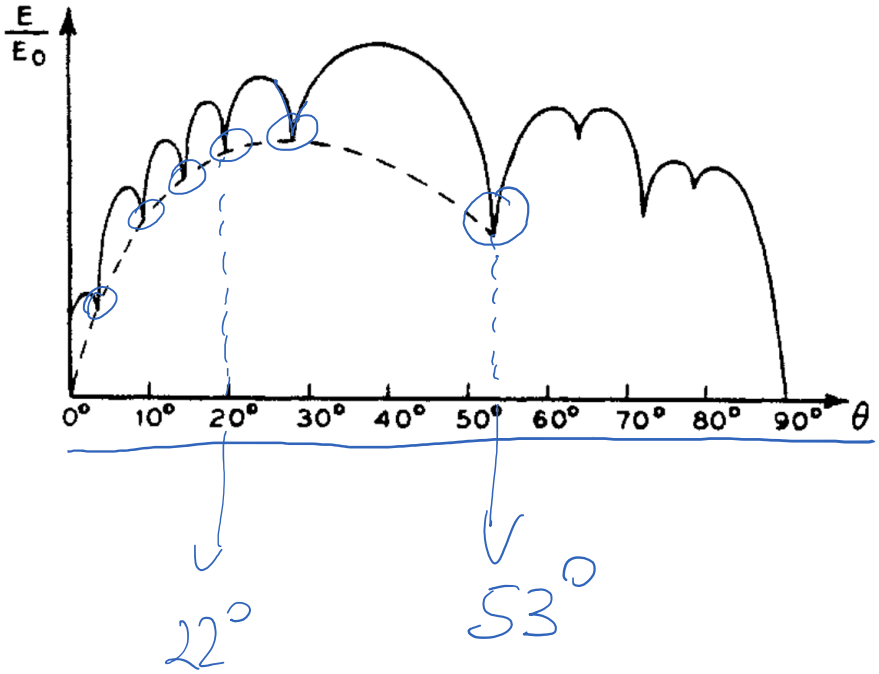

$sc$, $\mathbf{u} = \langle 001 \rangle$,
$\mathbf{n} = (100)$, $\theta = 18$



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



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



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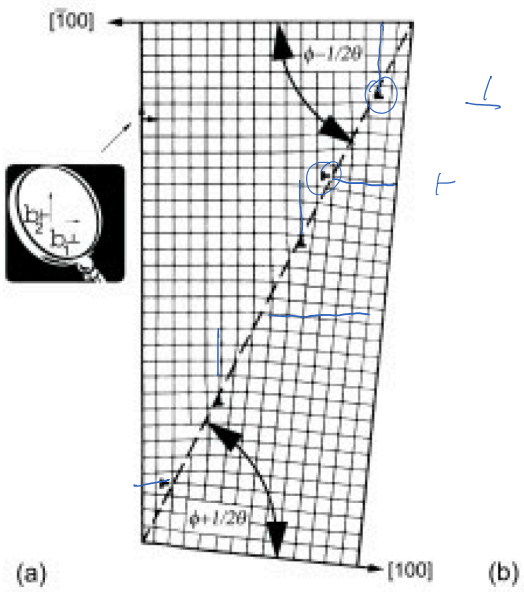
# Asymmetric Tilt Grain Boundaries



