

Coherent and Semi-coherent Grain Boundaries

Lesson 10

MSE 304

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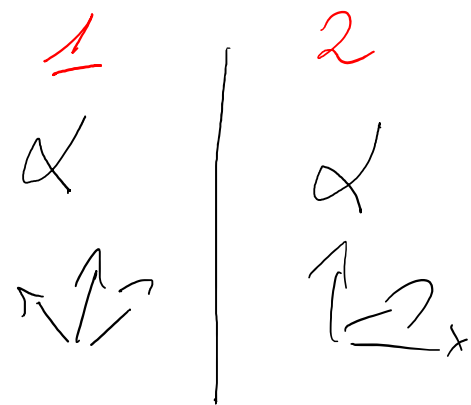
Reading for this Class

Chapter 13 Howe book

misfit dislocations $\rightarrow +14$

Homophase Interfaces (Grain Boundaries)

Homop. Interfaces $\leftrightarrow$ homophase G. Bound.



homophase
1 and 2 have
the same:

- composition
- Bravais lattices

$\Rightarrow$ primitive cell

Key Topics in the Previous Class

$$\gamma_{ss} \sim \underbrace{\sum_{\text{b}} E_{bb}}_{L, \text{ small}} + E_e$$

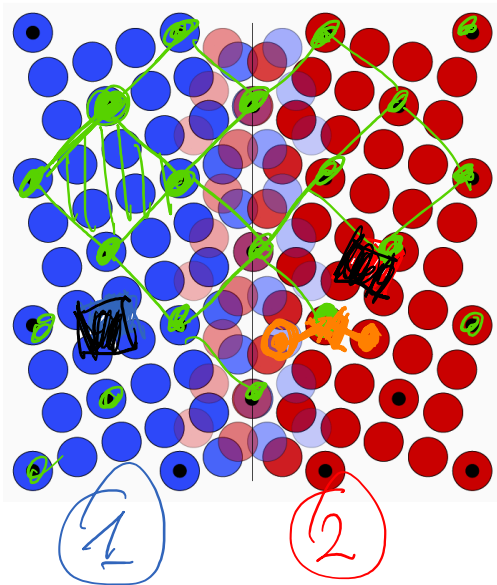
of broken bond
small compared to # of
interface atoms

homophase interface:

- 1) crystallographically describe the interface
- 2) determine the # broken bonds (# of dislocations)

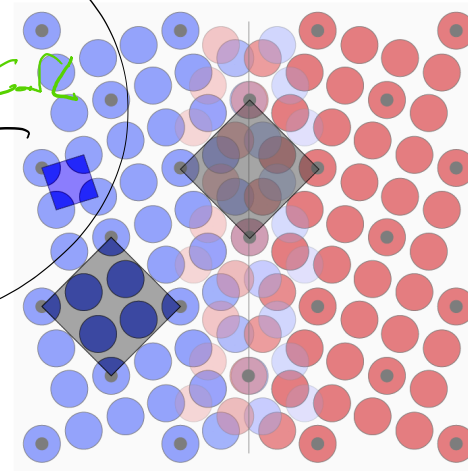
symmetric tilt g.b.
 $\theta = \frac{b}{L}$
 O-lattice
 Frank B

Coincidence Lattice Description of a Generic Grain Boundaries



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

$$\Sigma = \frac{\# \text{ p.c. C.L.}}{\# \text{ P.C.}}$$



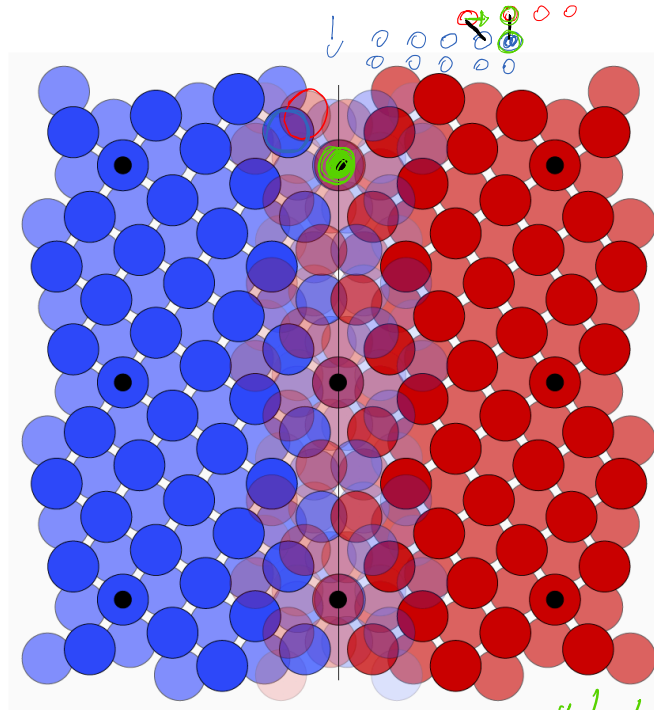
Atoms per unit cell: 1
 Atoms per CSL cell: 5

$$\Sigma = 5$$

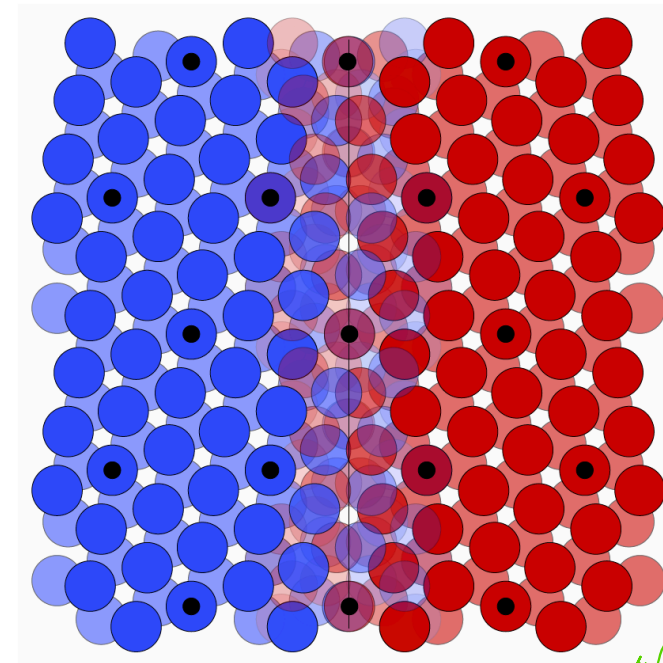
$sc, \mathbf{n} = (100),$
 $\mathbf{u} = \langle 001 \rangle, \theta = 36.9^\circ$

Coincidence Lattice Description of a Generic Grain Boundaries

$$\begin{aligned} \mathcal{K} &= 3 \\ \gamma &= 2 \\ g + l &= 12 \end{aligned}$$



$$\begin{aligned} \text{fcc, } \mathbf{n} &= (100), \quad \mathcal{K} = 1 \\ \mathbf{u} &= \langle 001 \rangle, \quad \theta = 22.6^\circ \\ \Sigma &= 13a \end{aligned}$$



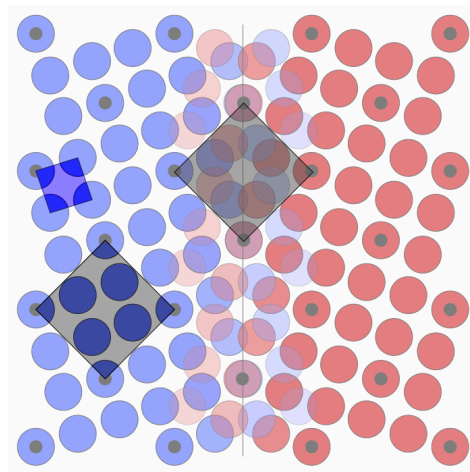
$$\begin{aligned} \text{fcc, } \mathbf{n} &= (1\bar{1}0), \quad \mathcal{K} = 3 \\ \mathbf{u} &= \langle 111 \rangle, \quad \theta = 38.21^\circ \\ \Sigma &= 7 \end{aligned}$$

