Difusão

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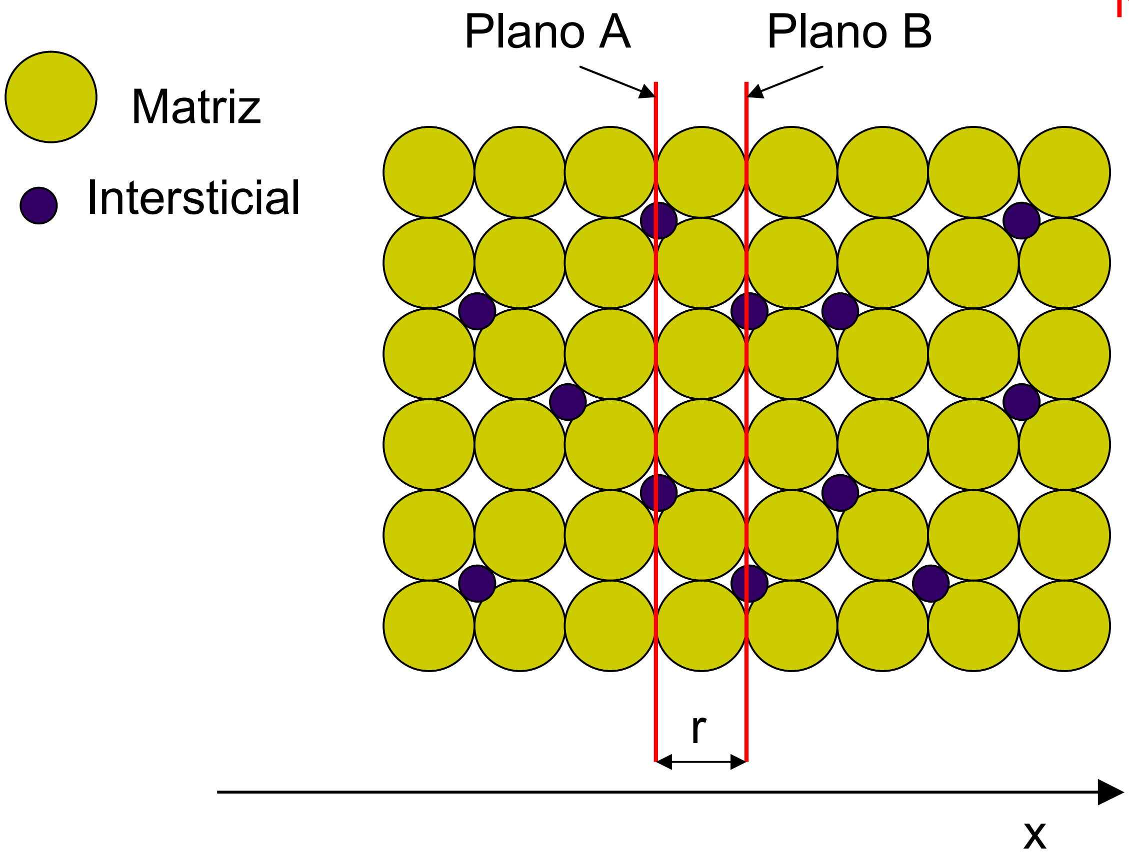
Difusão de Intersticiais