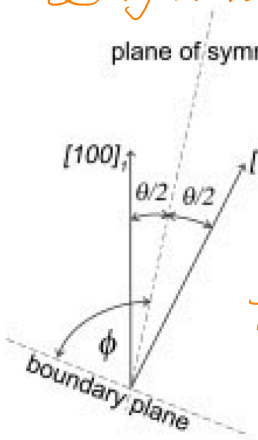
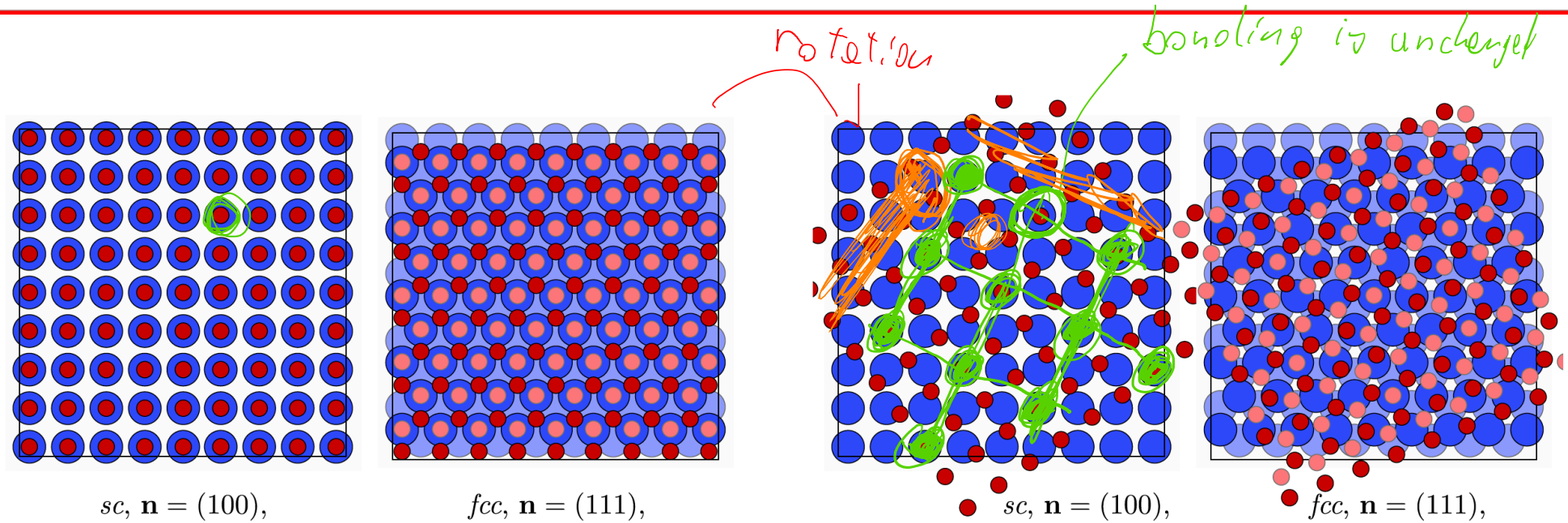




**Figure 1.5**: (a) Lattice dislocation arrangement [6] and (b) rotation angle $\theta$ and inclination $\phi$ of an asymmetric tilt SAGB [14]

# Twist Grain Boundaries




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

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

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

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

phase 1 and phase 2

# Twist Grain Boundaries

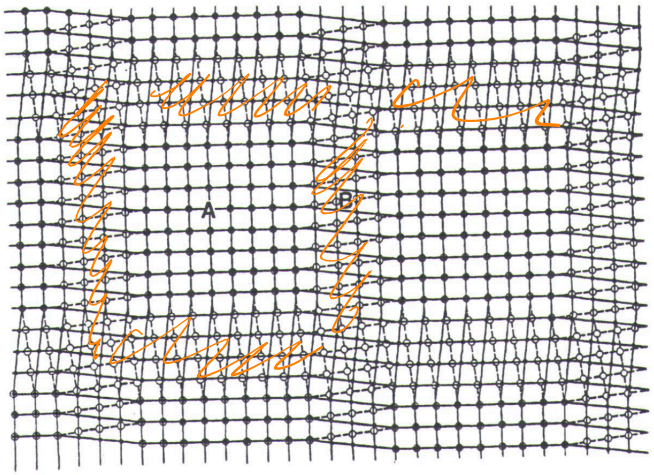
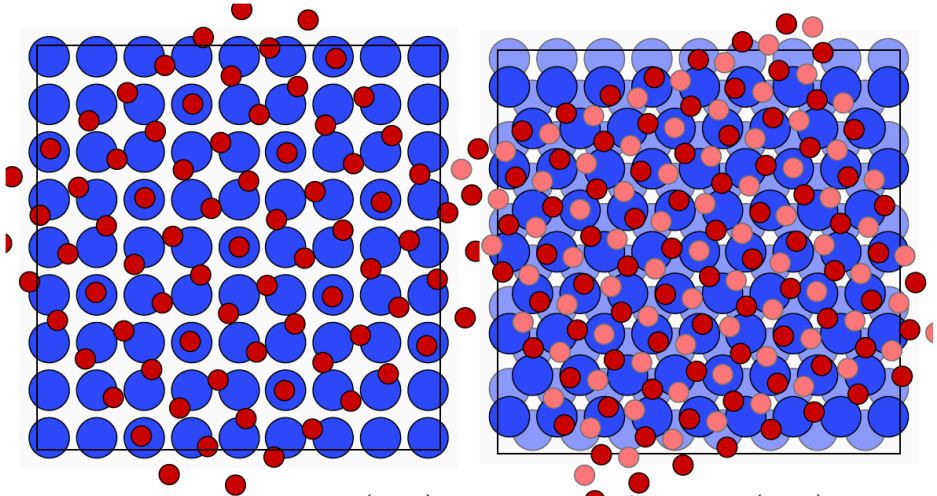



