# Fundamentos de Ciência e Engenharia de Materiais





#### **DEFEITOS CRISTALINOS**

Prof. Dr. André Paulo Tschiptschin



#### **Defeitos cristalinos**

- Defeito cristalino: imperfeição do reticulado cristalino
- Classificação dos defeitos cristalinos:
  - Defeitos puntiformes (associados com uma ou duas posições atômicas): lacunas e átomos intersticiais.
  - Defeitos de linha (defeitos unidimensionais): discordâncias
  - Defeitos bidimensionais (fronteiras entre duas regiões com diferentes estruturas cristalinas ou diferentes orientações cristalográficas): contornos de grão, interfaces, superfícies livres, contornos de macla, defeitos de empilhamento.
  - Defeitos volumétricos (defeitos tridimensionais): poros, trincas e inclusões.



# **Defeitos puntiformes**

(Lacunas e auto-intersticiais)

- Lacuna: ausência de um átomo em um ponto do reticulado cristalino.
- Podem ser formadas durante a solidificação ou como resultado de vibrações atômicas.
- Existe uma concentração de equilíbrio de lacunas.

$$N_L = N \exp\left(-\frac{Q_L}{kT}\right)$$

onde: N ≡ número total de posições atômicas

 $N_I \equiv número de lacunas$ 

Q<sub>I</sub> ≡ energia de ativação para formação de lacunas

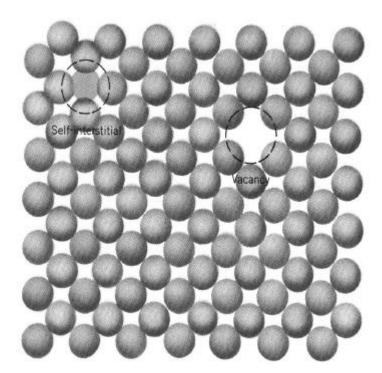
k ≡ constante de Boltzmann

 $T \equiv temperatura absoluta$ 

# **Defeitos puntiformes**

(Lacunas ou auto-intersticiais)

- Auto-intersticial: é um átomo que ocupa um interstício da estrutura cristalina.
- Os auto-intersticiais causam uma grande distorção do reticulado cristalino a sua volta.



Representação de uma lacuna e de um auto-intersticial

## Defeitos pontuais

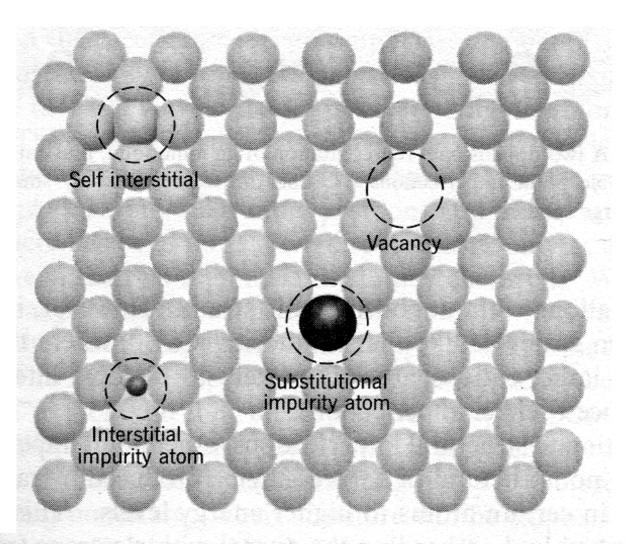
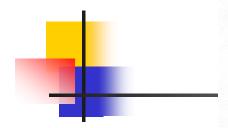


Figure 4.1 A two-dimensional representation of a simple crystalline solid, illustrating some of the point imperfections that are possible.



# Defeitos pontuais

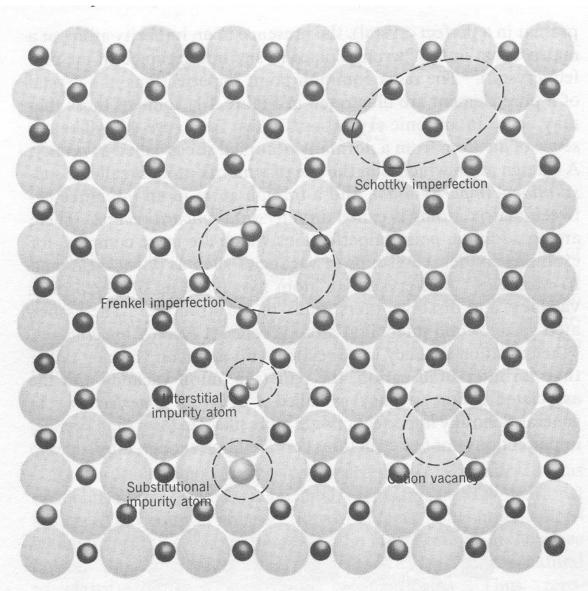
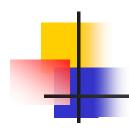
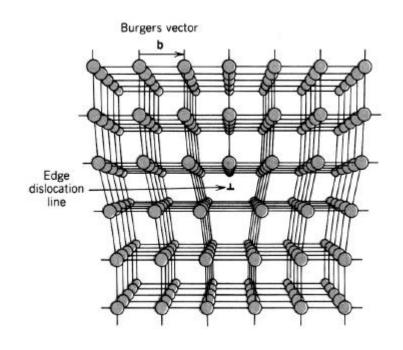


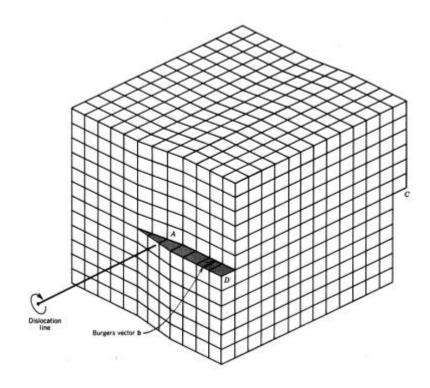
Figure 4.2 A two-dimensional representation of an ionic solid, illustrating a number of possible point imperfections. Cations are represented by small spheres, anions by large spheres.



# Defeitos de linha



Arranjo dos átomos em torno de uma discordância em cunha



Discordância em hélice

#### Discordância em hélice

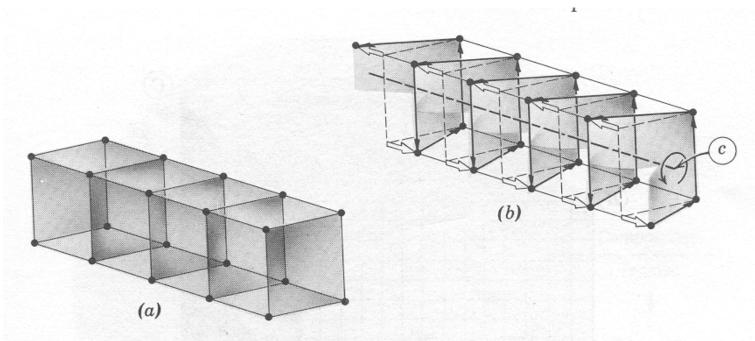
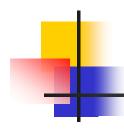
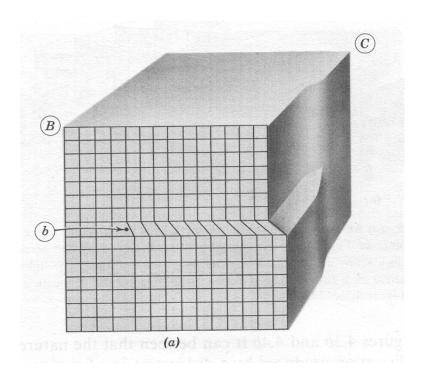
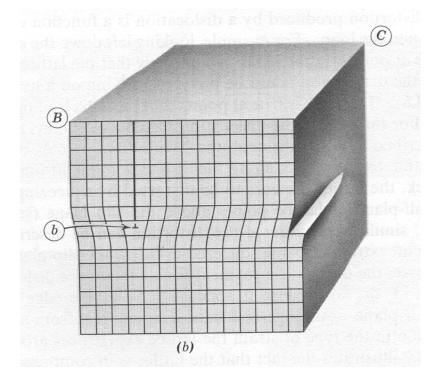


Figure 4.5 (a) An array of four-unit cells in an ideal simple cubic lattice. (b) The lattice points of Figure 4.5a after having been displaced by the broad arrows, resulting in a screw dislocation along the heavy dashed line. The lighter arrows trace a helical path through the distorted lattice around the dislocation. Point c refers to Figure 4.3b.



