2009 fall

Phase Transformation of Materials

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Contents for previous class

- Boundaries in Single-Phase Solids

  (a) Low-Angle and High-Angle Boundaries

  (b) Special High-Angle Grain Boundaries

  (c) Equilibrium in Polycrystalline Materials

- Thermally Activated Migration of Grain Boundaries

  - Grain coarsening at high T, annealing due to metastable equilibrium of grain boundary

- The Kinetics of Grain Growth

  - Grain boundary migration by thermally activated atomic jump

  - mobility of grain boundary ~ grain boundary segregation

- Grain Growth

  - Normal grain growth ⟺ Abnormal grain growth

  Effect of second-phase particle - Zener Pinning

$$\bar{D}_{max} = \frac{4r}{3f_v}$$

Contents for today's class

- **Interphase Interfaces in Solid (α/β)**

  - Second-Phase Shape: Interface Energy Effects

  - Second-Phase Shape: Misfit Strain Effects

  - Coherency Loss

  - Glissil Interfaces

  - Solid/Liquid Interfaces

- **Interphase migration**

  - Diffusion controlled and Interface controlled growth

3.4 Interphase Interfaces in Solids

Interphase boundary
- different two phases : different crystal structure
different composition

{ **coherent,** **semicoherent** **incoherent**

3.4.1 Coherent interfaces

Perfect atomic matching at interface

화학적인 것은 무시한 채 계면에서 양쪽 상이 같은 원자배열을 갖고, 두 결정이 특정한 방위를 이루고 있는 경우

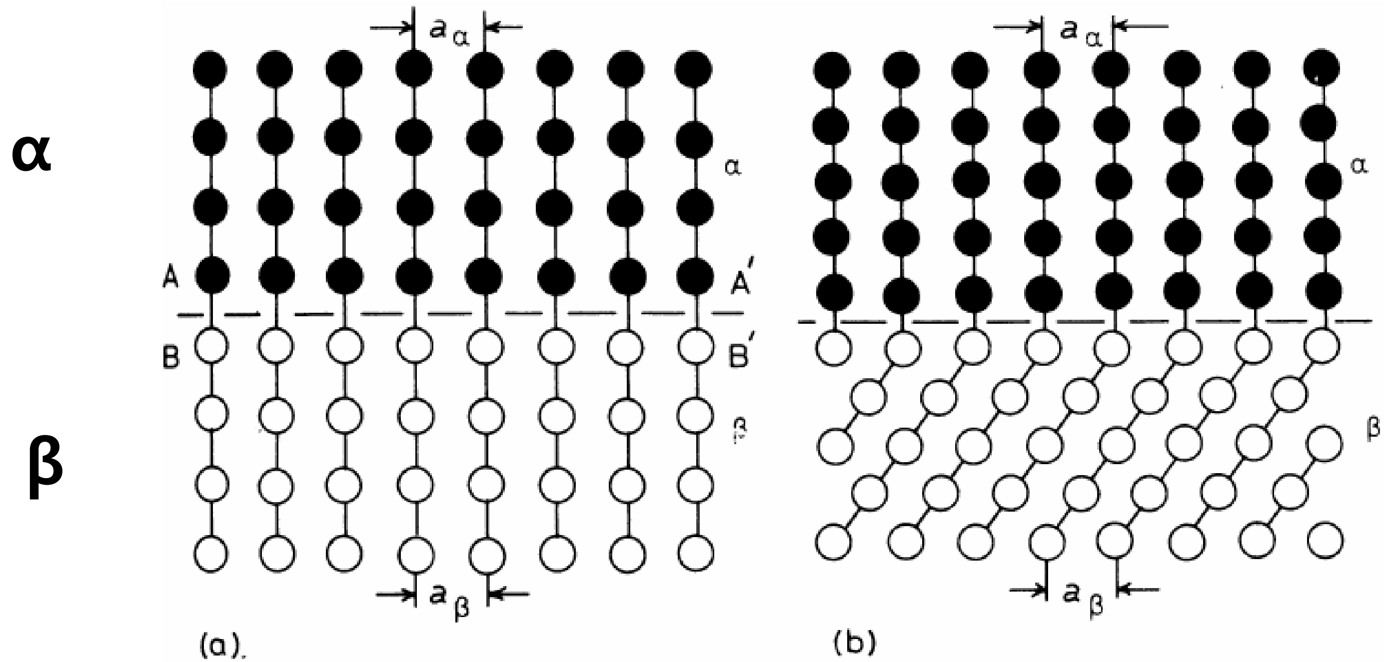


Fig. 3.32 Strain-free coherent interfaces. (a) Each crystal has a different chemical composition but the same crystal structure. (b) The two phases have different lattices.