$$\begin{aligned} \mathcal{K} &= 2 \\ \gamma &= 1 \\ \Sigma &= 7 \end{aligned}$$

CSL Selection Rules

x, y are integers

$$\Sigma = x^2 + Ny^2$$



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

$$\Sigma = 5$$

$$N=1$$

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

$$N = 1^2 + 0^2 + 0^2 = N = 1$$

$$N = u^2 + v^2 + w^2$$

$$\Sigma = 4 + 1 = 5$$

$$x = 2 \quad y = 1$$



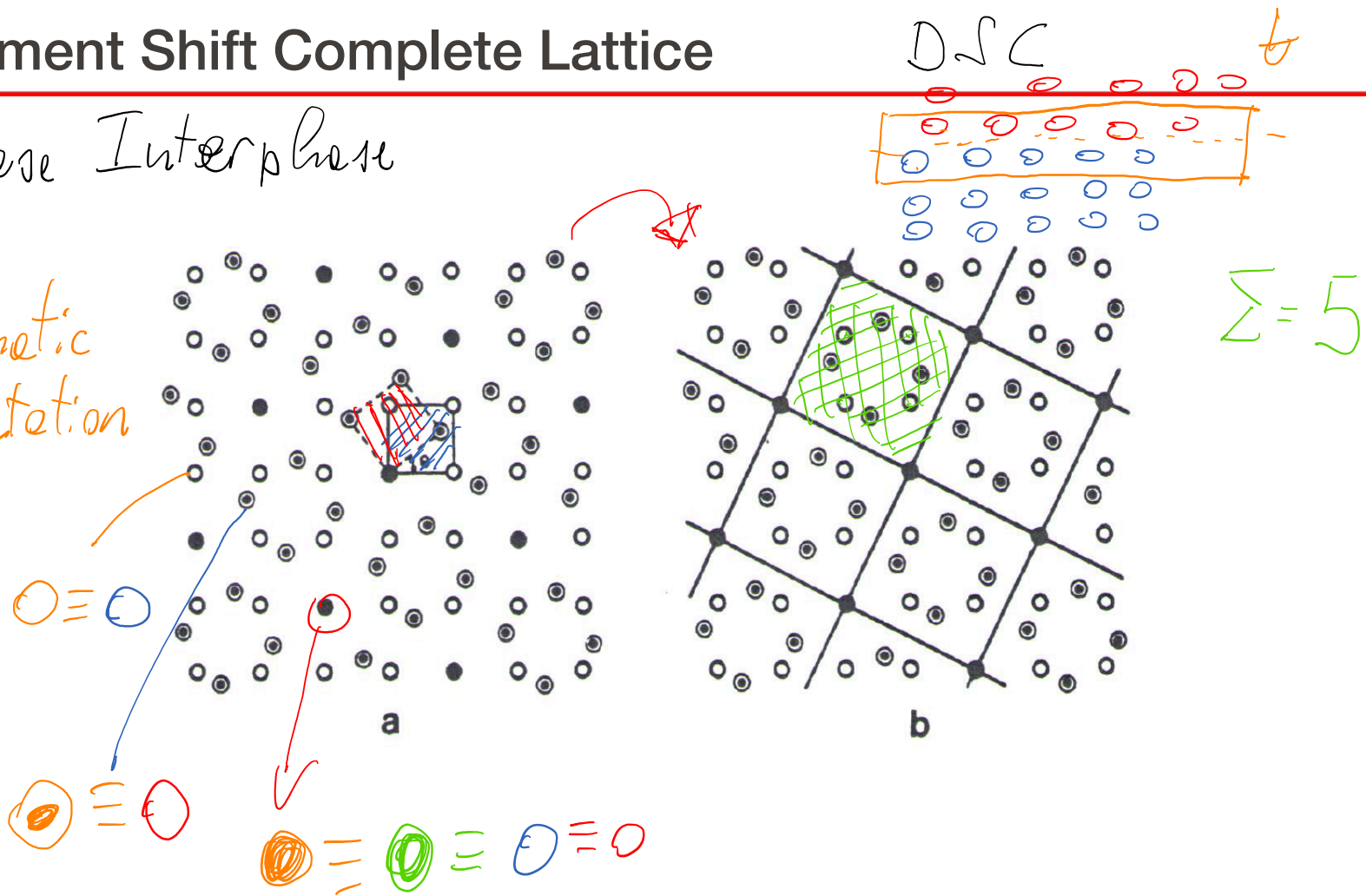
$$\theta = 2 \tan^{-1} \left(\frac{y}{x} \right) N^{\frac{1}{2}}$$

x, y, N

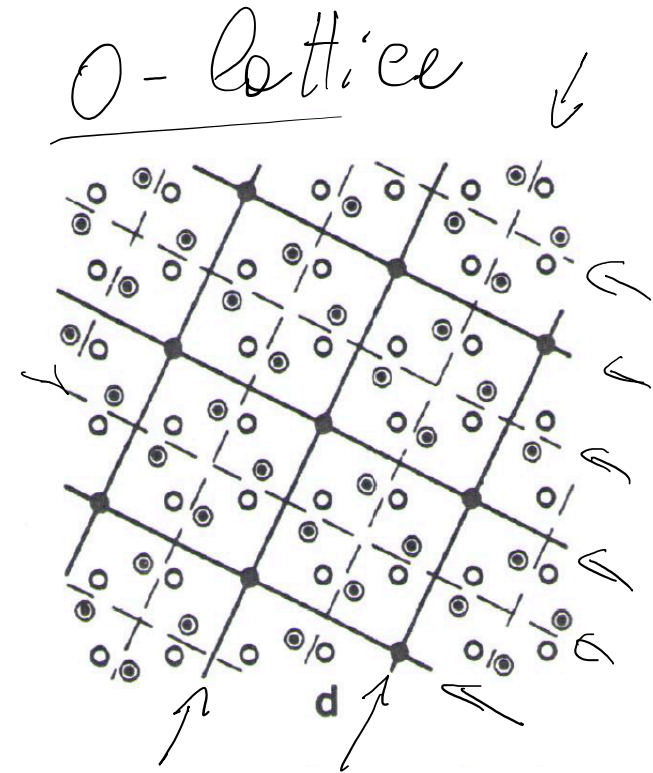
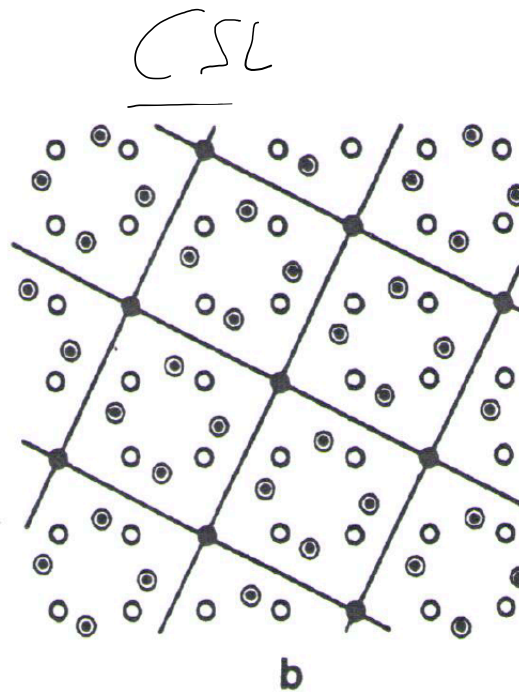
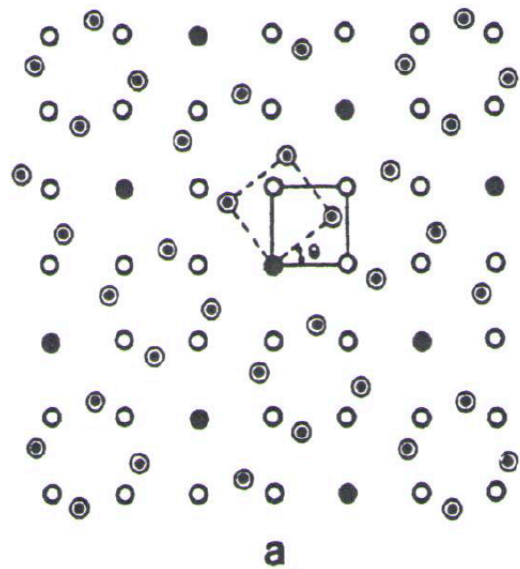
Displacement Shift Complete Lattice