# **Defeitos de linha**





Discordância em hélice

Discordância em cunha



# Campos de tensão

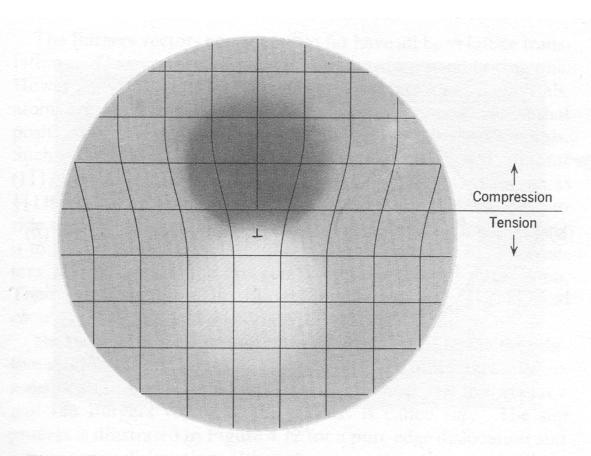
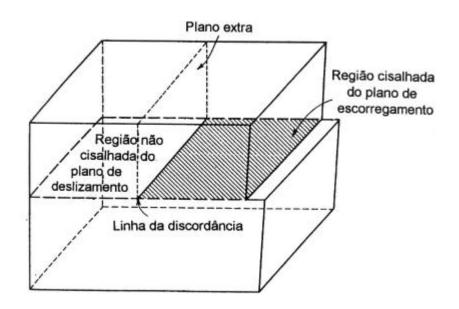


Figure 4.7 The regions of tension (light) and compression (dark) around an edge dislocation in a simple cubic lattice.



#### Defeitos de linha

- A linha de discordância delimita as regiões cisalhada e não cisalhada.
- Uma discordância não pode terminar no interior de um cristal.

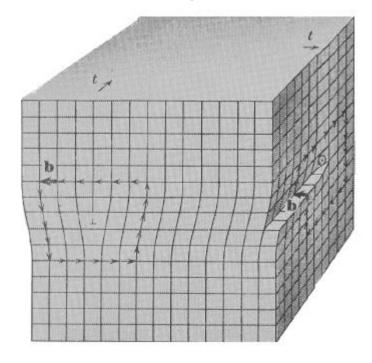


Linha de discordância e plano de escorregamento

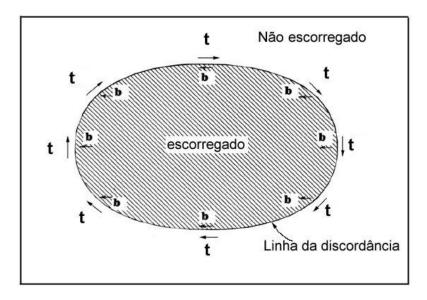


#### Defeitos de linha

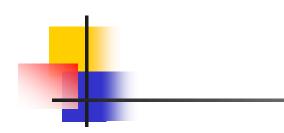
- A magnitude e a direção da distorção do reticulado associada a uma discordância podem ser expressas em termos do vetor de Burgers, b.
- O vetor de Burgers é determinado por meio do circuito de Burgers.



Circuito de Burgers



Linha de discordância, plano de escorregamento e vetor de Burgers



# Discordâncias parciais

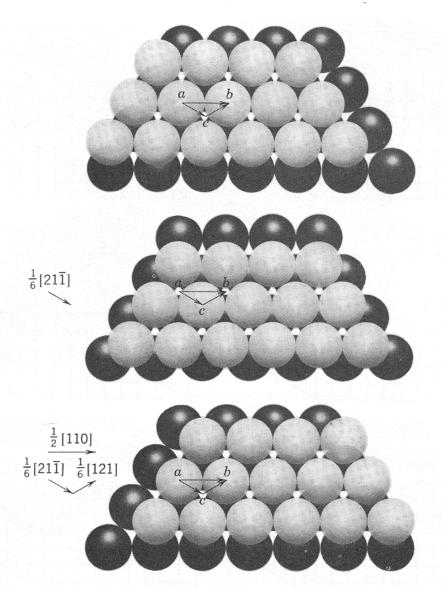
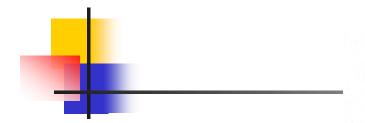


Figure 4.11 The zig-zag motion of one (111) plane over another in a FCC crystal, illustrating the meaning of partial dislocations. The sum of the Burgers vectors of the two partials,  $\frac{1}{6}[21\overline{1}]$  and  $\frac{1}{6}[121]$ , is a lattice translation vector, that is, the Burgers vector of a whole dislocation.



# **Escorregamento**

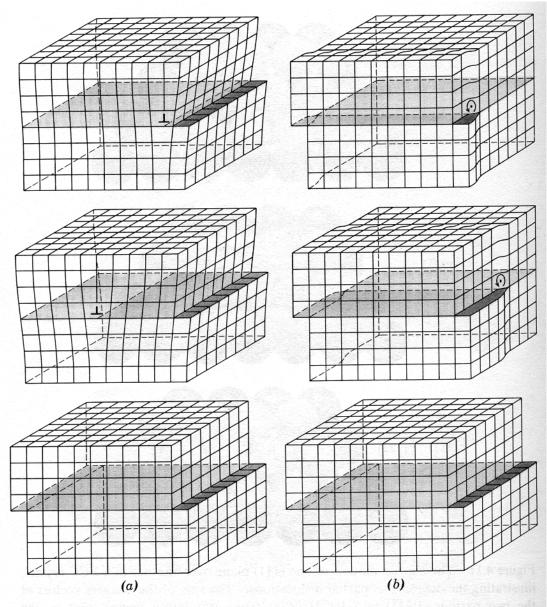
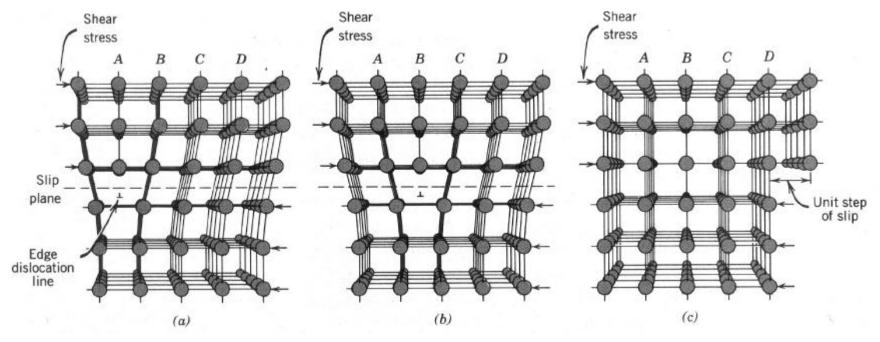


Figure 4.12 (a) Slip resulting from the movement (right to left) of a pure edge dislocation through a simple cubic lattice. (b) Slip resulting from the movement (front to back) of a pure screw dislocation through a simple cubic lattice. The dislocations in (a) and (b) have the same Burgers vector so they result in the same amount and direction of slip.