Número de Intersticiais no plano
Área do Plano
Saltos/segundo

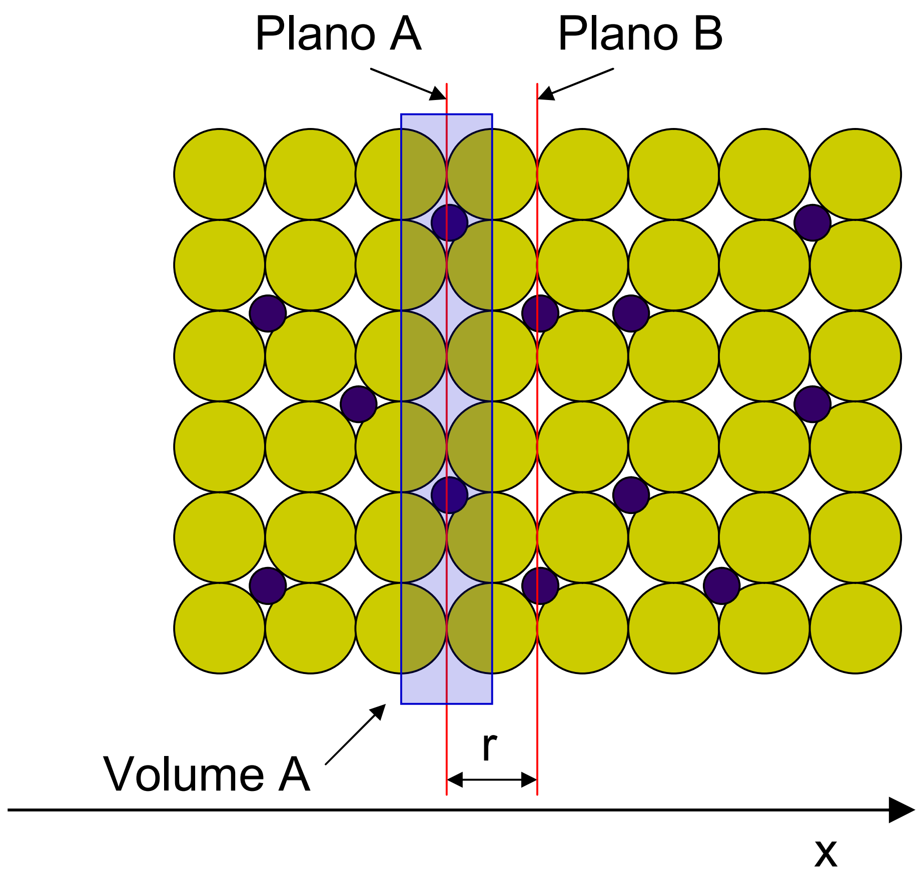
$$\vec{J}_x = \frac{1}{6}\Gamma\frac{n_A}{A}$$

$$\overleftarrow{J}_x = -\frac{1}{6}\Gamma\frac{n_B}{A}$$

$$J_x = \frac{1}{6}\Gamma\frac{(n_A - n_B)}{A}$$

(átomos/m²/s)