Homophase Interphase

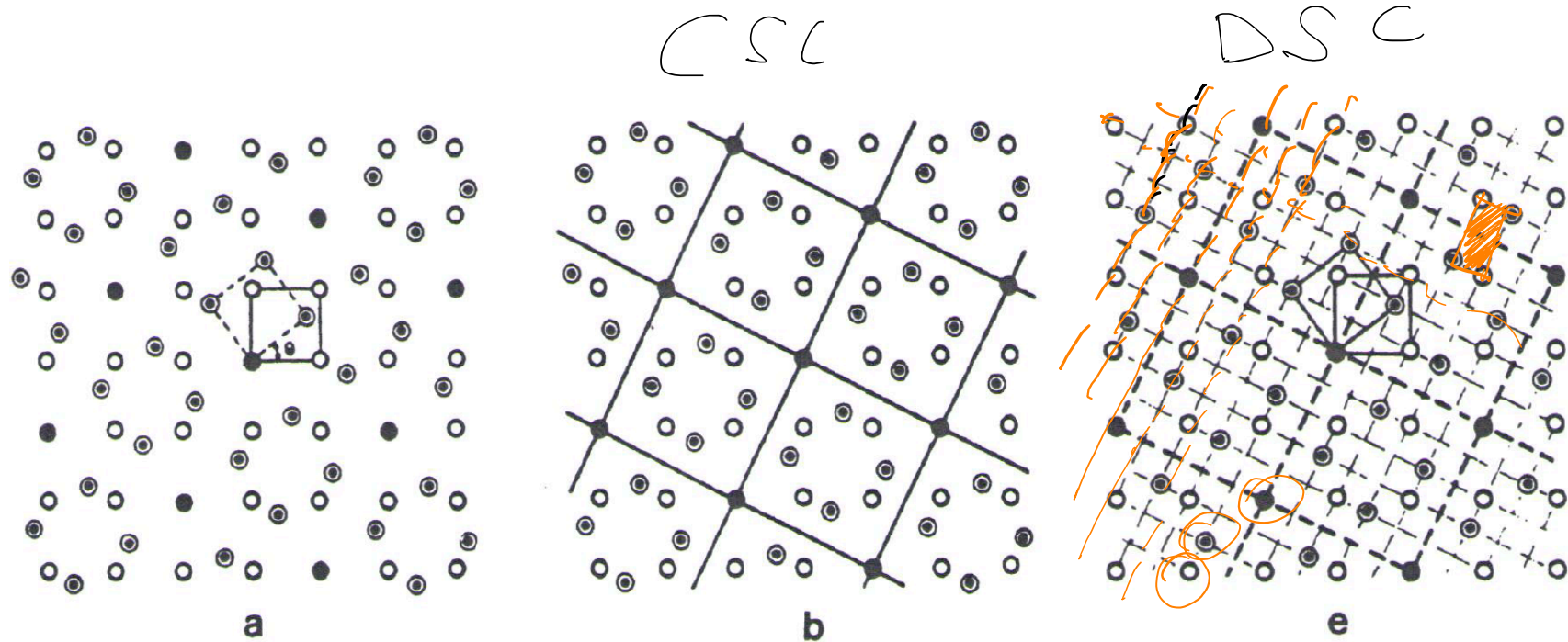
di chromatic
representation



Displacement Shift Complete Lattice

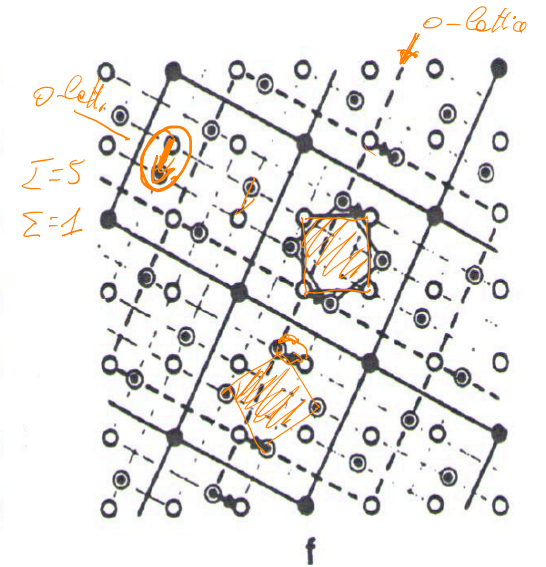
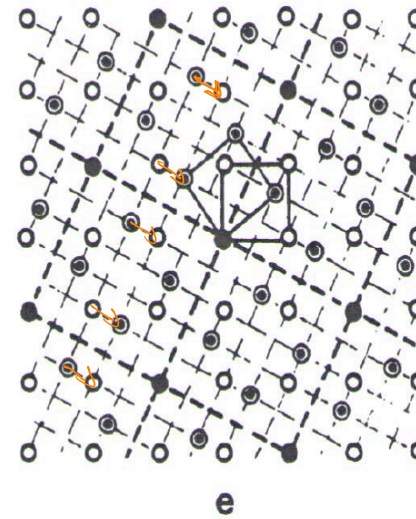
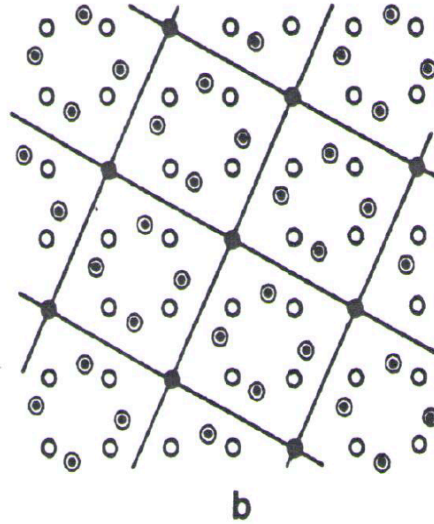
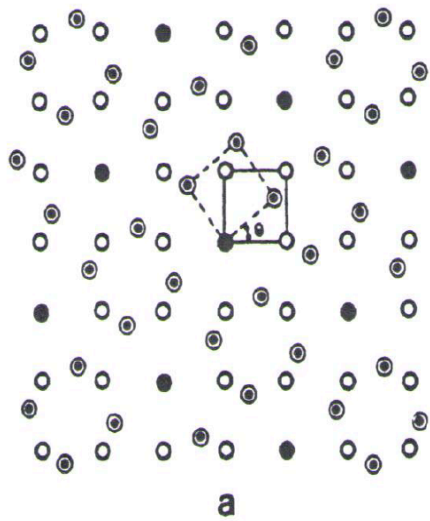


Displacement Shift Complete Lattice

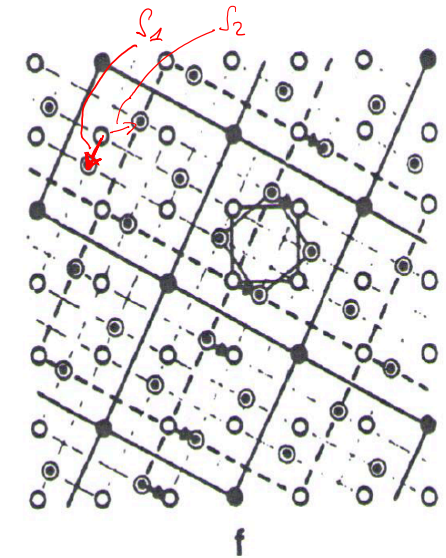
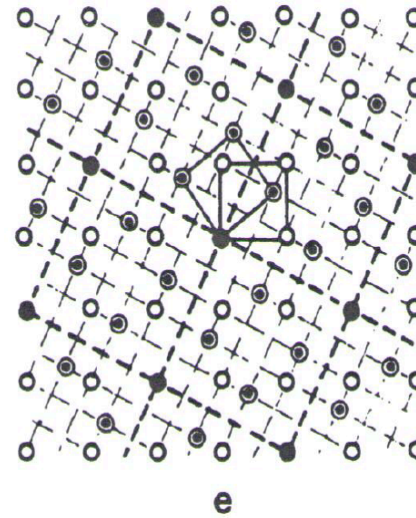
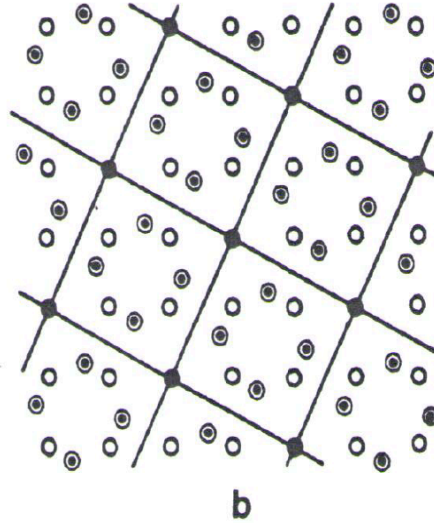
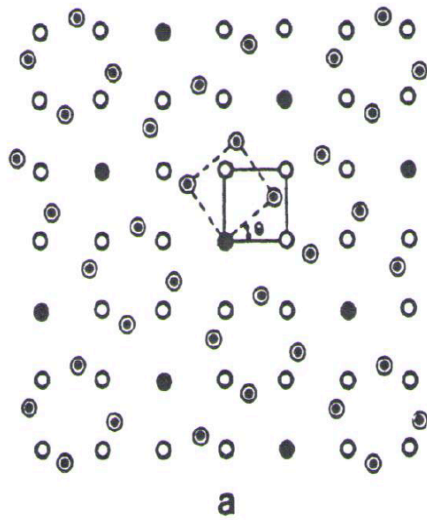