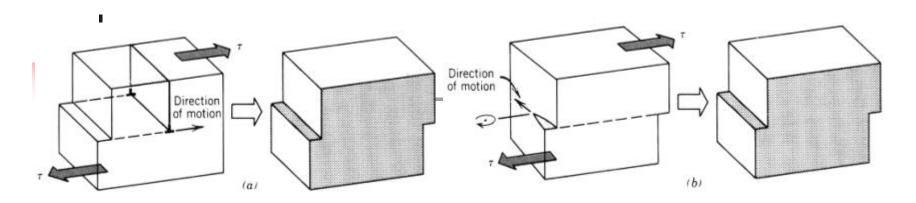
# Deformação plástica

O mecanismo de deformação plástica é diferente para materiais cristalinos e materiais amorfos. Nos materiais cristalinos o principal mecanismo de deformação plástica consiste no escorregamento de planos atômicos através da movimentação de discordâncias, já nos materiais amorfos consiste no escoamento viscoso.

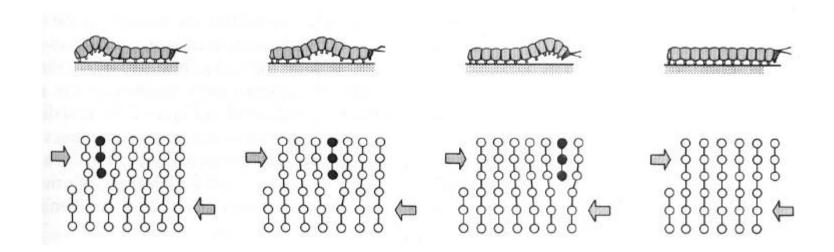


Deformação plástica produzida pela movimentação de uma discordância em cunha

# Deformação plástica



Formação de um degrau na superfície de um metal pela movimentação de (a) uma discordância em cunha e (b) uma discordância em hélice.



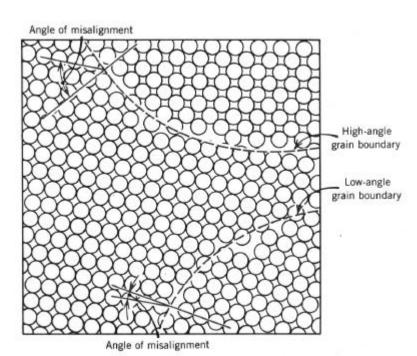
Analogia entre a movimentação de uma lagarta e de uma discordância.



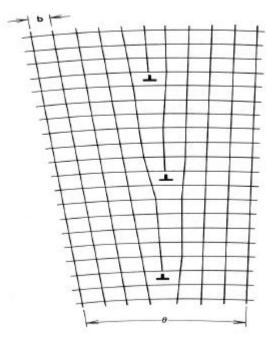
- Interface: contorno entre duas fases diferentes.
- Contornos de grão: contornos entre dois cristais sólidos da mesma fase.
- Superfície externa: superfície entre o cristal e o meio que o circunda
- Contorno de macla: tipo especial de contorno de grão que separa duas regiões com uma simetria tipo "espelho".
- Falhas de empilhamento: ocorre nos materiais quando há uma interrupção na sequência de empilhamento, por exemplo na sequência ABCABCABC.... dos planos compactos dos cristais CFC.

(contornos de grão)

Quando o desalinhamento entre os grãos vizinhos é grande (maior que ~15°), o contorno formado é chamado contorno de grão de alto ângulo. Se o desalinhamento é pequeno (em geral, menor que 5°), o contorno é chamado contorno de pequeno ângulo.



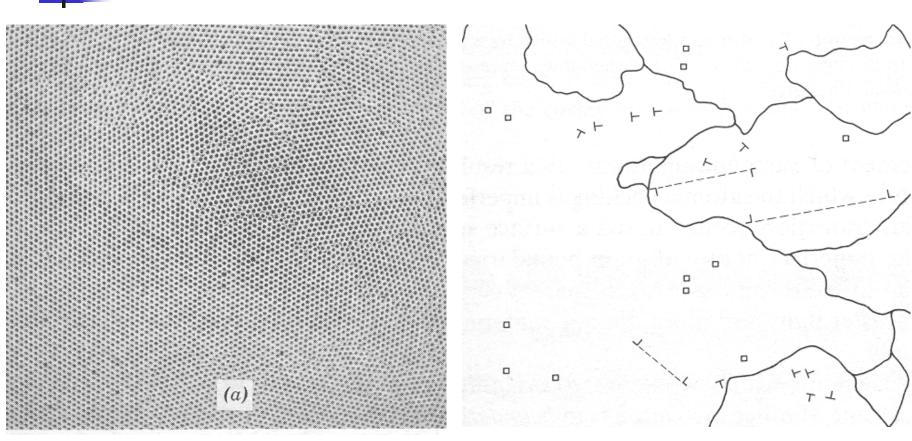
Contornos de grão e de sub-grão



Contorno de pequeno ângulo resultante do alinhamento de discordâncias em cunha



(contornos de grão)



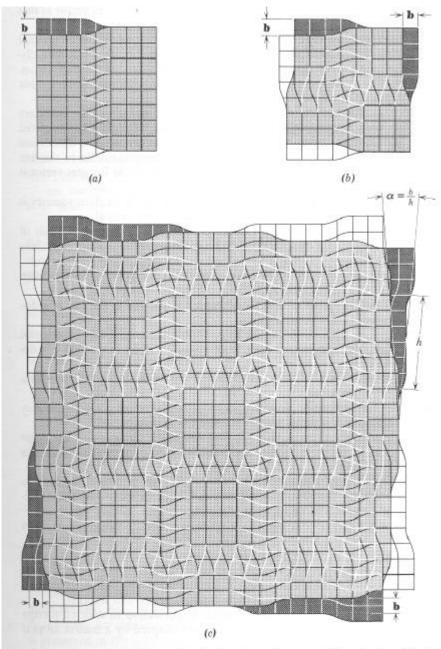
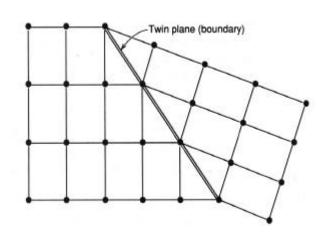


Figure 4.17 (a) A view normal to the slip plane of a screw dislocation in a simple cubic lattice. (b) Two intersecting screw dislocations in a simple cubic lattice. (c) A simple twist boundary composed of two sets of intersecting screw dislocations in a simple cubic lattice.

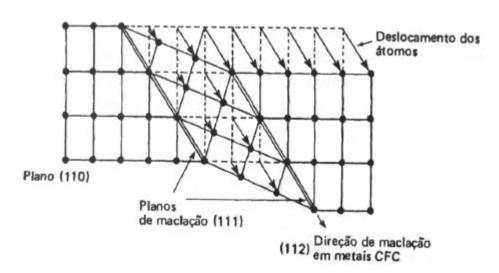
# Contornos de pequeno ângulo (torção)

(contornos de macla)

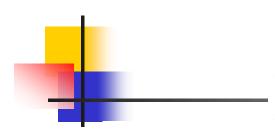
- A macla é um tipo de defeito cristalino que pode ocorrer durante a solidificação, deformação plástica, recristalização ou crescimento de grão.
- Tipos de macla: maclas de recozimento e maclas de deformação.
- A maclação ocorre em um plano cristalográfico determinado segundo uma direção cristalográfica específica. Tal conjunto plano/direção depende do tipo de estrutura cristalina.