Difusão de Instersticiais



$$C_A = \frac{n_A}{V_A} = \frac{n_A}{r.A}$$

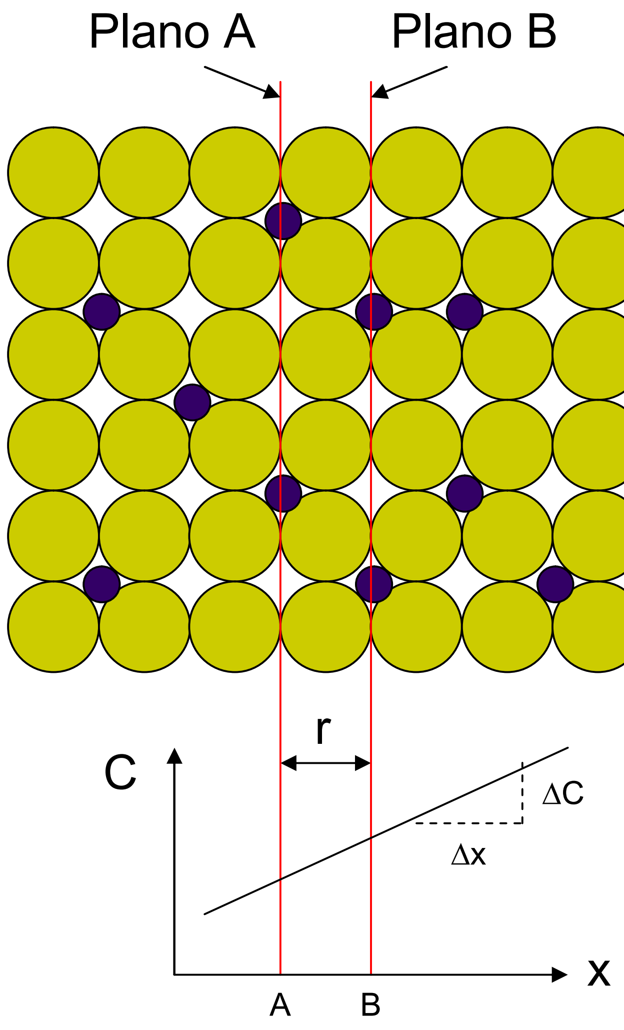
$$C_B = \frac{n_B}{r.A}$$

$$J_x = \frac{1}{6}\Gamma\frac{(n_A - n_B)}{A}$$

$$J_x = \frac{1}{6}\Gamma r \cancel{A}\frac{(C_A - C_B)}{\cancel{A}}$$

$$\boxed{J_x = \frac{1}{6}\Gamma r(C_A - C_B)}$$

Difusão de Instersticiais



$$\frac{\Delta C}{\Delta x} = \frac{C_B - C_A}{r}$$

$$C_A - C_B = -r.\frac{\Delta C}{\Delta x}$$

$$J_x = \frac{1}{6}\Gamma r(C_A - C_B)$$

$$J_x = -\frac{1}{6}\Gamma r^2 \frac{\Delta C}{\Delta x}$$

1ª lei de Fick

$$J_x = -\frac{1}{6}\Gamma r^2 \frac{\Delta C}{\Delta x}$$

$$\Delta x \to 0 \qquad J_x = -\frac{1}{6}\Gamma r^2 \frac{\partial C}{\partial x}$$

D

$$J_x = -D\frac{\partial C}{\partial x}$$

$$J = -D\left(\frac{\partial C}{\partial x} + \frac{\partial C}{\partial y} + \frac{\partial C}{\partial z}\right)$$

$$J = -D\nabla C$$

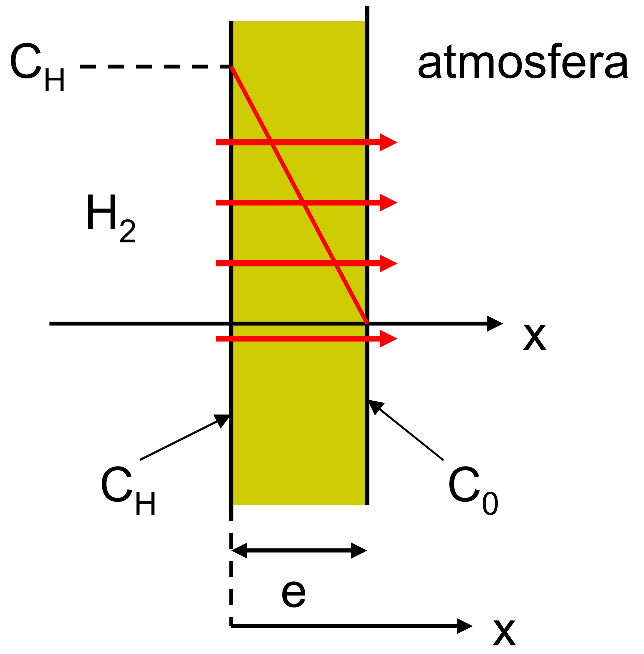
A força motriz para a difusão é o gradiente de concentração

Aplicação da 1ª lei de Fick

- Regimes estacionários

$$\frac{\partial C}{\partial t} = 0 \qquad \frac{\partial C}{\partial x} = constante \qquad J_x = constante$$

- Exemplo



$$C_H = \underline{cte}$$

$$C_0 = 0$$

$$\frac{\partial C}{\partial x} = \underline{cte} = \frac{\Delta C}{\Delta x} = \frac{C_0 - C_H}{e} = \frac{-C_H}{e}$$

$$J_x = -D\frac{\partial C}{\partial x} = -D\frac{-C_H}{e}$$

$$\boxed{J_x = D\frac{C_H}{e}}$$

O coeficiente de difusão

$$D = \frac{1}{6}\Gamma r^2$$

$$\Gamma = z\nu \exp\left(\frac{-\Delta G_m}{RT}\right) \qquad \Delta G = \Delta H - T\Delta S$$