DSC is the lattice of the discomm. crystal

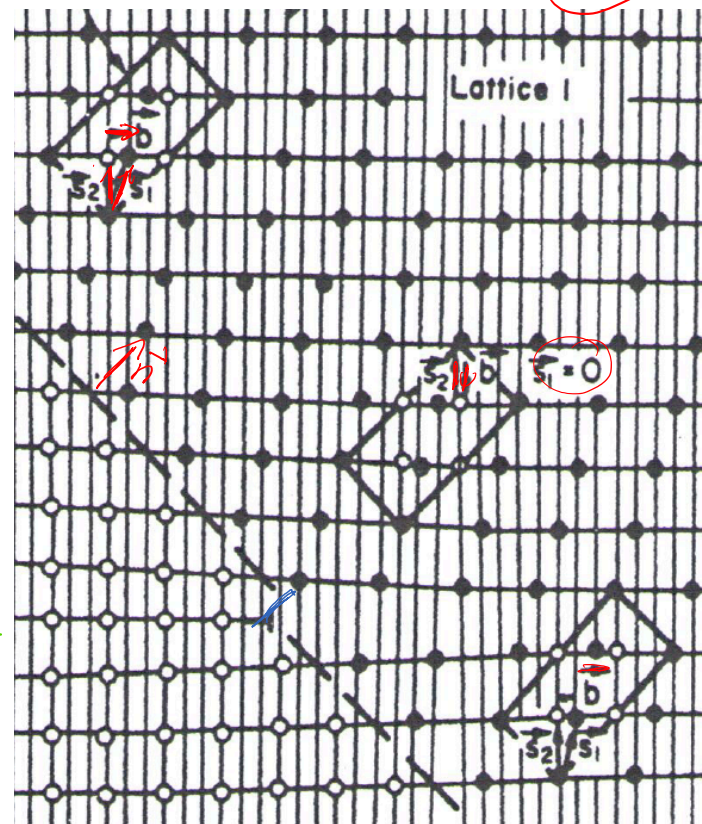
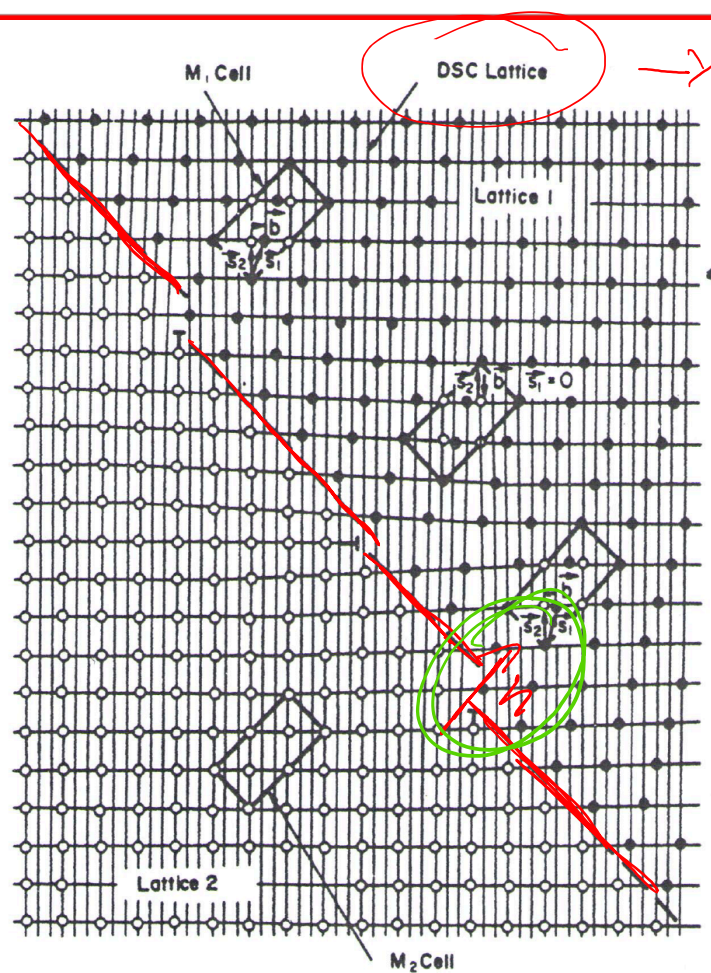
Displacement Shift Complete Lattice



Displacement Shift Complete Lattice



Defects at a Coherent Homophase Interface (CHI)