Contorno de macla



Maclação mecânica em metais CFC



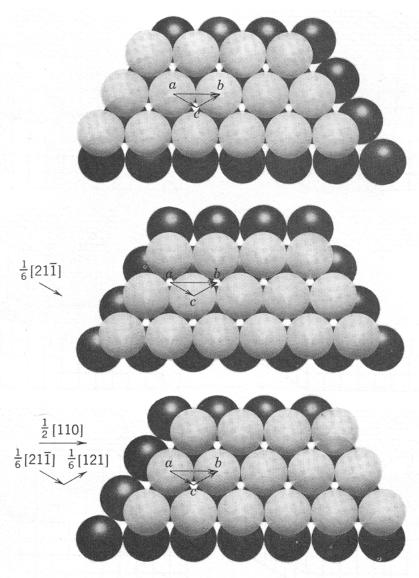


Figure 4.11 The zig-zag motion of one (111) plane over another in a FCC crystal, illustrating the meaning of partial dislocations. The sum of the Burgers vectors of the two partials,  $\frac{1}{6}[21\overline{1}]$  and  $\frac{1}{6}[121]$ , is a lattice translation vector, that is, the Burgers vector of a whole dislocation.

# Falha de empilhamento



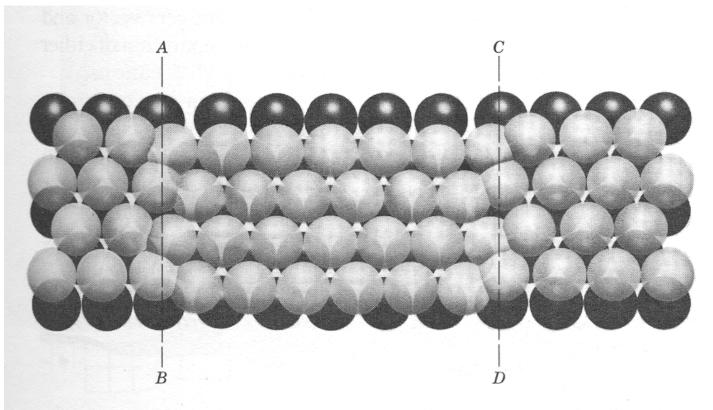
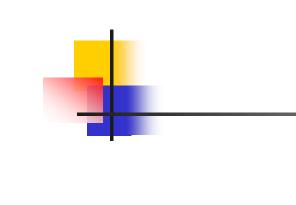
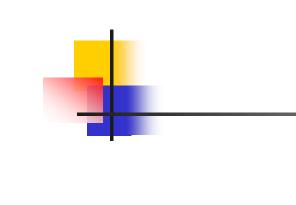


Figure 4.15 A view normal to a stacking fault between the lines AB and CD on a close-packed plane, in either a FCC or a HCP metal. If the stacking fault is viewed as resulting from the dissociation of a dislocation into two partials, AB and CD are the lines of the partial dislocations.





# Observação microestrutural

- Observação estrutural: macroestrutura e microestrutura.
- Observação da macroestrutura: a olho nu ou com baixos aumentos (até ~10X).
- Observação da microestrutura: microscopia óptica e microscopia eletrônica.

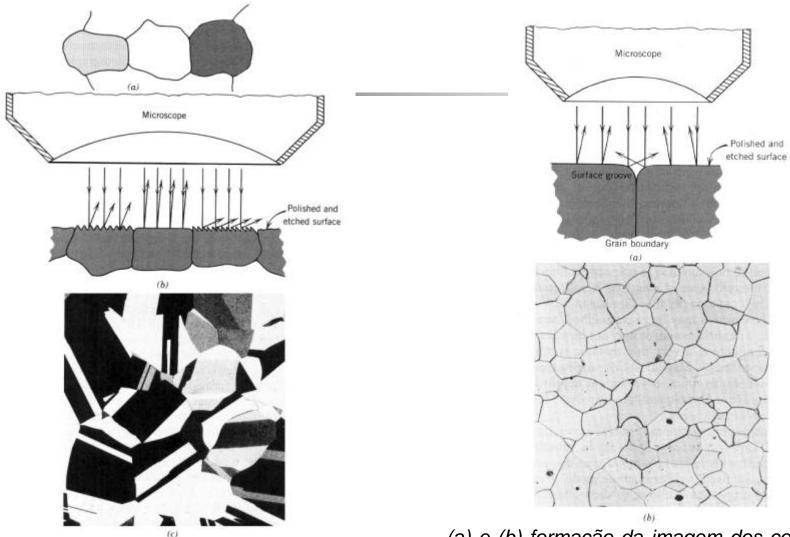


Macroestrutura de um lingote de chumbo apresentando os diferentes grãos.

Aumento: 0,7X

### Observação microestrutural

(microscopia óptica)



- (a) e (b) formação do contraste entre grãos.
- (c) Micrografia óptica de um latão (Cu-Zn) policristalino. Aumento: 60X.
- (a) e (b) formação da imagem dos contornos de grão.
- (c) Micrografia óptica de uma liga Fe-Cr. Aumento: 100X.



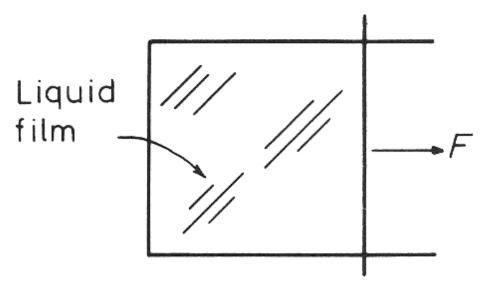


Fig. 3.1 A liquid film on a wire frame.



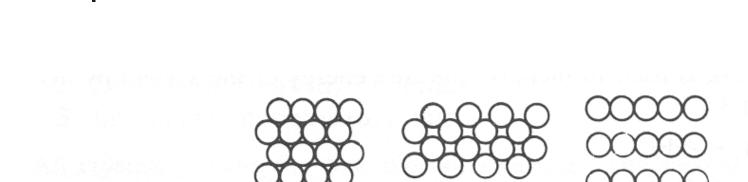


Fig. 3.2 Atomic configurations on the three closest-packed planes in fcc crystals: (111), (200) and (220).



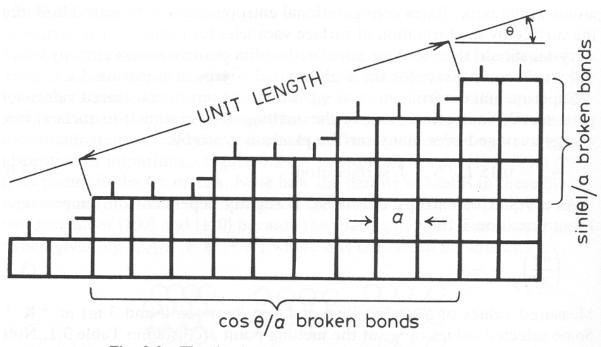


Fig. 3.3 The 'broken-bond' model for surface energy.



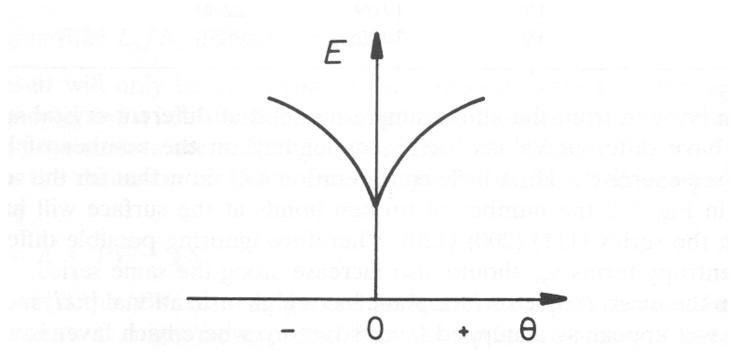


Fig. 3.4 Variation of surface energy as a function of  $\theta$  in Fig. 3.3.