Configuração do interstício

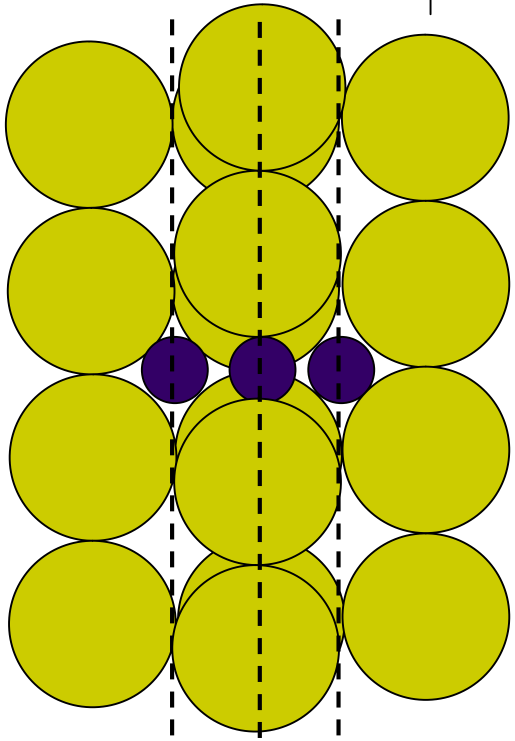
Freqüência de vibração atômica

Probabilidade de sucesso

$$\Gamma = z\nu \exp\left(\frac{\Delta S_m}{R}\right)\exp\left(\frac{-\Delta H_m}{RT}\right)$$

$$D = \frac{1}{6} r^2 z\nu \exp\left(\frac{\Delta S_m}{R}\right)\exp\left(\frac{-\Delta H_m}{RT}\right)$$