3.4.1 Coherent interfaces

Which plane and direction will be coherent between FCC and HCP?

: **Interphase interface will make lowest energy and thereby the lowest nucleation barrier**

ex) hcp silicon-rich κ phase in fcc copper-rich α matrix of Cu-Si alloy

→ the same atomic configuration

원자간 거리도 동일

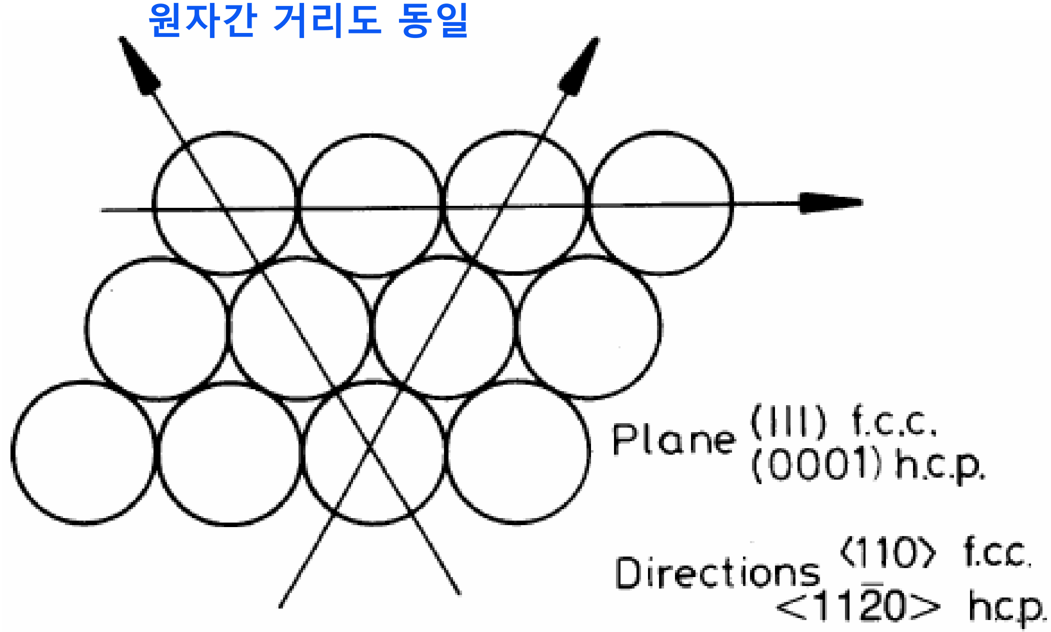


Fig. 3.33 The close-packed plane and directions in fcc and hcp structures.

hcp/ fcc 계면의 경우: 정합을 이루는 면은 하나만 존재

→ Orientation relation

$$(111)_\alpha // (0001)_\kappa$$

$$[\bar{1}10]_\alpha // [11\bar{2}0]_\kappa$$

$\gamma_{\alpha\text{-}\kappa}$ of Cu-Si ~ 1 mJM^{-2}

In general,

γ (coherent) ~ 200 mJM^{-2}

$$\gamma_{coherent} = \gamma_{structure} + \gamma_{chemical}$$

$$= \gamma_{chemical}$$

γ (coherent) = γ_{ch}

When the atomic spacing in the interface is not identical between the adjacent phase, what would happen?

Lattice가 같지 않아도 Coherent interface를 만들 수 있다.