**Figure 13.10.** A pure (relaxed) twist boundary between two simple cubic crystals. The boundary is in the plane of the figure and the two grains have a small rotation about the cube axis normal to the boundary. The open circles represent atoms just above the plane of the boundary in one grain and the 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].

screw dislocation



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

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

# Twist Grain Boundaries

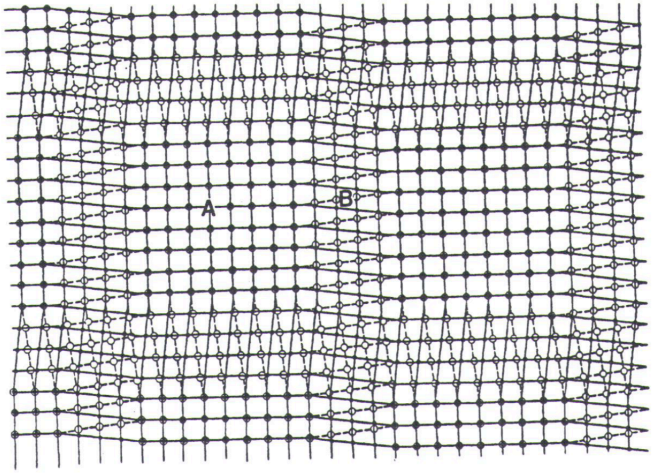



**Figure 13.10.** A pure (relaxed) twist boundary between two simple cubic crystals. The boundary is in the plane of the figure and the two grains have a small rotation about the cube axis normal to the boundary. The open circles represent atoms just above the plane of the boundary in one grain and the 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].

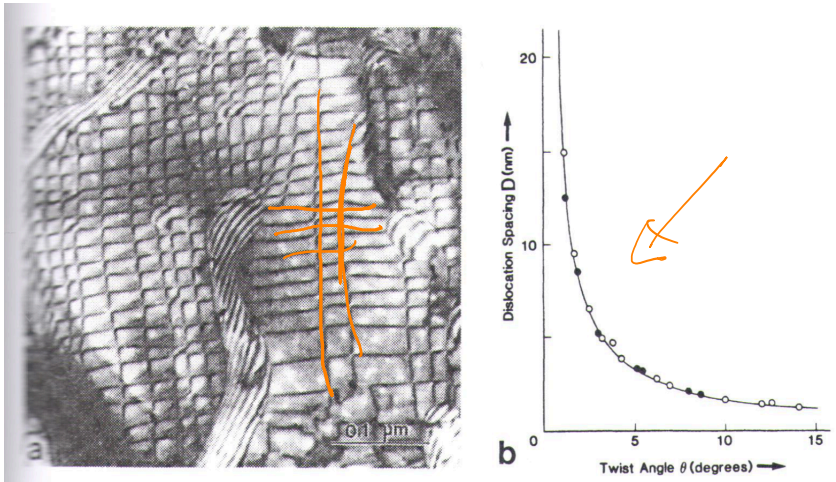
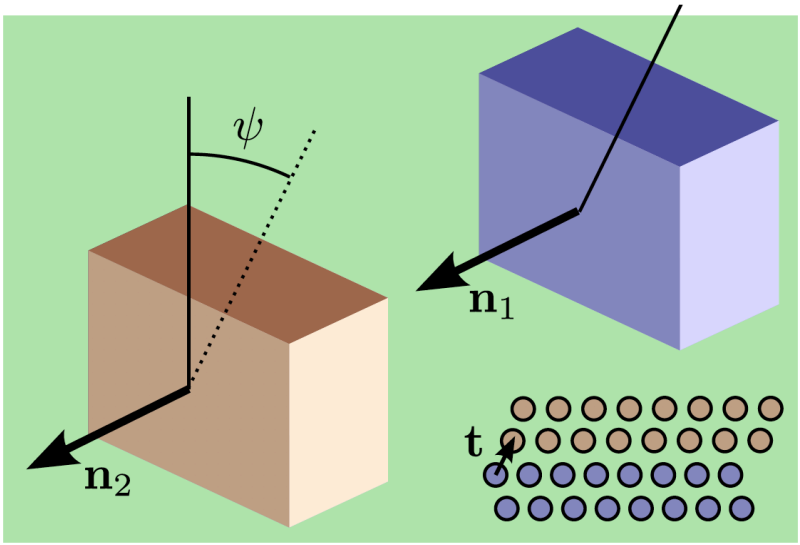