$$D = D_0 \exp\left(\frac{-\Delta H_m}{RT}\right)$$

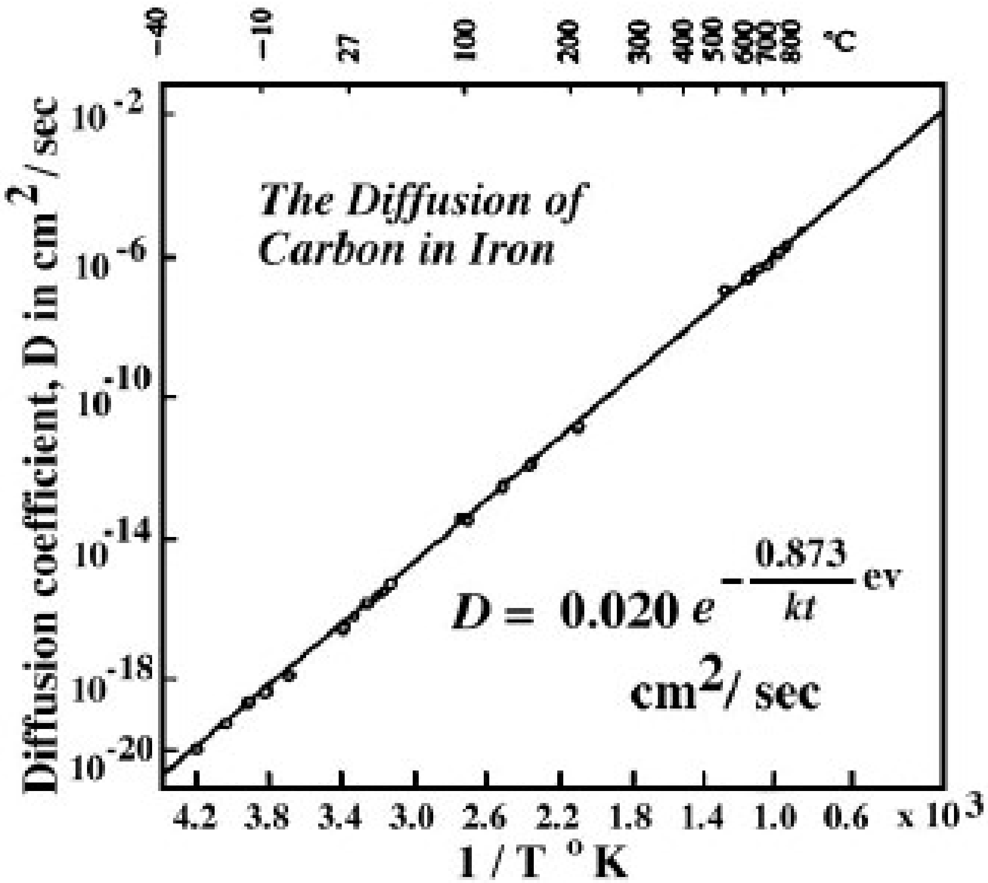


A temperatura ativa a difusão

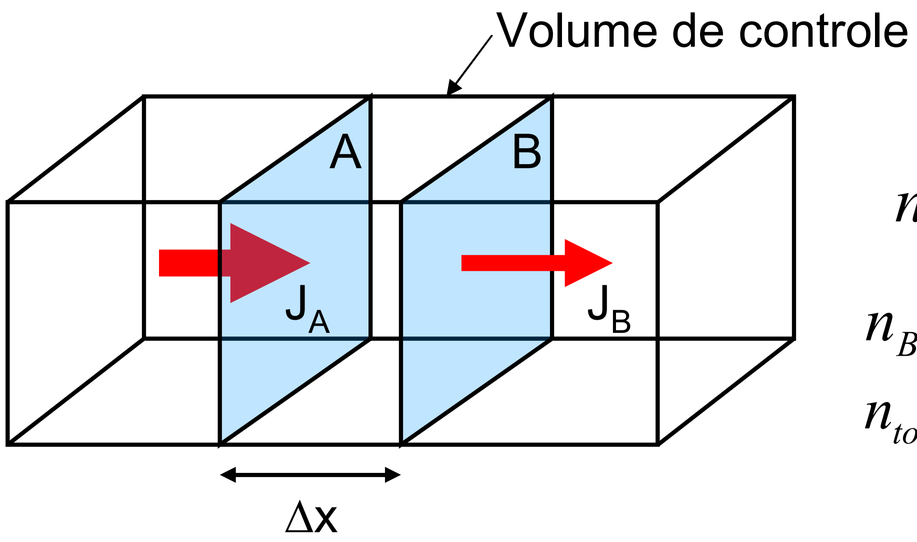
O coeficiente de difusão

$$D = D_0 \exp\left(\frac{-\Delta H}{RT}\right)$$

$$\ln D = \ln D_0 - \frac{\Delta H}{RT}$$



Difusão em regime transiente



$$n_A = J_A.A.\Delta t$$

$$n_B = J_B.A.\Delta t$$

$$n_{total} = n_A - n_B = (J_A - J_B).A.\Delta t$$

$$\Delta C = \frac{n_{total}}{V}$$

$$\frac{\Delta C}{\Delta t} = -\frac{\Delta J}{\Delta x} \qquad \begin{matrix} \Delta x \to 0 \\ \Delta t \to 0 \end{matrix} \qquad \boxed{\frac{\partial C}{\partial t} = -\frac{\partial J}{\partial x}}$$

2ª lei de Fick

$$\frac{\partial C}{\partial t} = -\frac{\partial J}{\partial x} \qquad J = -D\frac{\partial C}{\partial x}$$

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial x}\left(D\frac{\partial C}{\partial x}\right)$$