→ lattice distortion

→ Coherency strain

→ strain energy

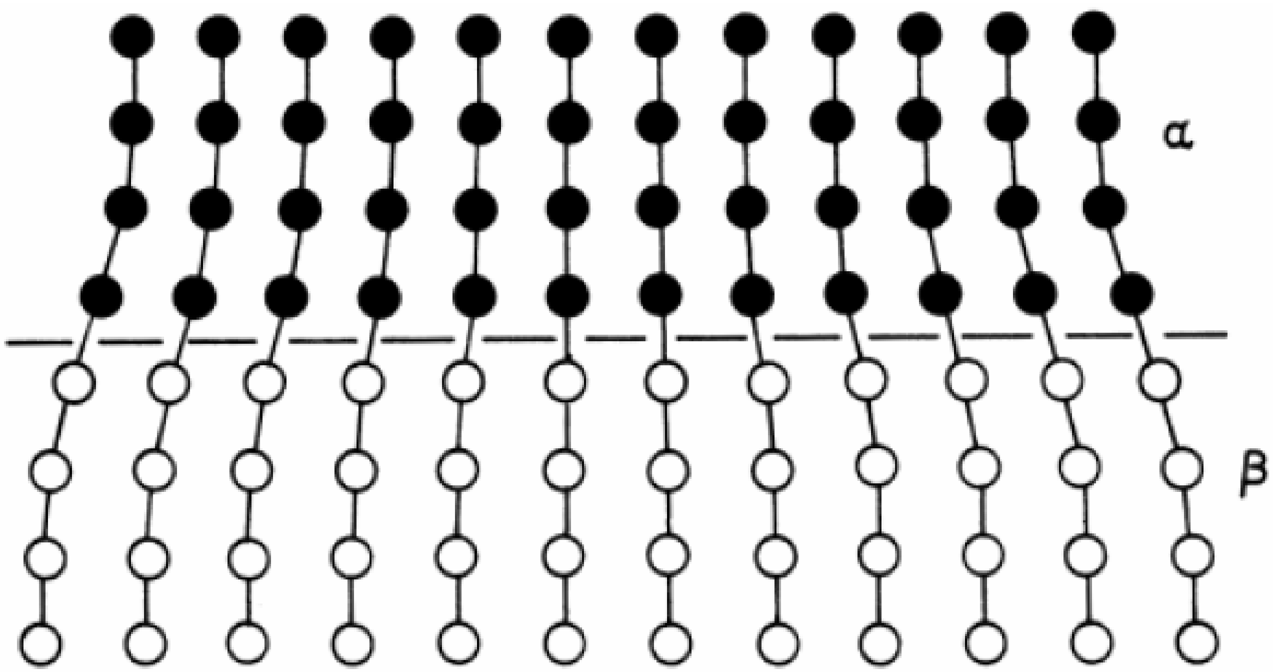


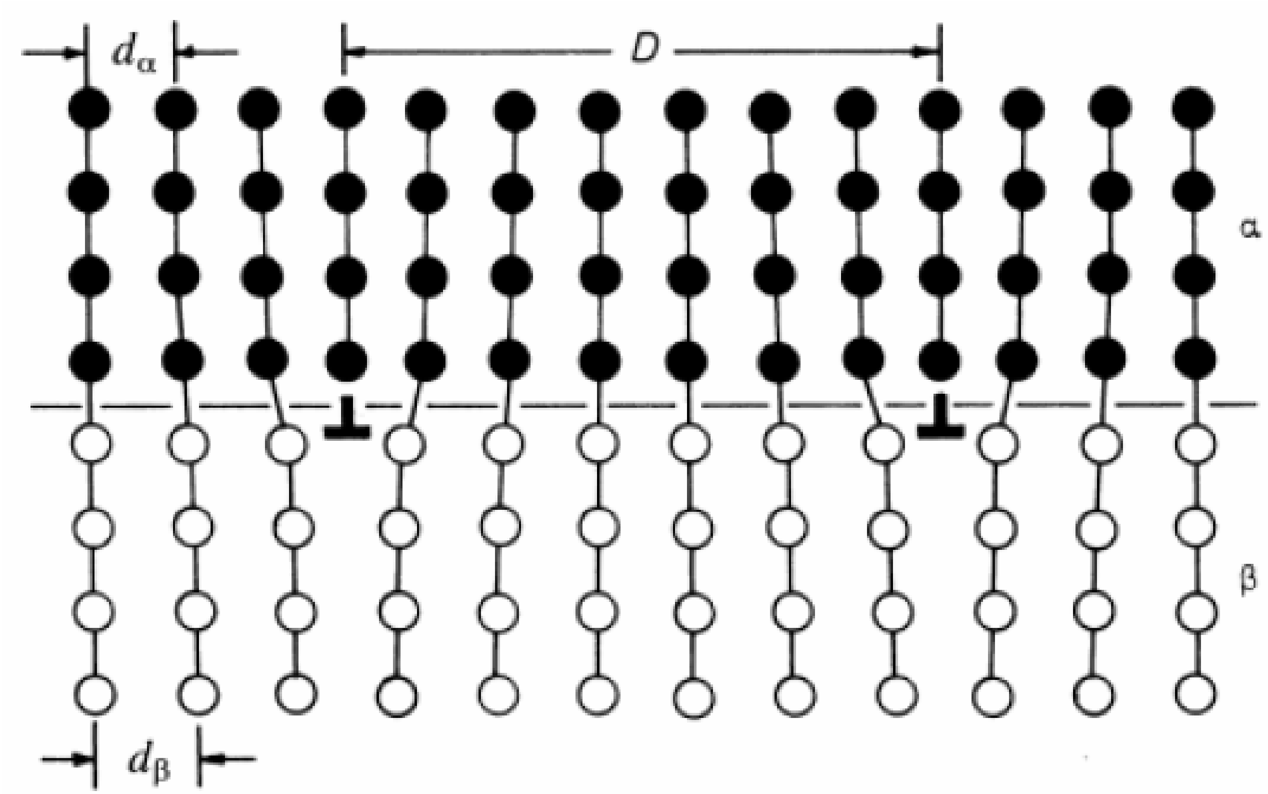
Fig. 3.34 A coherent interface with slight mismatch leads to coherency strains in the adjoining lattices.

정합 계면에서 형성된 strain은 계의 총 에너지를 증가시킴.

How can this coherent strain can be reduced?

If coherency strain energy is sufficiently large, → "misfit dislocations"

→ semi-coherent interface



$$\delta = \frac{d_\beta - d_\alpha}{d_\alpha}$$

δ가 작다면,

$$D = \frac{b}{\delta}$$