$$\vec{S}_1 \quad \vec{S}_2$$

$$\vec{b} = \vec{S}_1 - \vec{S}_2$$

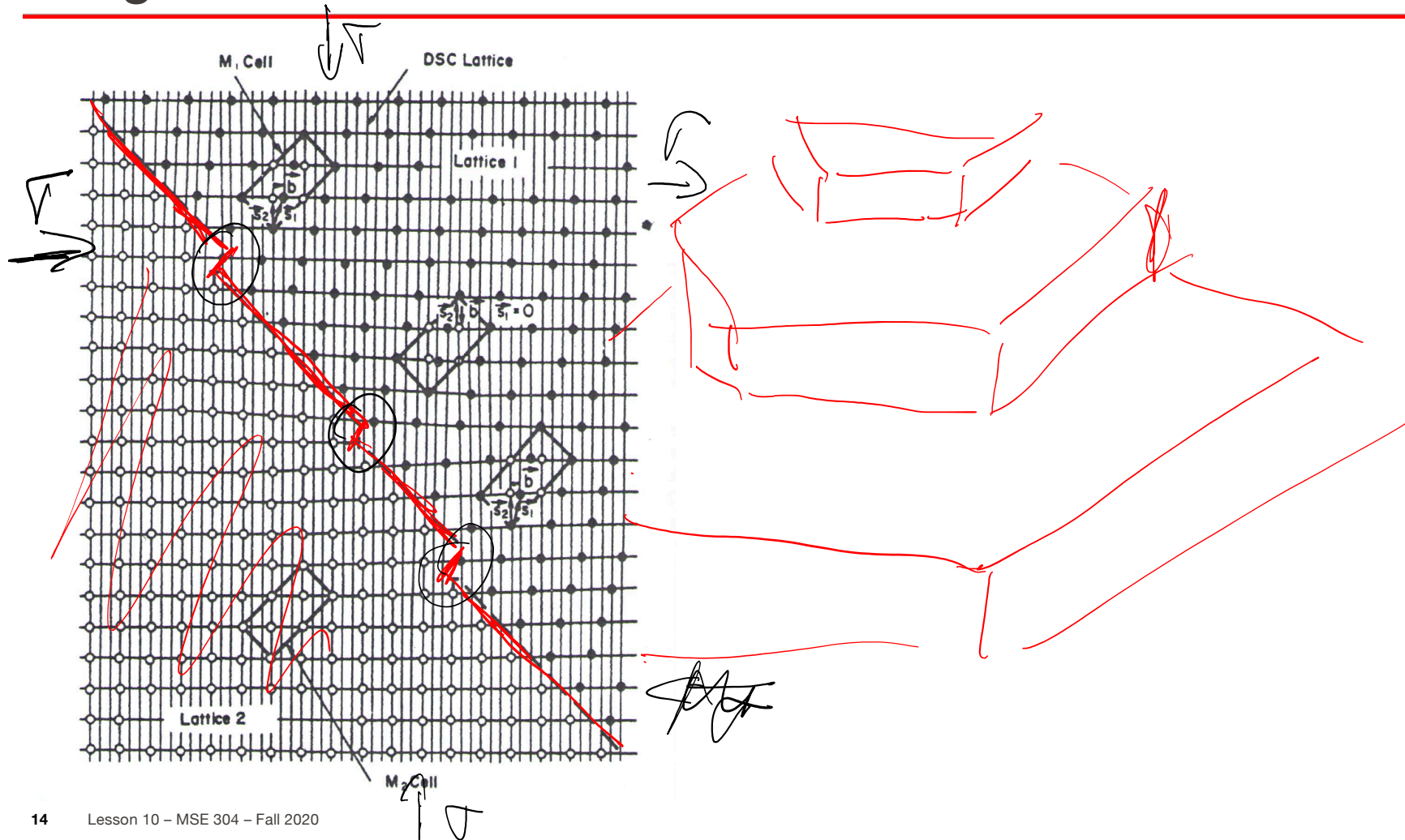
misfit

$\vec{b} \in \text{plane of the interface}$

$$\vec{S}_1 \cdot \vec{n} = \vec{S}_2 \cdot \vec{n}$$

$\perp$ plane of the interface

Ledges and Grain Boundaries



Misfit Dislocation in CHI

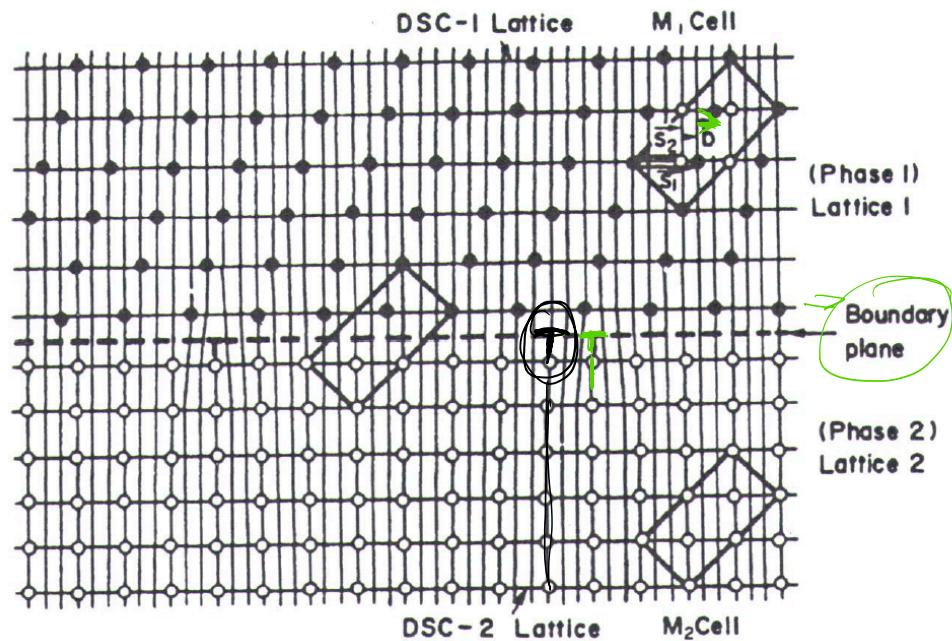


Figure 13.24. The interphase boundary between two different lattices (phases) M_1 and M_2 , which form a planar interface containing interfacial dislocations with a spacing determined by O-lattice theory. The Burgers vector and ledge vectors of the interfacial dislocations are shown in the diagram in the upper right. The DSC lattice is indicated by fine lines in the figure. Reprinted with permission from [53] by Elsevier Science Ltd., Oxford, England.

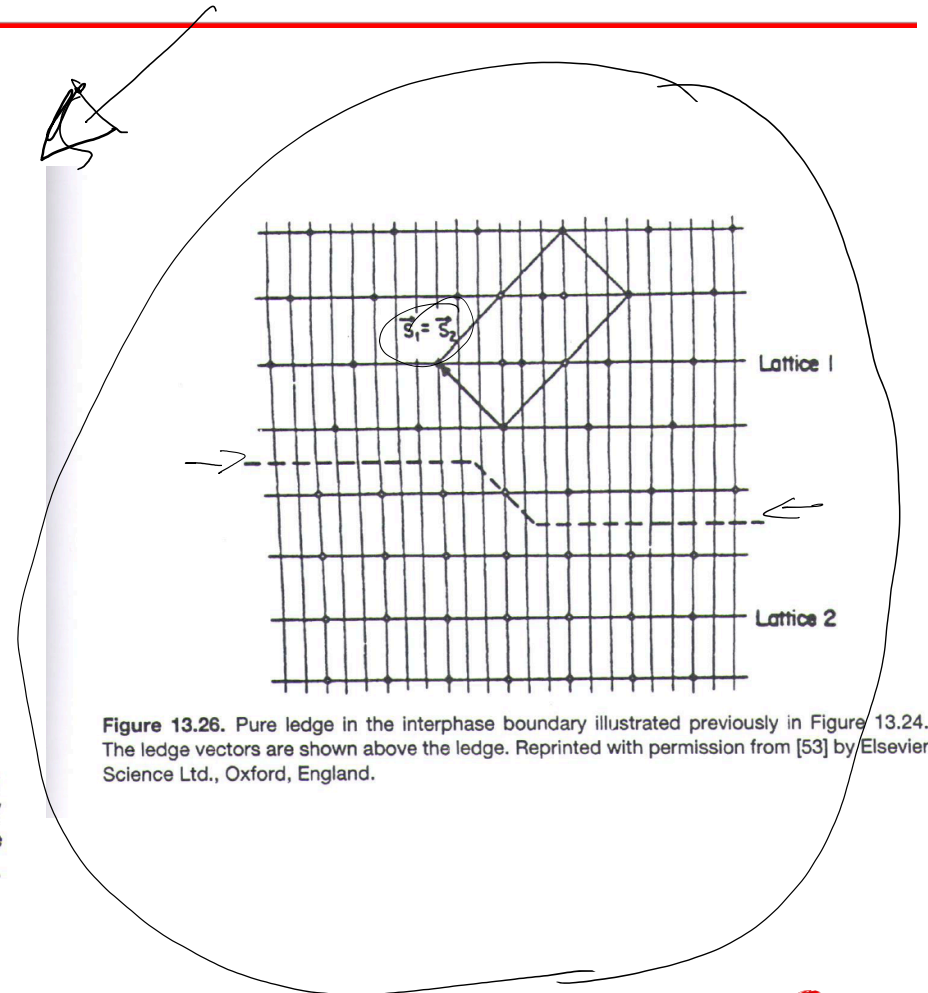


Figure 13.26. Pure ledge in the interphase boundary illustrated previously in Figure 13.24. The ledge vectors are shown above the ledge. Reprinted with permission from [53] by Elsevier Science Ltd., Oxford, England.

Misfit Dislocations in Semi-coherent Interfaces

α / β

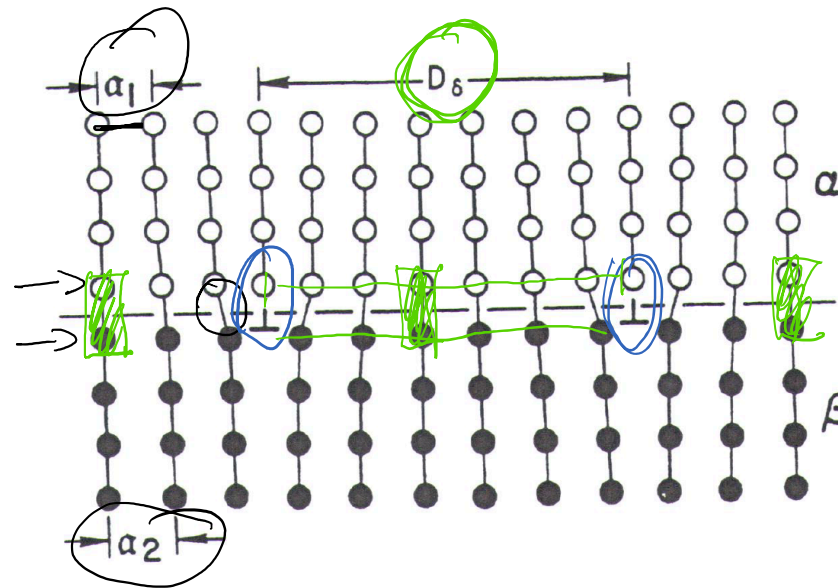
$$a_1 \neq a_2$$

same Bravais
lattice

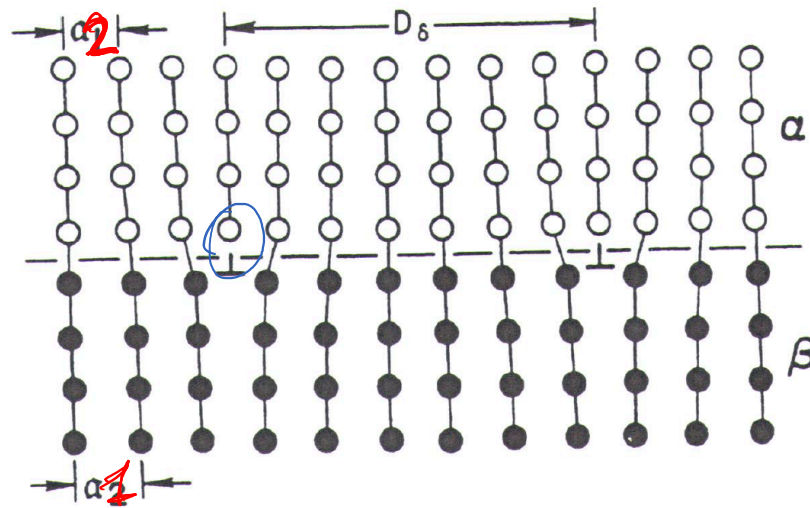
interface has
the same $\vec{n}$

but α and β

have at least 1 unit of the primitive cell
that is different



Misfit Dislocations in Semi-coherent Interfaces



$$D_\delta = n a_1 = (n+1) a_2$$

$$n = \frac{a_2}{a_1 - a_2}$$

$$a' = \frac{a_1 + a_2}{2}$$

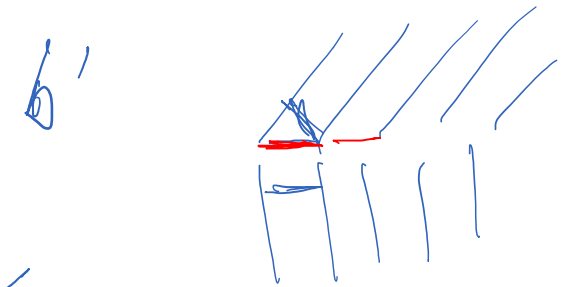
$$D_\delta = \left(n + \frac{1}{2}\right) a'$$