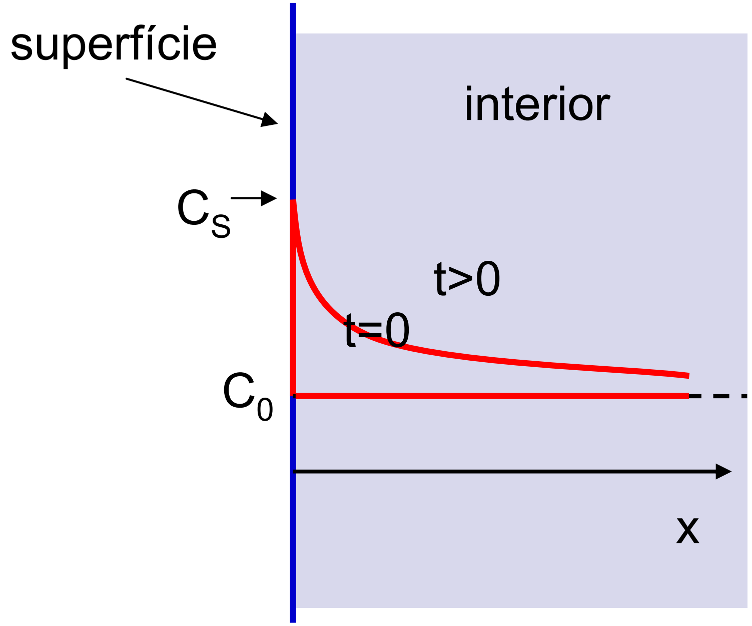
$$\boxed{\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2}}$$

$$\frac{\partial C}{\partial t} = D\left(\frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2} + \frac{\partial^2 C}{\partial z^2}\right) \qquad \boxed{\frac{\partial C}{\partial t} = D\nabla^2 C}$$

Uma solução da segunda lei

- Sólido semi-infinito de superfície plana
- C_s = cte
- $C_{(x)} = C_0$ para qualquer x > 0 quando t = 0
- Para t > 0, $C_{(\text{infinito})} = C_0$

$$\frac{C_{(x,t)} - C_0}{C_S - C_0} = 1 - erf\left(\frac{x}{2\sqrt{Dt}}\right)$$



Função erro

z	erf(z)	z	erf(z)	z	erf(z)
0	0.0000	**0.55**	0.5633	**1.3**	0.9340
0.025	0.0282	**0.60**	0.6038	**1.4**	0.9523
0.05	0.0564	**0.65**	0.6420	**1.5**	0.9661
0.10	0.1125	**0.70**	0.6778	**1.6**	0.9763
0.15	0.1680	**0.75**	0.7111	**1.7**	0.9838
0.20	0.2227	**0.80**	0.7421	**1.8**	0.9891
0.25	0.2763	**0.85**	0.7707	**1.9**	0.9928
0.30	0.3286	**0.90**	0.7969	**2.0**	0.9953
0.35	0.3794	**0.95**	0.8209	**2.2**	0.9981
0.40	0.4284	**1.00**	0.8427	**2.4**	0.9993
0.45	0.4755	**1.1**	0.8802	**2.6**	0.9998
0.50	0.5205	**1.2**	0.9103	**2.8**	0.9999

Aplicação da segunda lei

- Cementação
  - $C_0 = 0,2\%$
  - $C_S = 1\%$
  - T = 900ºC
  - t = 6 horas
  - C a 1 mm da superfície?