**Figure 13.12.** (a) Bright field TEM image of a cross-grid of screw dislocations in a pure twist boundary (θ = 1°) in gold. From [34] copyright Taylor & Francis Ltd. (b) Comparison of experimental and calculated spacings of dislocations for (001) twist boundaries in gold. From [33]. The filled circles 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

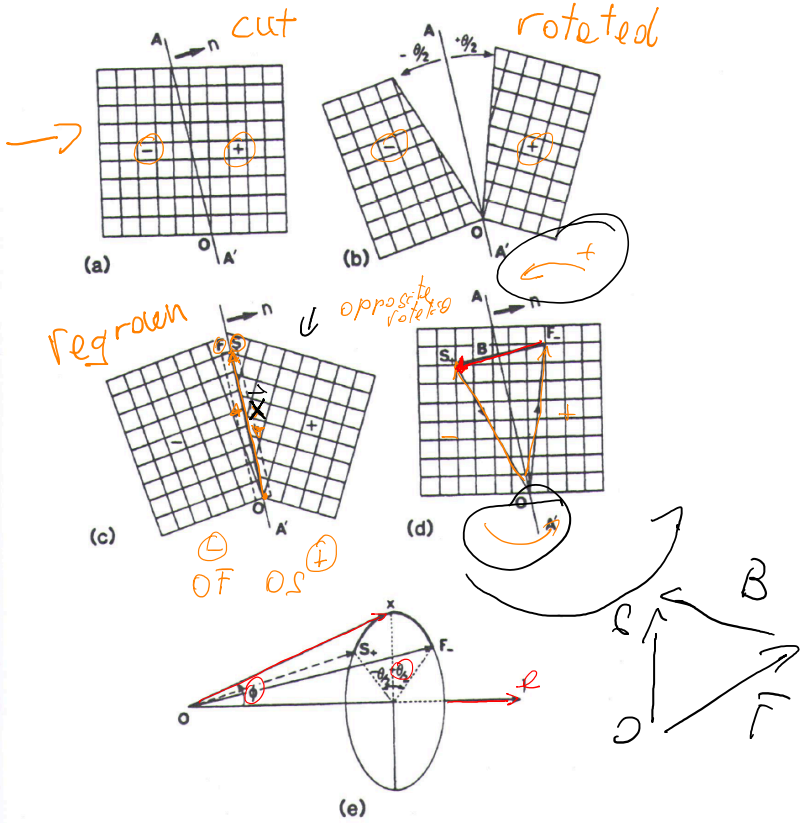



**Figure 13.15.** Illustration of the derivation of the net Burgers vector **B** crossing a vector **x** in a planar grain boundary *AA'* with unit normal **n**, where lattice + is rotated with respect to lattice − by an angle θ in a right-handed sense about an axis **l** directed into the plane of the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