δ: misfit (disregistry)

b: Burgers vector of disl.

[$b=(d_\alpha + d_\beta)/2$]

Fig. 3.35 A semicoherent interface. The misfit parallel to the interface is accommodated by a series of edge dislocations.

(2) Semicoherent interfaces

$$\gamma(semicoherent) = \gamma_{ch} + \gamma_{st}$$

$d_\alpha < d_\beta$

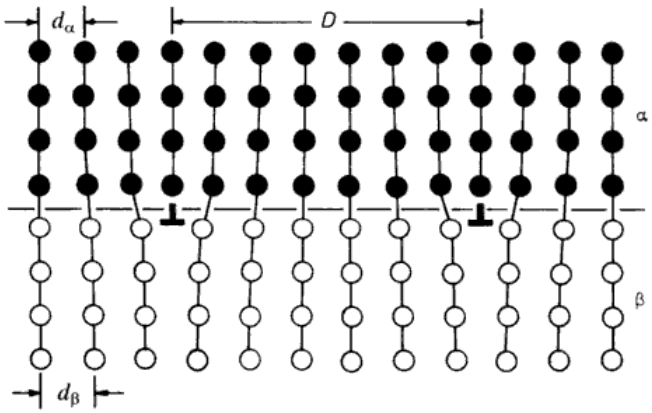


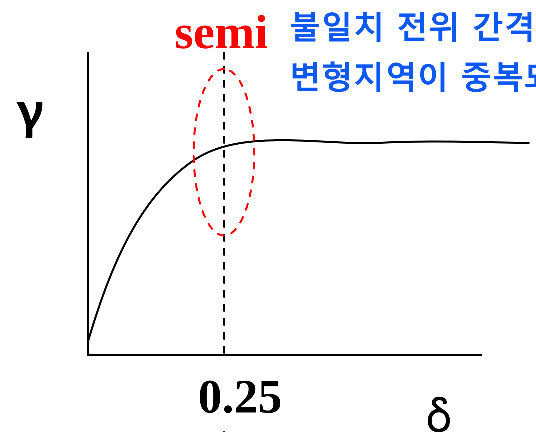
Fig. 3.35 A semicoherent interface. The misfit parallel to the interface is accommodated by a series of edge dislocations.