$$\frac{C_{(x,t)} - C_0}{C_S - C_0} = 1 - erf\left(\frac{x}{2\sqrt{Dt}}\right)$$

$$\frac{C_{(x,t)} - 0,2}{1 - 0,2} = 1 - erf\left(\frac{x}{2\sqrt{Dt}}\right)$$

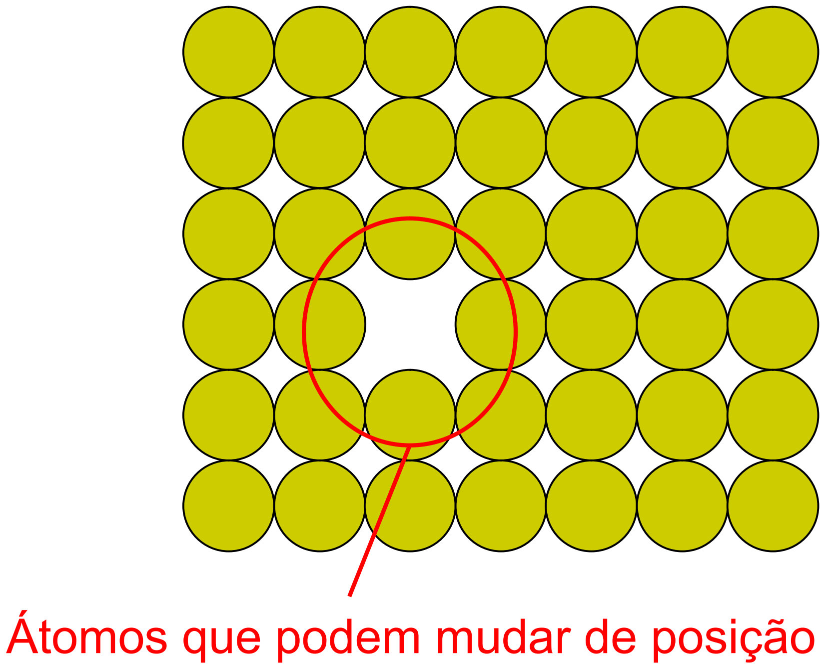
$$C_{(x,t)} = 1 - 0,8.erf\left(\frac{x}{2\sqrt{Dt}}\right)$$

$$z = \frac{x}{2\sqrt{Dt}} = \frac{0,1cm}{2\sqrt{3,55x10^{-6}\frac{cm^2}{s}.6.3600s}} = 0,255$$

$$erf(0,255) \cong 0,28$$

$$C_{(x,t)} \cong 1 - 0,8.0,28 \cong 0,77\%$$

Autodifusão



$$D = \frac{1}{6}\Gamma r^2$$

$$\Gamma = z\nu . C_v . \exp\left(\frac{-\Delta G_m}{RT}\right)$$

Concentração de vacâncias

$$C_v = \exp\left(\frac{-\Delta G_v}{RT}\right)$$

$$\Gamma = z\nu . \exp\left(\frac{-\Delta G_v}{RT}\right) . \exp\left(\frac{-\Delta G_m}{RT}\right)$$

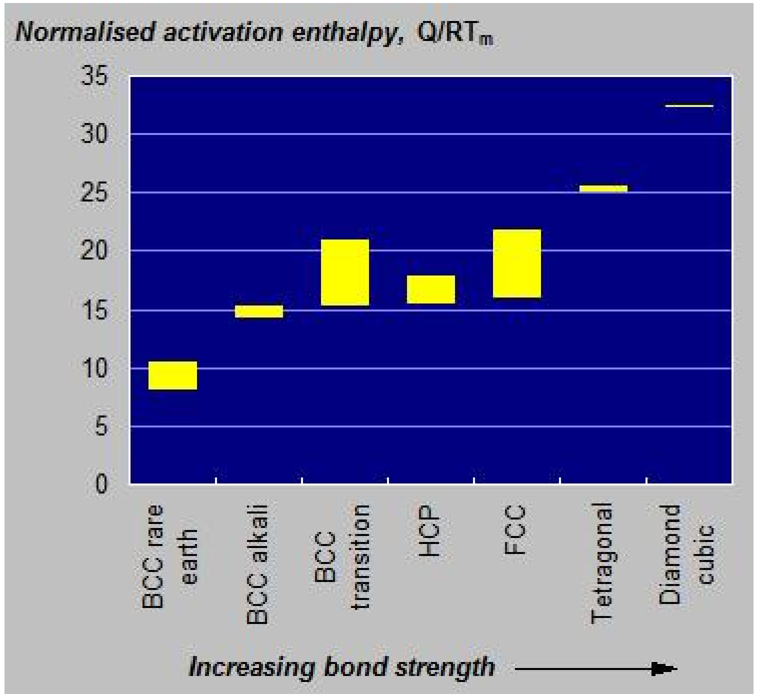
$$D = \frac{1}{6} r^2 z\nu \exp\left(\frac{-\Delta G_m - \Delta G_v}{RT}\right)$$