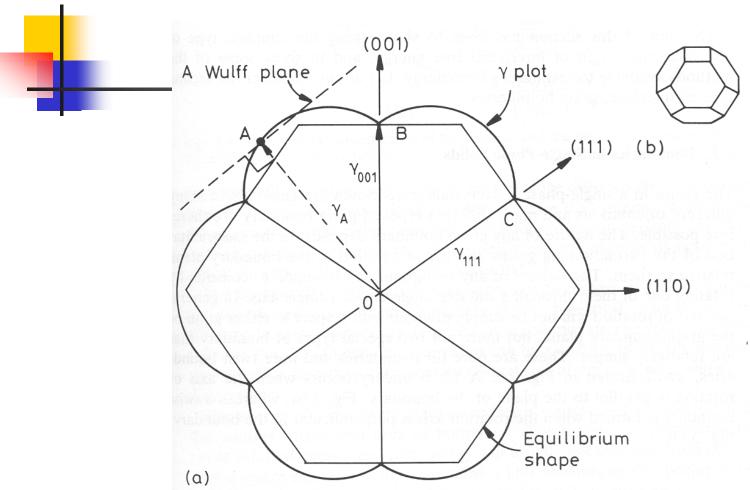


Fig. 3.5 (a) A possible  $(1\bar{1}0)$  section through the  $\gamma$ -plot of an fcc crystal. The length OA represents the free energy of a surface plane whose normal lies in the direction OA. Thus OB =  $\gamma_{(001)}$ , OC =  $\gamma_{(111)}$ , etc. Wulff planes are those such as that which lies normal to the vector OA. In this case the Wulff planes at the cusps (B, C, etc.) give the inner envelope of all Wulff planes and thus the equilibrium shape. (b) The equilibrium shape in three dimensions showing  $\{100\}$  (square faces) and  $\{111\}$  (hexagonal faces).

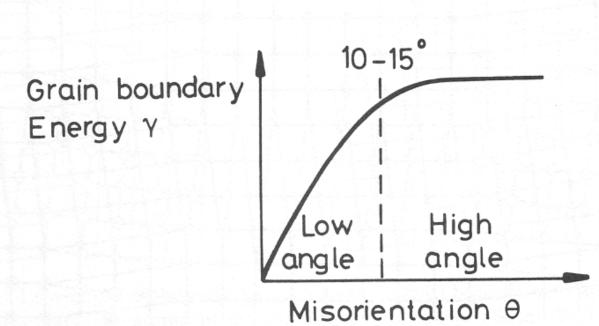
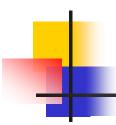


Fig. 3.9 Variation of grain boundary energy with misorientation (schematic).



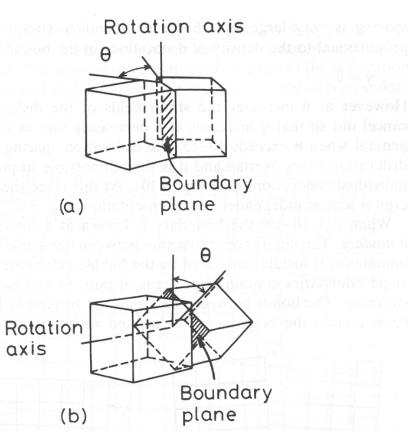


Fig. 3.6 The relative orientations of the crystals and the boundary forming (a) a tilt boundary (b) a twist boundary.



## Energia livre de superfície de alguns metais

Crystal	$T_{\rm m}/^{\circ}{\rm C}$	$\gamma_{\rm sv}/{\rm mJ~m^{-2}}$
S and said Sn	232	o aoi 680 a se battolo si sin l
Al	660	
Ag Ag	961	1120
da zomala zo Au wold	1063	1390
Cu	1084	to ve 1720 vol la betterol ed stol
δ-Fe stud	1536	2080
Pt	1769	2280
W	3407	2650



# Energia de contorno de grão de alguns metais

Crystal	$\gamma_b/mJ m^{-2}$	T/°C	$\gamma_{\rm b}/\gamma_{\rm sv}$
Sn	164	223	0.24
Al	324	450	0.30
Ag	375	950	0.33
Au	378	1000	0.27
Cu	625	925	0.36
γ-Fe	756	1350	0.40
δ-Fe	468	1450	0.23
Pt	660	1300	0.29
W	1080	2000	0.41



### Energia de interface

### Energia de contorno de grão de alguns metais

Crystal	Coherent twin boundary energy	Incoherent twin boundary energy	Grain boundary energy
Cu	21	498	623
Ag	8	126	377
Fe-Cr-Ni (stainless steel type 304)	19	209	835

### Contornos de pequeno ângulo



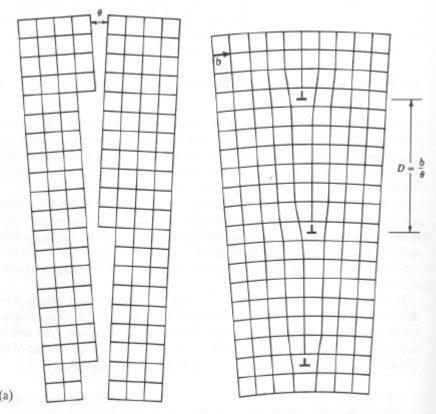


Fig. 3.7 (a) Low-angle tilt boundary, (b) low-angle twist boundary: ○ atoms in crystal below boundary, ● atoms in crystal above boundary. (After W.T. Read Jr., Dislocations in Crystals, McGraw-Hill, New York, 1953.)





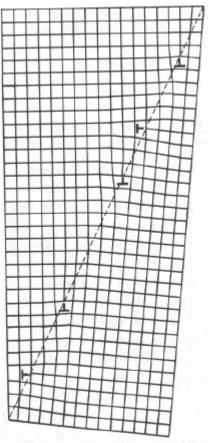


Fig. 3.8 An unsymmetric tilt boundary. Dislocations with two different Burgers vectors are present. (After W.T. Read Jr., *Dislocations in Crystals*, McGraw-Hill, New York, 1953.)



### Contornos de grande ângulo

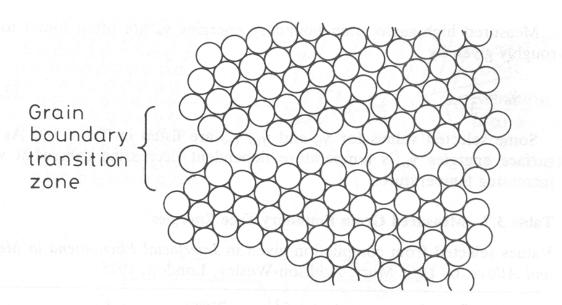


Fig. 3.10 Disordered grain boundary structure (schematic).





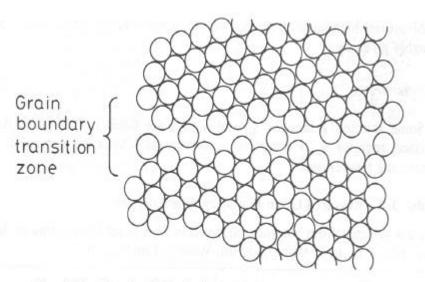
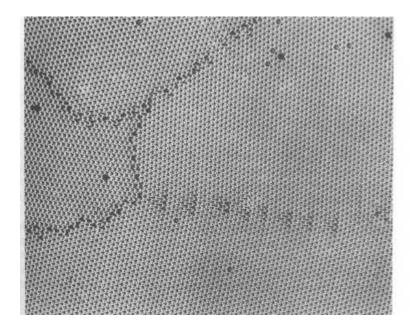


Fig. 3.10 Disordered grain boundary structure (schematic).