γ_{st} → due to structural distortions caused by the misfit dislocations

$$\gamma_{st} \propto \delta \text{ for small } \delta$$

In general,
γ (semicoherent) ~ 200~500 mJM^{-2}

불일치 전위 간격이 감소함에 따라 변형지역이 중복되어 서로 상쇄됨.



1 dislocation per 4 lattices
δ=4

$\delta = (d_\beta - d_\alpha)/ d_\alpha$: misfit

→ D vs. δ vs. n

$(n+1)\, d_\alpha = n\, d_\beta = D$

$\delta = (d_\beta / d_\alpha) - 1$, $(d_\beta / d_\alpha) = 1 + 1/n = 1 + \delta$

→ $\delta = 1/n$

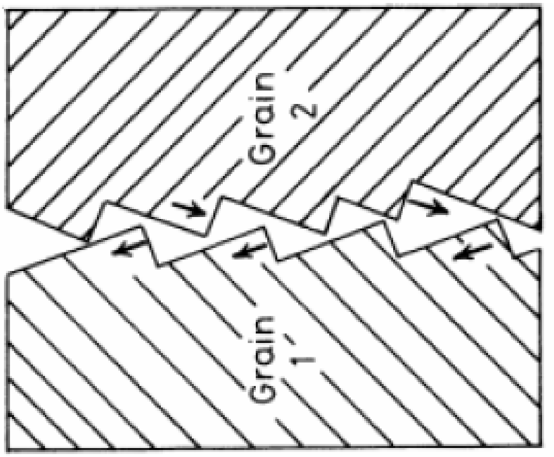
$D = d_\beta / \delta \approx b / \delta$ $\quad$ [$b=(d_\alpha + d_\beta)/2$]

δ가 작다면,

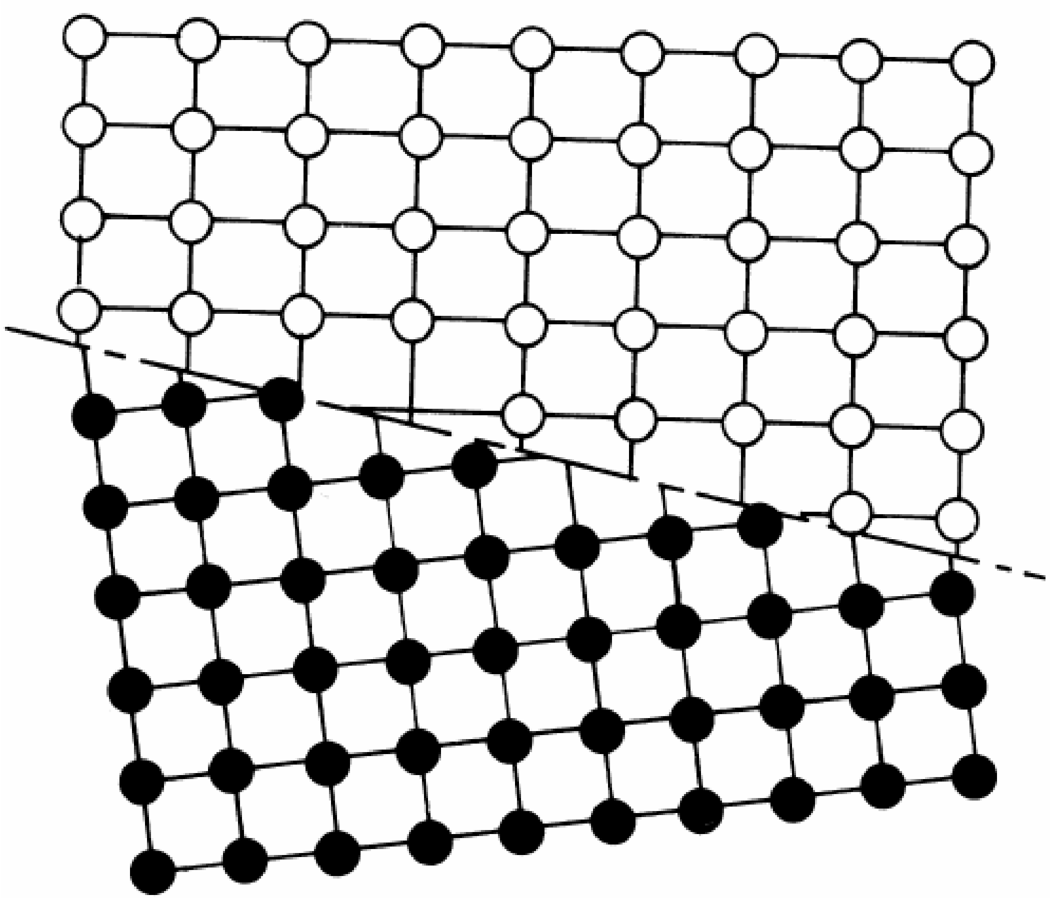
3) Incoherent Interfaces ~ high angle grain boudnary