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

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

Frank



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# O-Lattice Description of a Generic Grain Boundary

$$\vec{B} = \vec{OS} - \vec{OF} = R^{+}\vec{X} - R^{-}\vec{X} = (R^{+} - R^{-})\vec{X}$$

$$= \vec{OS} - \vec{OF} = I\vec{X} - R\vec{X} = (I - R)\vec{X}$$

homoplane

etoroplane $R \rightarrow A$

$$\vec{B} = (I - R)\vec{X} \leftarrow$$

$$\frac{\vec{B}}{\vec{X}} = (I - A)$$

# O-Lattice Description of a Generic Grain Boundary

for a green lattice point

there will be a $\vec{x}_2$ that describes it on Lattice 2

there will be a $\vec{x}_1 + \vec{b}_L$ that describes it on Lattice 1

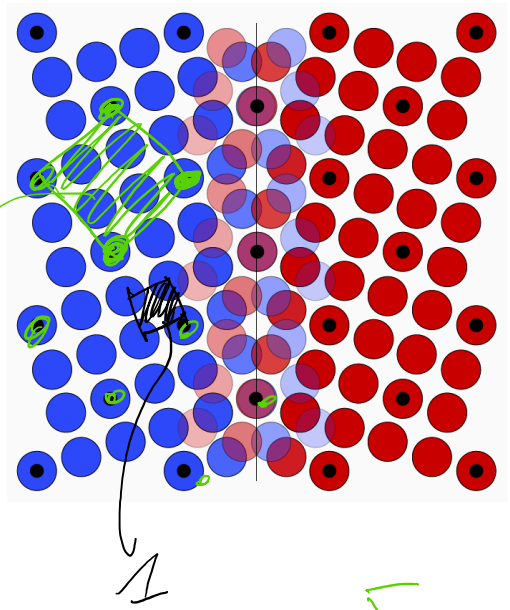
where $\vec{b}_L$ is an allowed translation in Lattice 1

$A\vec{x}_1 = \vec{x}_2 = \vec{x}_1 + \vec{b}_L \rightarrow \vec{b}_L = (I - A)\vec{x}_1$

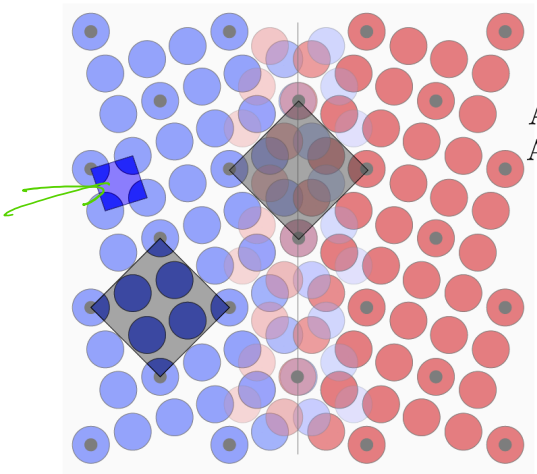
if A (transformation matrix A) $\vec{x}_2 = A\vec{x}_1$

O-lattice

# 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

$\boxed{\Sigma = 5}$

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

$$\Sigma = \frac{\#\text{ atoms in the coincidence U.C.}}{\#\text{ atoms in the primitive U.C.}}$$

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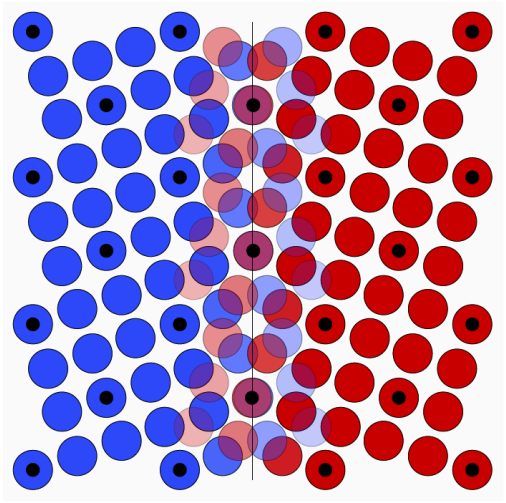
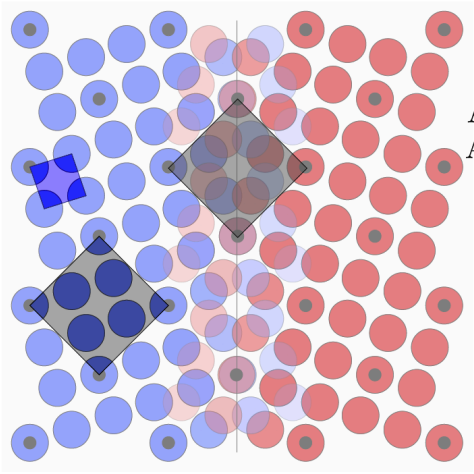