#### Contornos de macla

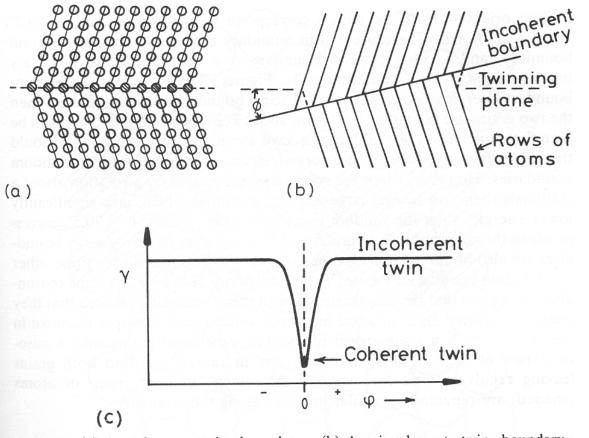
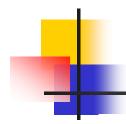
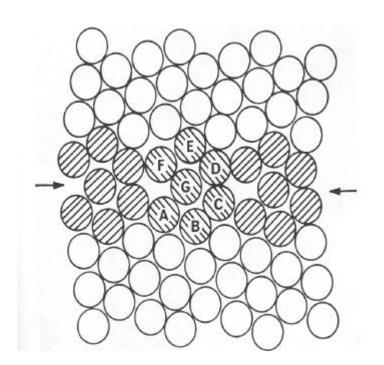
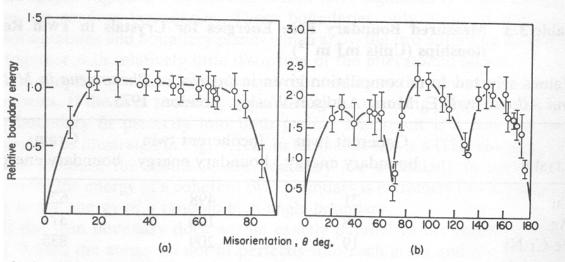


Fig. 3.12 (a) A coherent twin boundary. (b) An incoherent twin boundary. (c) Twin-boundary energy as a function of the grain boundary orientation.



### **Contornos especiais**

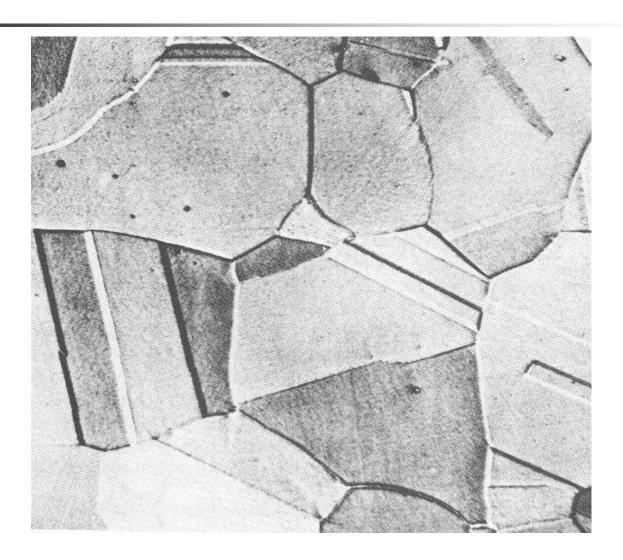




3.13 Measured grain boundary energies for symmetric tilt boundaries in Al when the rotation axis is parallel to  $\langle 100 \rangle$ , (b) when the rotation axis is parallel to  $\rangle$ . (After G. Hasson and C. Goux, *Scripta Metallurgica*, 5 (1971) 889.)



### Aço austenítico



### **Tensão interfacial**

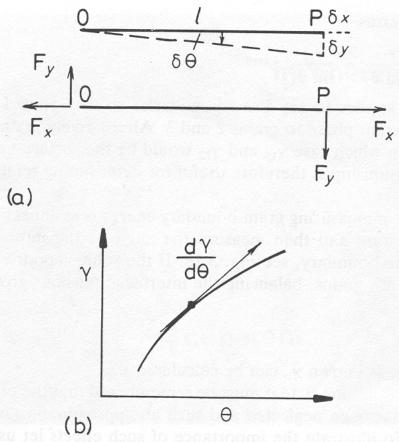


Fig. 3.16 (a) Equilibrium forces  $F_x$  and  $F_y$  supporting a length l of boundary OP. (b) The origin of  $F_y$ .

#### Tensão interfacial

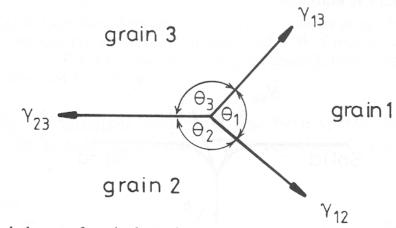


Fig. 3.17 The balance of grain boundary tensions for a grain boundary intersection in metastable equilibrium.

$$\frac{\gamma_{23}}{\sin \,\theta_1} = \frac{\gamma_{13}}{\sin \,\theta_2} = \frac{\gamma_{12}}{\sin \,\theta_3}$$



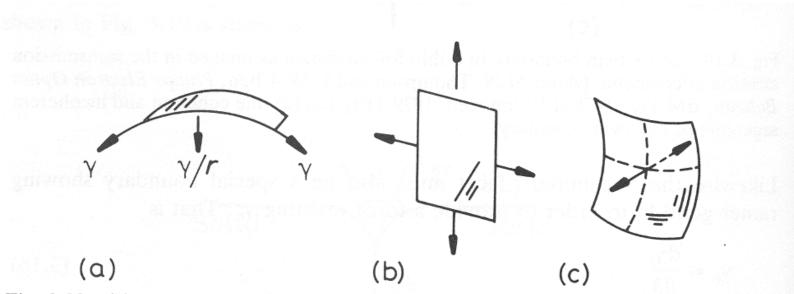


Fig. 3.20 (a) A cylindrical boundary with a radius of curvature r is acted on by a force  $\gamma/r$ . (b) A planar boundary with no net force. (c) A doubly curved boundary with no net force.



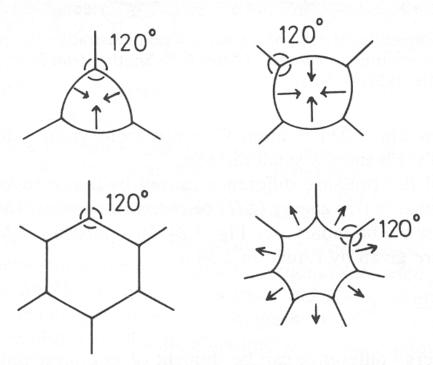


Fig. 3.21 Two-dimensional grain boundary configurations. The arrows indicate the directions boundaries will migrate during grain growth.



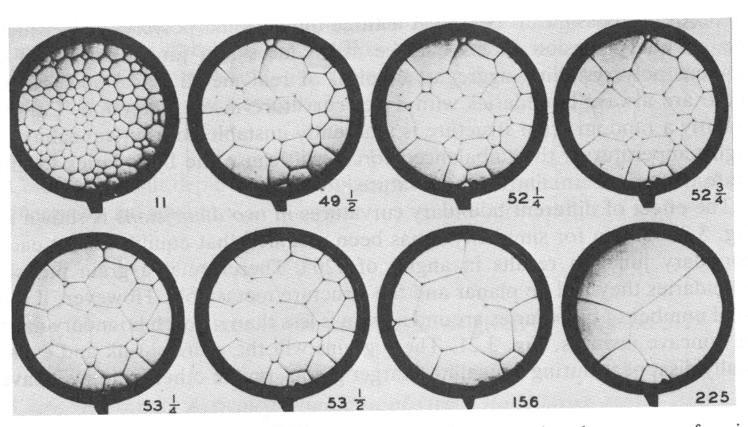


Fig. 3.22 Two-dimensional cells of a soap solution illustrating the process of grain growth. Numbers are time in minutes. (After C.S. Smith, *Metal Interfaces*, American Society for Metals, 1952, p. 81.)