1) δ > 0.25 격자가 잘 일치하는 것이 불가능해짐

2) different crystal structure (in general)



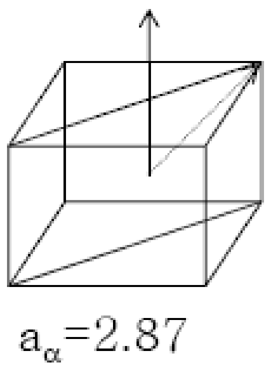
In general,
γ (incoherent) ~ 500~1000 mJM^{-2}

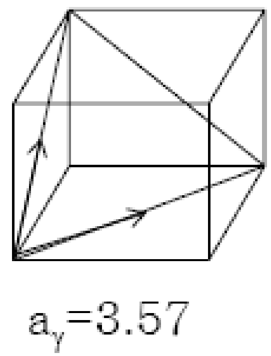


incoherent

Fig. 3.37 An incoherent interface.

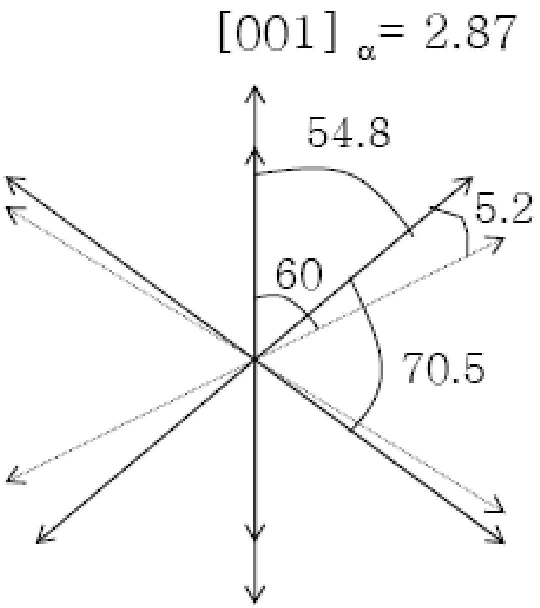
4) Complex Semicoherent Interfaces





If bcc α is precipitated from fcc γ, which interface is expected?

Which orientation would make the lowest interface energy?



Nishiyama-Wasserman (N-W) Relationship

$$(110)_{bcc} // (111)_{fcc}, \quad [001]_{bcc} // [\bar{1}01]_{fcc}$$

Kurdjumov-Sachs (K-S) Relationships

$$(110)_{bcc} // (111)_{fcc}, \quad [1\bar{1}1]_{bcc} // [0\bar{1}1]_{fcc}$$

(두 방위관계의 유일한 차이점은 조밀면에서 5.26°만큼 회전시킨 것임)

Complex Semicoherent Interfaces

Semicoherent interface observed at boundaries formed by low-index planes. (atom pattern and spacing are almost equal.)