$sc$, $\mathbf{n} = (100)$,
$\mathbf{u} = \langle 001 \rangle$, $\theta = 36.9°$



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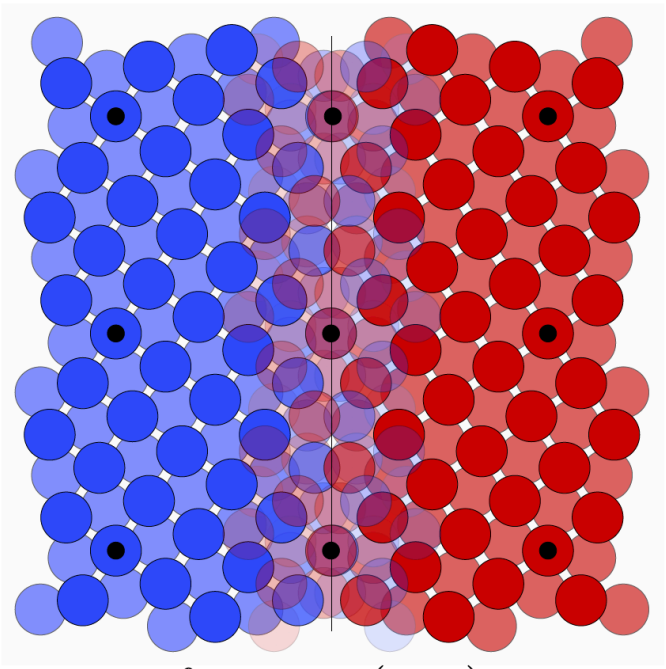
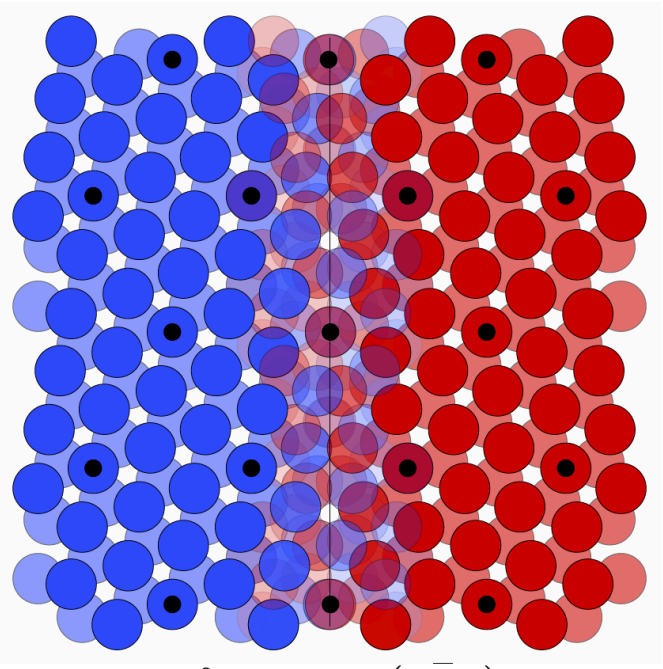


$fcc$, $\mathbf{n} = (100)$,
$\mathbf{u} = \langle 001 \rangle$, $\theta = 22.6°$

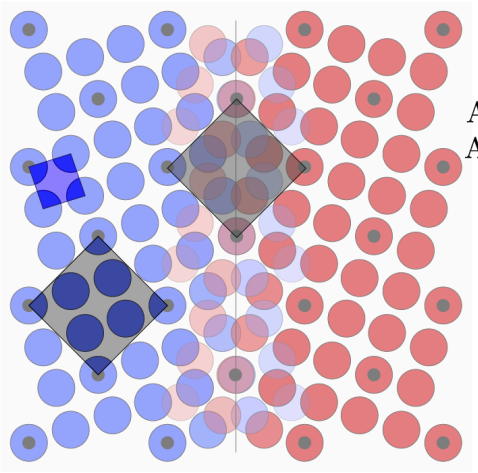
$\boxed{\Sigma = 13a}$



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

$\boxed{\Sigma = 7}$

# 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

atomically flat interfaces

≠ pure

generic interface that has no volume

# Conclusions

in isolated g. boundary

$\gamma_{gr} \propto$ # of dislocation

↳ amount of elastic energy