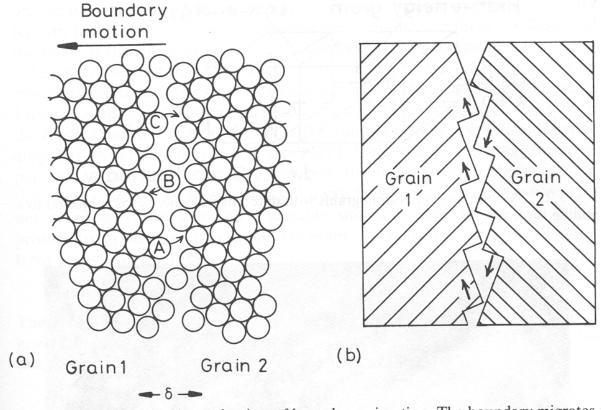


Fig. 3.23 (a) The atomic mechanism of boundary migration. The boundary migrates to the left if the jump rate from grain  $1 \rightarrow 2$  is greater than  $2 \rightarrow 1$ . Note that the free volume within the boundary has been exaggerated for clarity. (b) Step-like structure where close-packed planes protrude into the boundary.



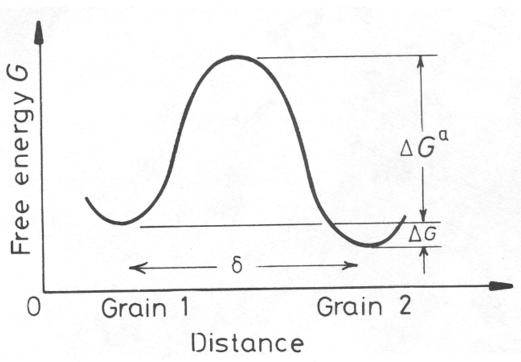
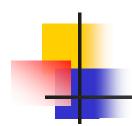


Fig. 3.24 The free energy of an atom during the process of jumping from one grain to the other.



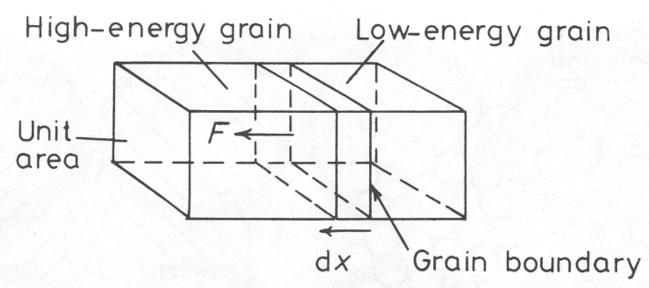


Fig. 3.25 A boundary separating grains with different free energies is subjected to a pulling force F.

# Migração de contornos induzida por deformação

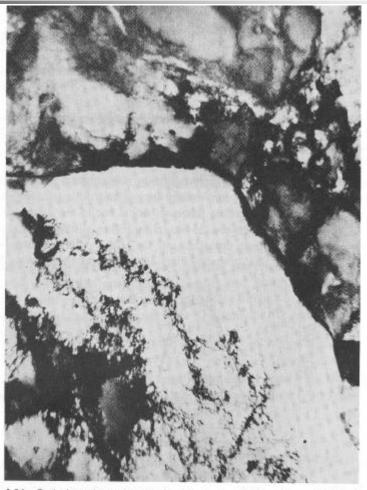
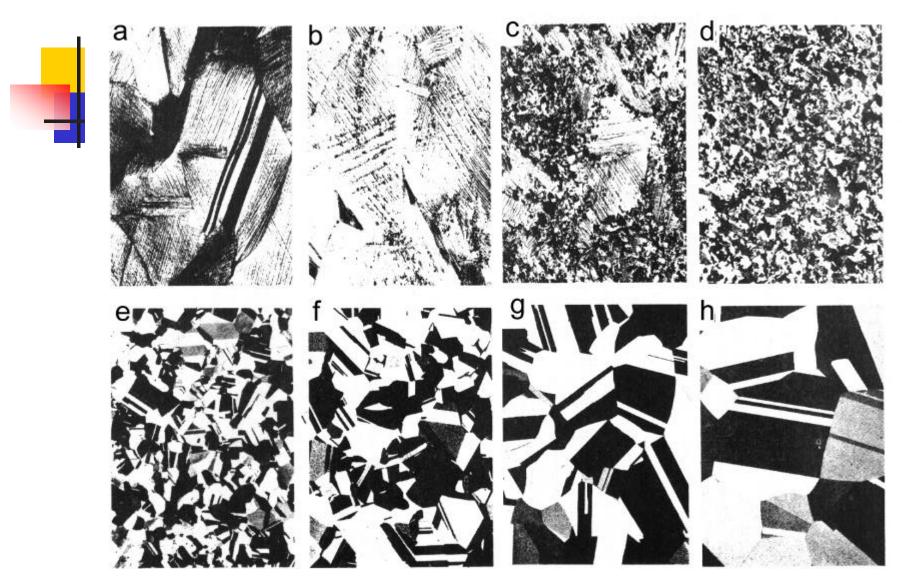


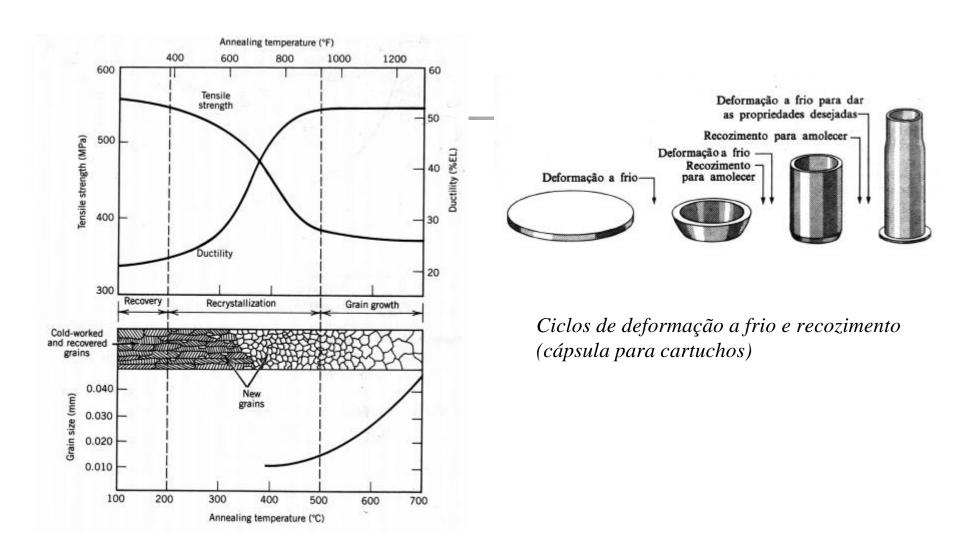
Fig. 3.26 Grain boundary migration in nickel pulled 10% and annealed 10 min at 425 °C. The region behind the advancing boundary is dislocation-free. (After J. Bailey and P. Hirsch, *Proceedings of the Royal Society*. London A267 (1962) 11)

### Recristalização e crescimento de grão



Recristalização de latão encruado (40X). De (a) a (h) pode-se ver a recristalização e o crescimento dos grãos em temperaturas elevadas.

### Recristalização e crescimento de grão



Influência da temperatura de recozimento na resistência à tração e na ductilidade de uma liga de Cu-Zn.

### **Interfaces**

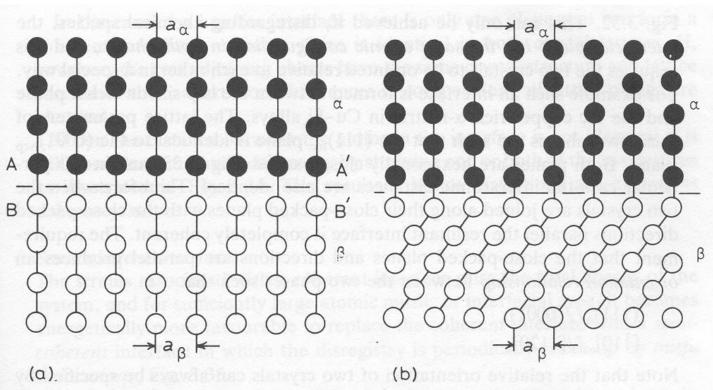
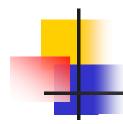


Fig. 3.32 Strain-free coherent interfaces. (a) Each crystal has a different chemical composition but the same crystal structure. (b) The two phases have different lattices.