$$D_\delta = \frac{(a_1 + a_2)^2}{4(a_1 - a_2)}$$

$$\delta = \frac{2(a_1 - a_2)}{a_1 + a_2} = \frac{a_1 - a_2}{a'} = \frac{\Delta a}{\langle a \rangle}$$

$$D_\delta = \frac{a'}{\delta} = \frac{b}{\delta}$$

$Q' = \langle Q_1, Q_2 \rangle$

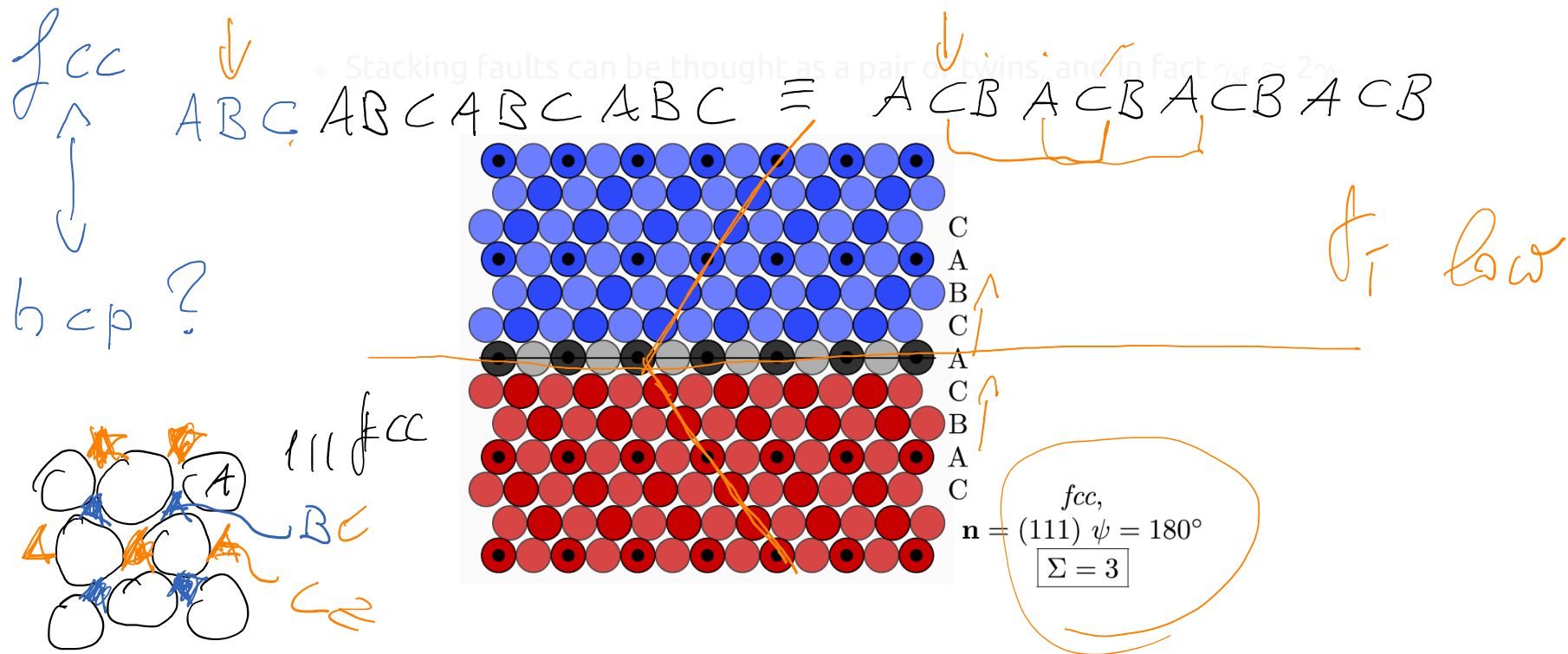


$[\%] \sim 100$ unit-less

$D_\delta = \frac{b}{\delta}$
symm. tilt boundary

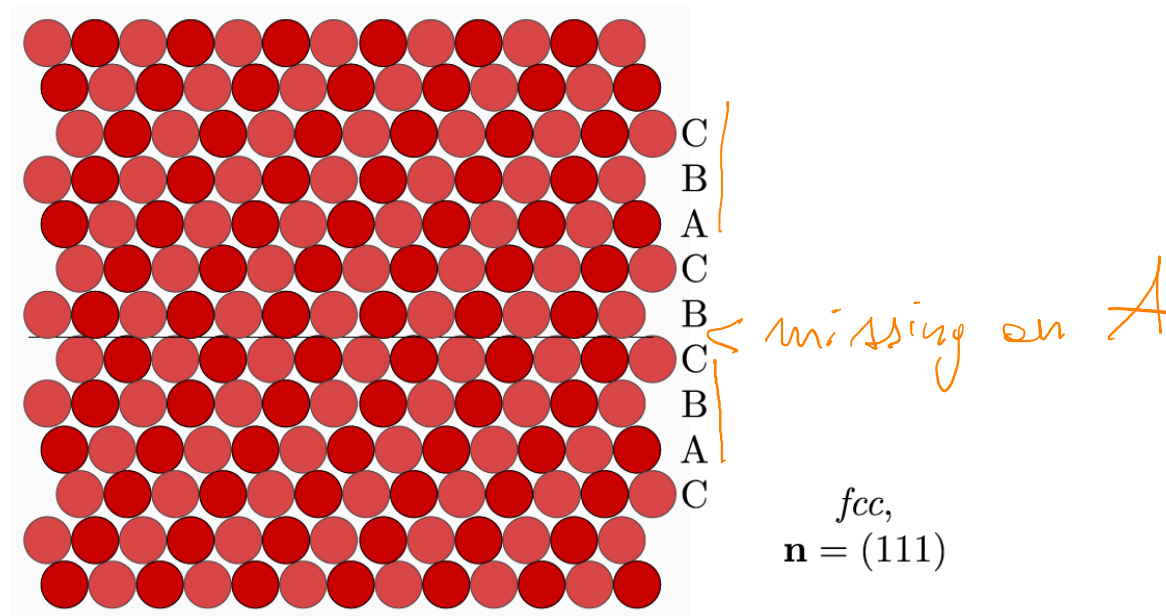
Twin Boundaries

- Close-packed *fcc* have very low-energy **twin** grain boundaries, that correspond to reversal of the ABCABC stacking order