N-W relationship

격자가 잘 일치하는 부분: 점선 영역으로 제한됨.

이러한 넓은 계면은 부정합 임.

K-S 방위관계에서도 유사한 거동 나타남.

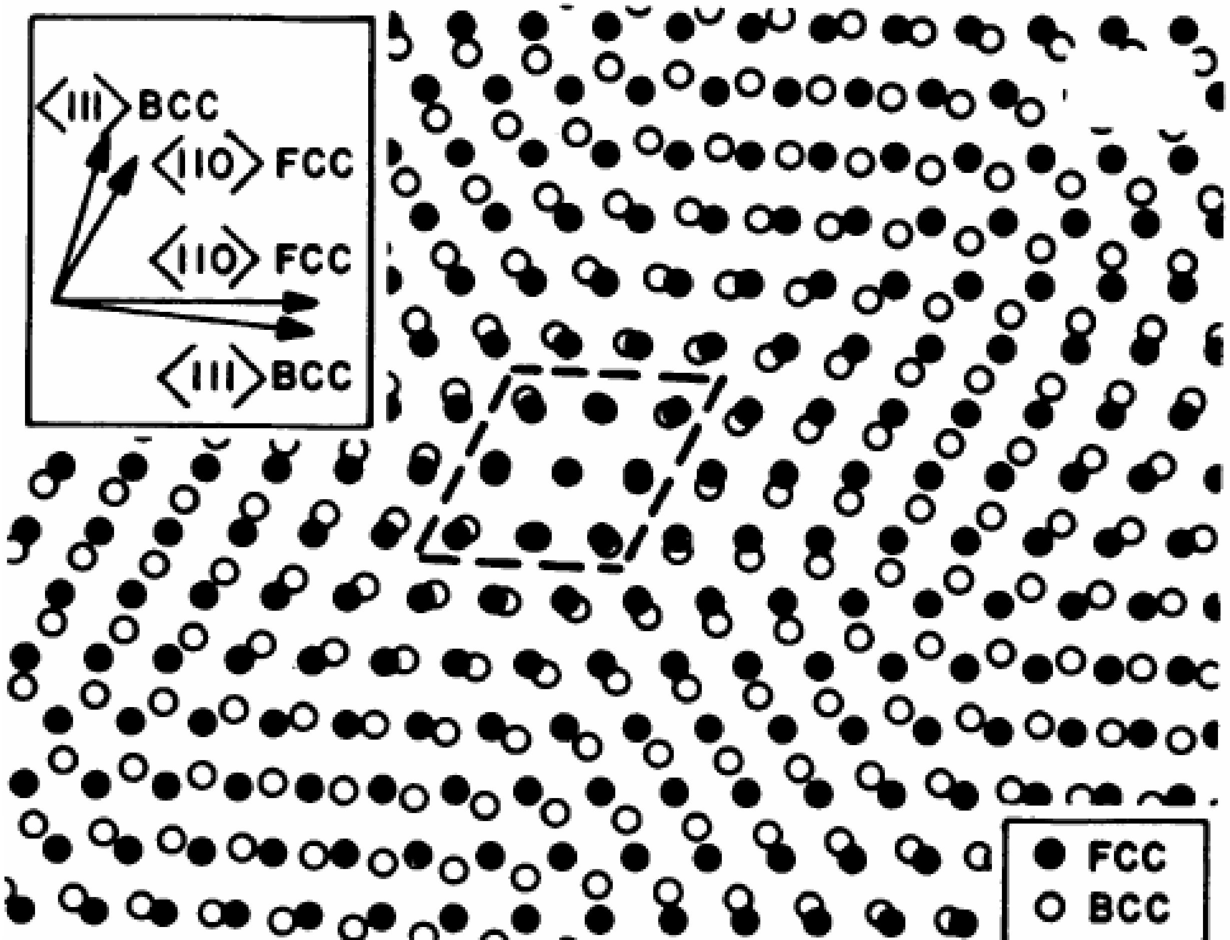
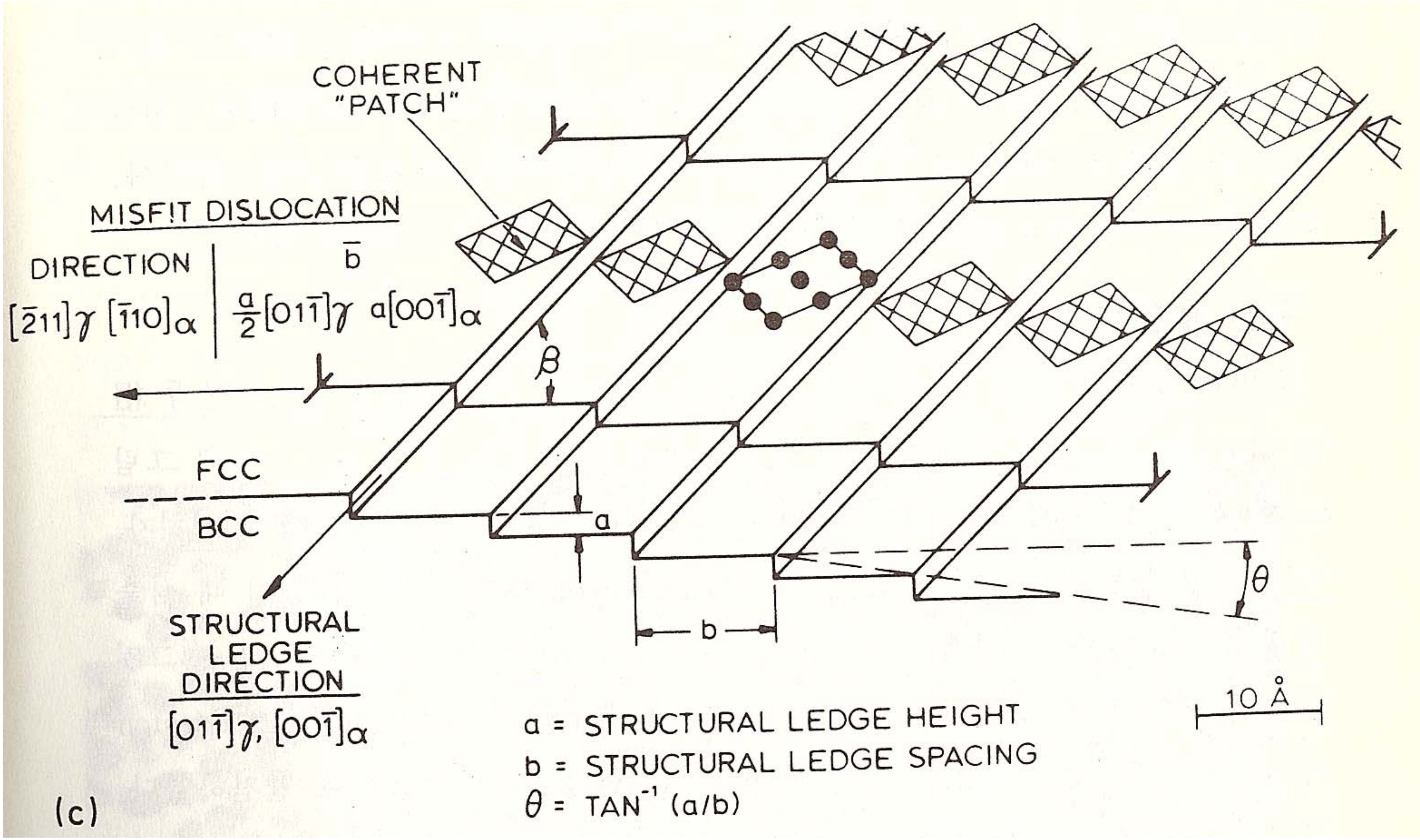


Fig. 3.38 Atomic matching across a $(111)_{fcc}/(11)_{bcc}$ interface bearing the NW orientation relationship for lattice parameters closely corresponding to the case of fcc and bcc iron. (M.G. Hall *et al*., *Surface Science*, 31 (1972)257).

Complex Semicoherent Interfaces



The degree of coherency can, however, be greatly increased if a macroscopically irrational interface is formed. The detailed structure of such interfaces is , however, uncertain due to their complex nature.