### **Interfaces**

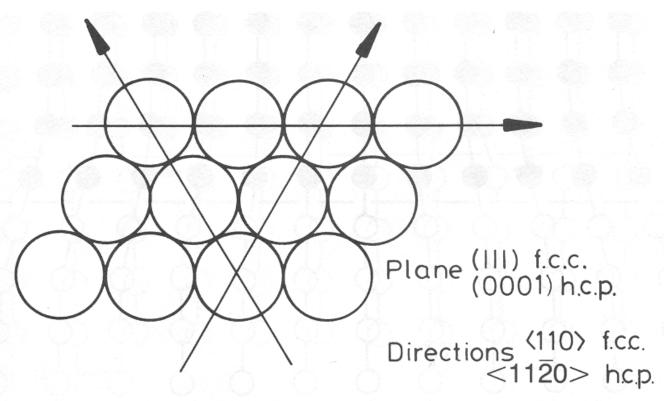
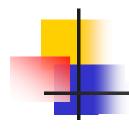


Fig. 3.33 The close-packed plane and directions in fcc and hcp structures.



### **Interfaces coerentes**

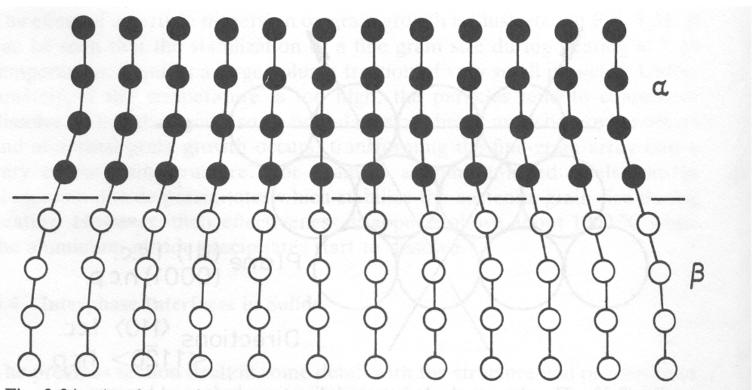


Fig. 3.34 A coherent interface with slight mismatch leads to coherency strains in the adjoining lattices.



### **Interfaces semi-coerentes**

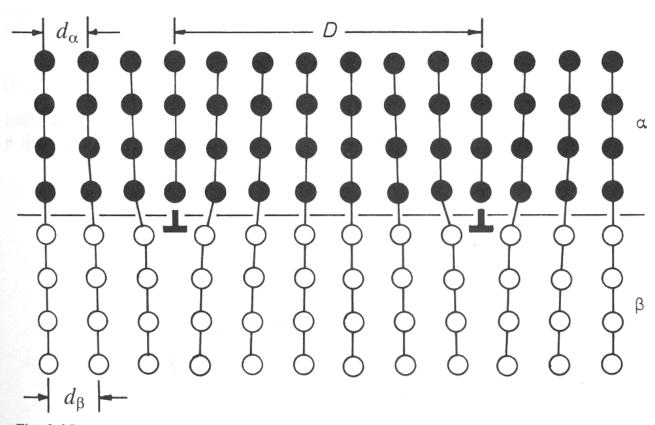


Fig. 3.35 A semicoherent interface. The misfit parallel to the interface is accommodated by a series of edge dislocations.



### **Interfaces incoerentes**

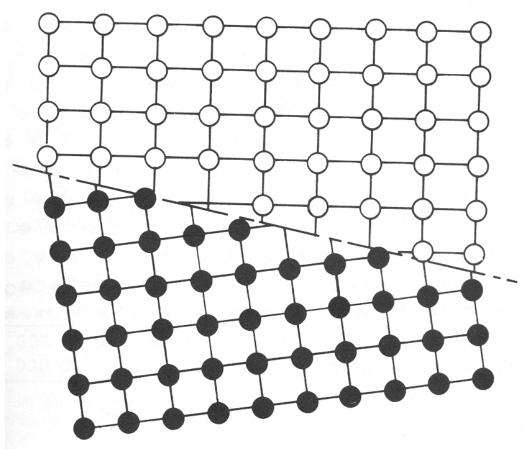


Fig. 3.37 An incoherent interface.

 $\begin{array}{c} (110)_{bcc}//(111)_{fcc}\,,\, [001]_{bcc}//[\bar{1}01]_{fcc} \\ \\ \text{and the so-called Kurdjumov-Sachs (K-S) relationship:} \\ \\ (110)_{bcc}//(111)_{fcc}\,,\, [1\bar{1}1]_{bcc}//[0\bar{1}1]_{fcc} \end{array}$ 

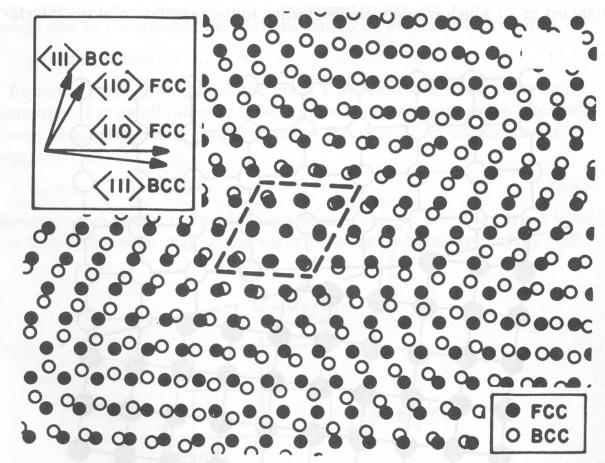
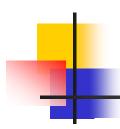


Fig. 3.38 Atomic matching across a  $(111)_{fcc}/(110)_{bcc}$  interface bearing the NW orientation relationship for lattice parameters closely corresponding to the case of fcc and bcc iron (M.G. Hall *et al.*, *Surface Science*, **31** (1972) 257).



#### Tensões de coerência

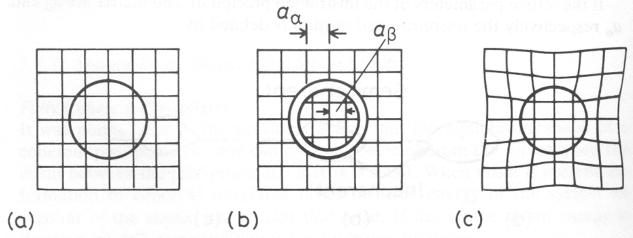
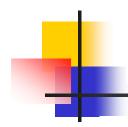


Fig. 3.47 The origin of coherency strains. The number of lattice points in the hole is conserved.

### Diferença de parâmetros

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



#### Tensões de coerência

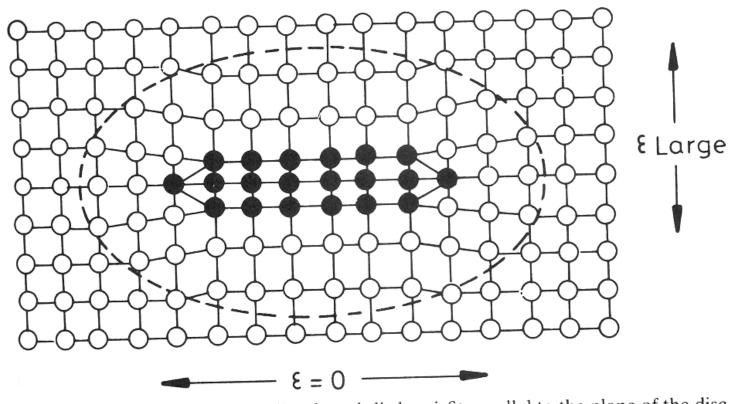


Fig. 3.48 For a coherent thin disc there is little misfit parallel to the plane of the disc. Maximum misfit is perpendicular to the disc.