Stacking Faults

- Twins are closely related to **stacking faults**, ABCBCAB or ABCBABC



Stacking Faults and Twin Boundaries

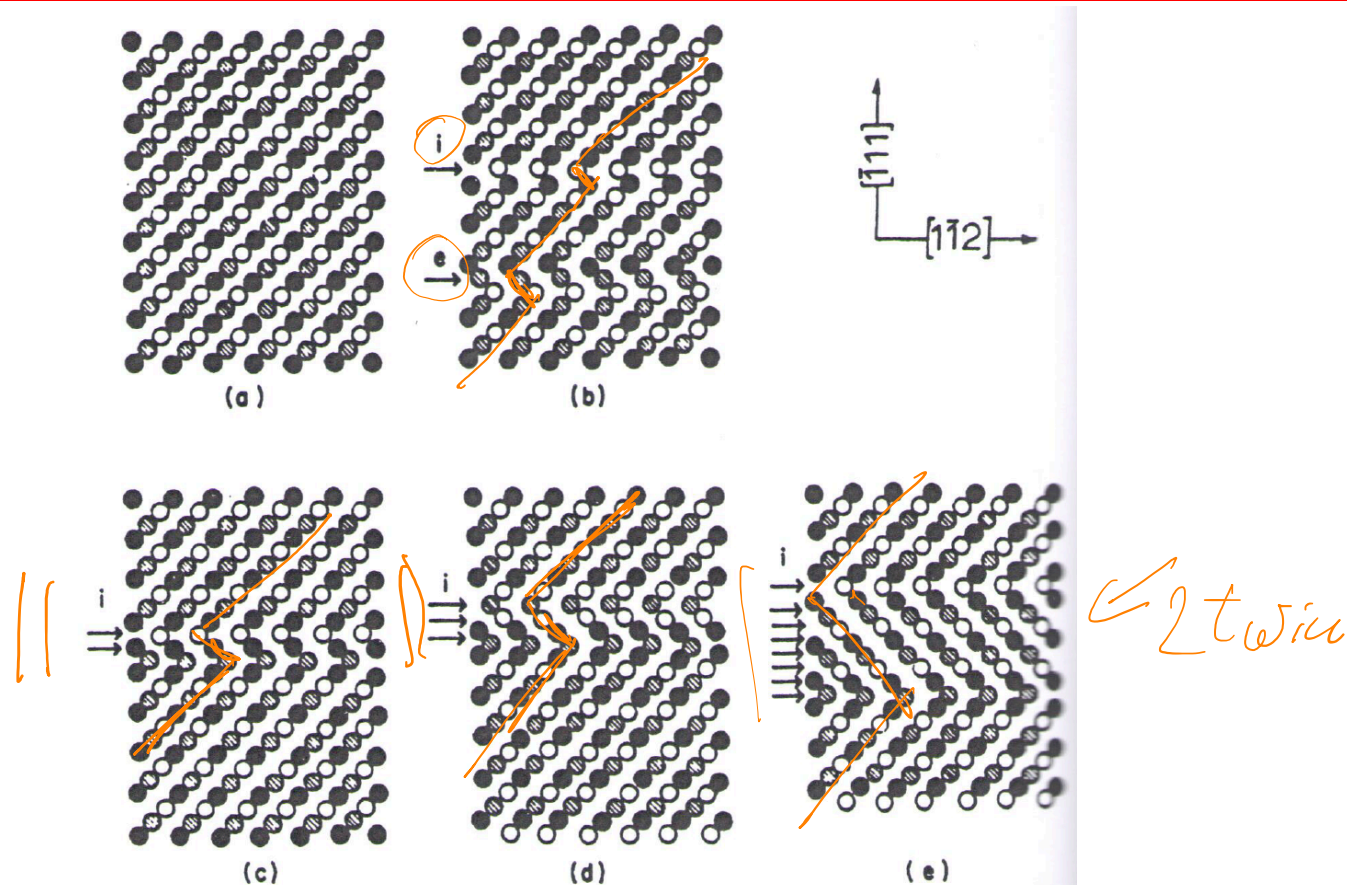
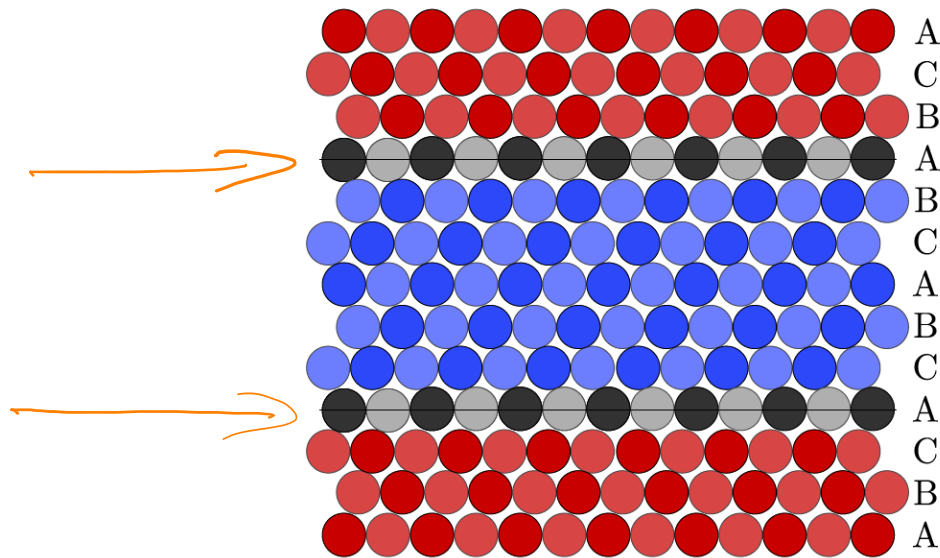


Figure 13.34. Idealized view of stacking faults and their development from perfect crystal in (a) to an n -layer twin in (e) in the close-packed f.c.c. structure. The viewing direction is along $[110]$. From [24].

Stacking Faults

- Twins are closely related to **stacking faults**, ABCBCAB or ABCBABC
- Stacking faults can be thought as a pair of twins, and in fact $\gamma_{sf} \approx 2\gamma_t$



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

Stacking Faults and Twin Boundaries

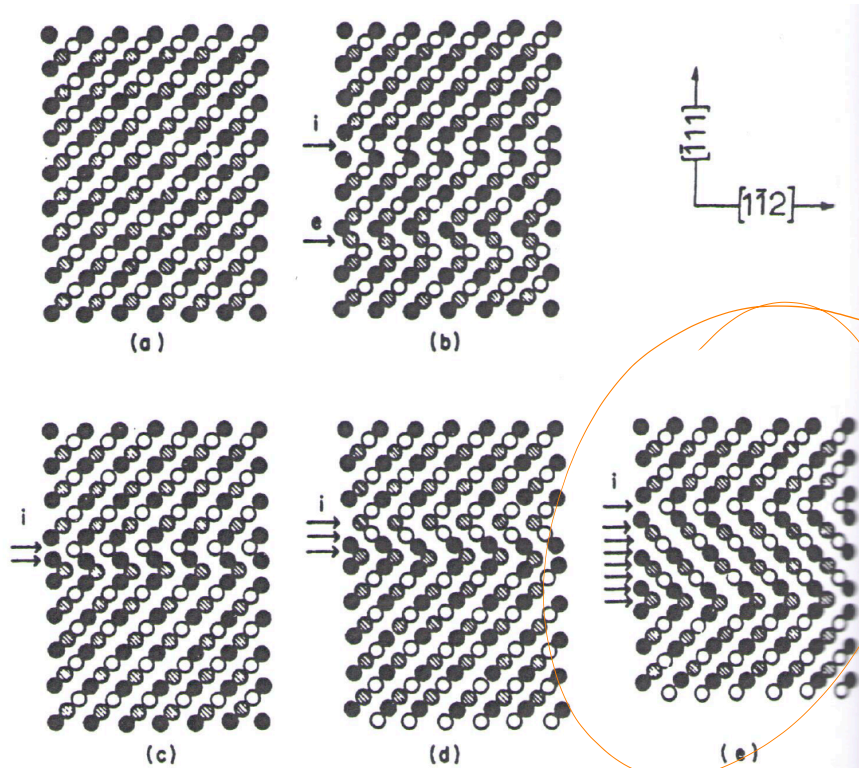


Figure 13.34. Idealized view of stacking faults and their development from perfect crystal in (a) to an n -layer twin in (e) in the close-packed f.c.c. structure. The viewing direction is along $[110]$. From [24].

$$\gamma_t = \sum [2n\phi_{3n} + n(\phi_{3n-1} + \phi_{3n+1})] \\ = \phi_2 + 2\phi_3 + \phi_4 + \dots, \quad (13.31)$$

$$\gamma_{esf} = \sum [2\phi_{3n-1} + (3n+1)\phi_{3n} + 3n\phi_{3n+1}] \\ = 2\phi_2 + 4\phi_3 + 3\phi_4 + \dots, \quad (13.32)$$

$$\gamma_{isf} = \sum [(3n-1)\phi_{3n-1} + 3n\phi_{3n}] \\ = 2\phi_2 + 3\phi_3 + 0\phi_4 + \dots, \quad (13.33)$$

$$\gamma_{hcp} = \sum [\Psi_{6n-2} + \Psi_{6n-3} + \Psi_{6n-4}] \\ = \phi_2 + \phi_3 + \phi_4 + \dots \quad (13.34)$$

Roughening at Domain Boundaries

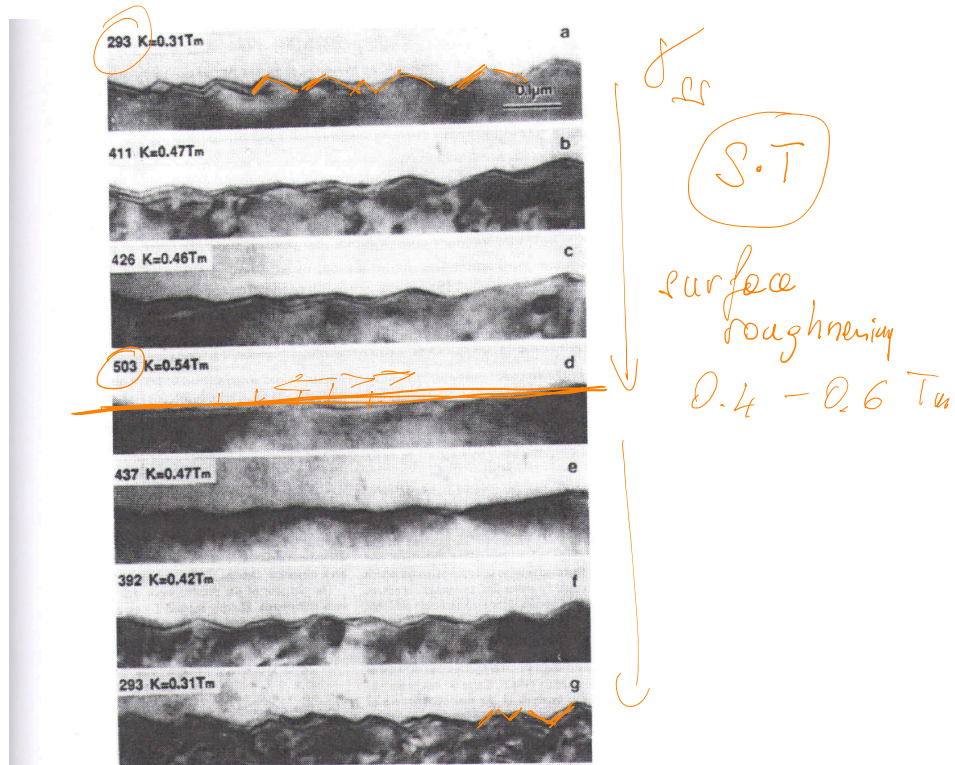


Figure 13.35. Reversible roughening-faceting transformation of an initially faceted $\Sigma = 3$ asymmetric $\langle 111 \rangle$ tilt boundary containing $\{112\}_1/\{112\}_2$ facets in aluminum as a function of step-wise heating (a-d) and subsequent cooling (d-g). Time at each temperature ≈ 30 min. Reprinted with permission from [75] by Elsevier Science Ltd., Oxford, England.

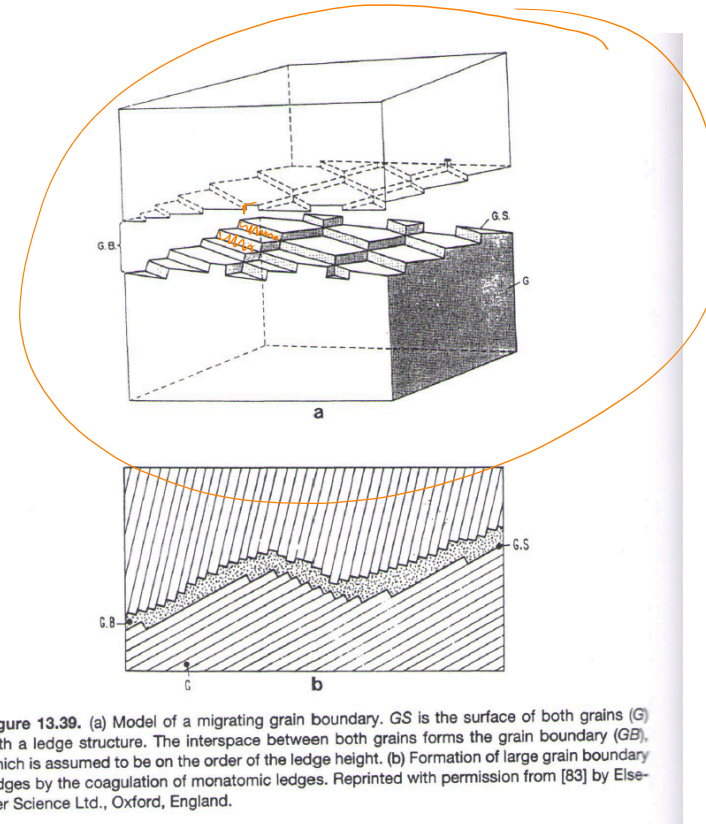
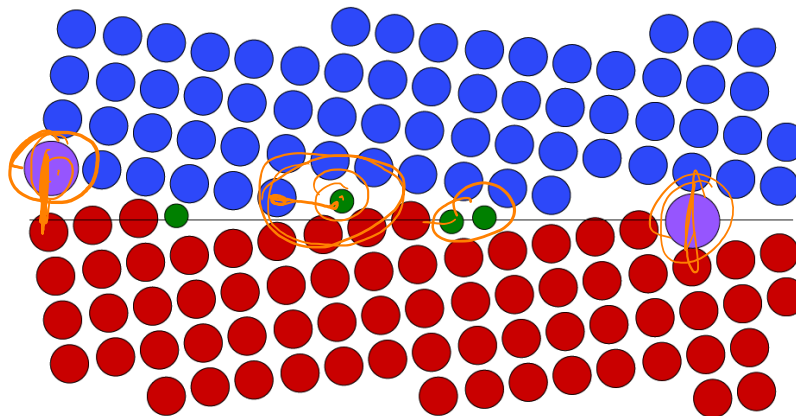


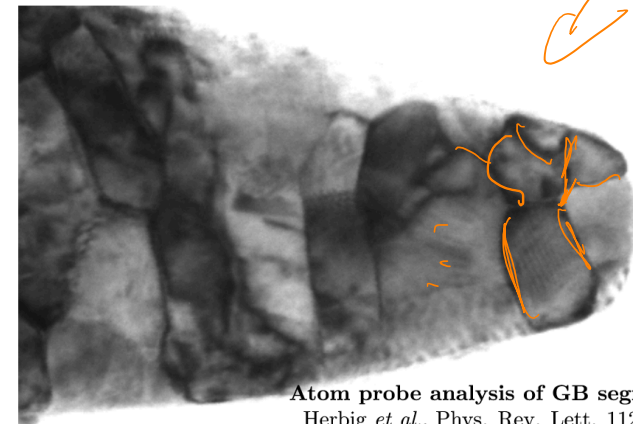
Figure 13.39. (a) Model of a migrating grain boundary. GS is the surface of both grains (G) with a ledge structure. The interspace between both grains forms the grain boundary (GB), which is assumed to be on the order of the ledge height. (b) Formation of large grain boundary ledges by the coagulation of monatomic ledges. Reprinted with permission from [83] by Elsevier Science Ltd., Oxford, England.

Segregation at Domain Boundaries

- 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}



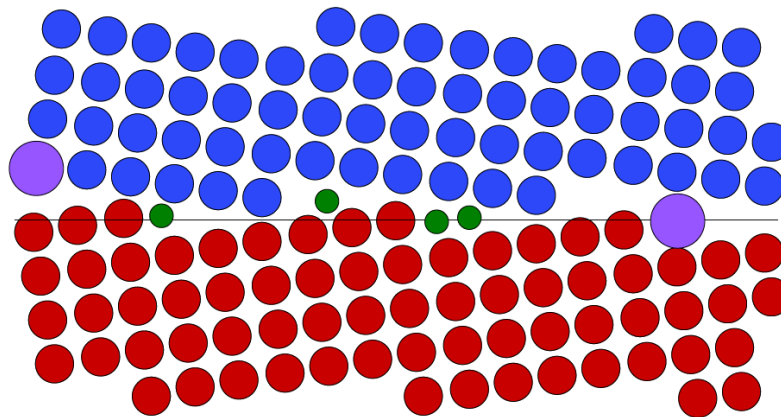
$$sc, \mathbf{u} = \langle 001 \rangle, \\ \mathbf{n} = (100), \quad \theta = 18^\circ$$



Atom probe analysis of GB segregation
Herbig *et al.*, Phys. Rev. Lett. 112 (2014)
Li *et al.*, Phys. Rev. Lett. 113 (2014)

Segregation at Domain Boundaries

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

$$\frac{X_{gb}}{1 - X_{gb}} = \frac{X_B}{X_B^{sat}} \exp \frac{-\Delta G'}{RT}, \quad (13.40)$$

$$\beta_{gb} = \frac{1}{X_B^{sat}} \exp \frac{-\Delta G'}{RT}. \quad (13.42)$$

Conclusions

DSC $\rightarrow$ dichromatic interface
lattice

$\vec{s}_1, \vec{s}_2 \rightarrow \vec{b}$

twin boundaries ; stacking faults

grain boundary accumulation
of defects