Autodifusão

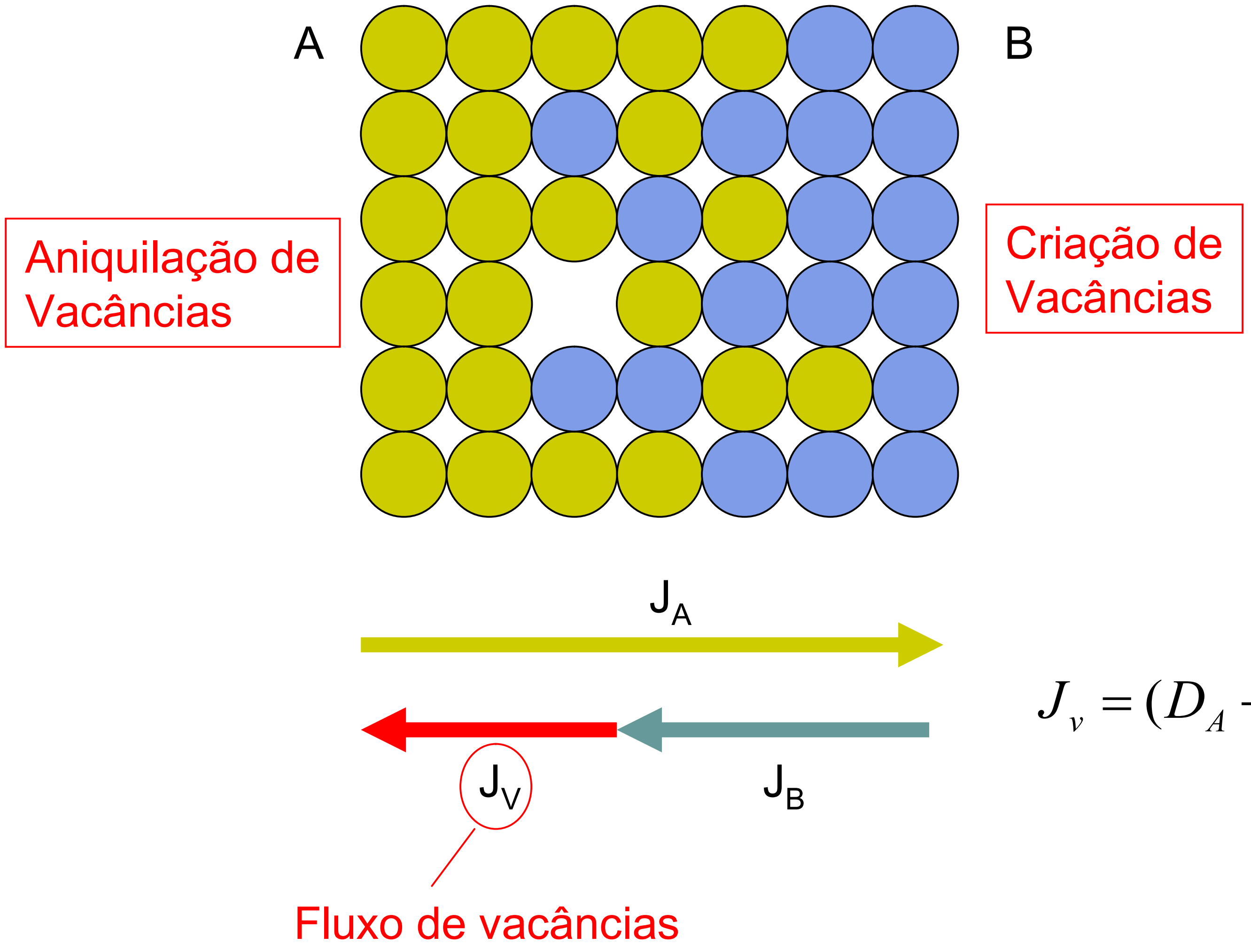
$$D = \frac{1}{6} r^2 z \nu \exp\left(\frac{-\Delta G_m - \Delta G_v}{RT}\right)$$

$$D = \frac{1}{6} r^2 z \nu \exp\left(\frac{\Delta S_m + \Delta S_v}{R}\right) \exp\left(\frac{-\Delta H_m - \Delta H_v}{RT}\right)$$

$$D = D_0 \exp\left(\frac{-\Delta H_A}{RT}\right)$$

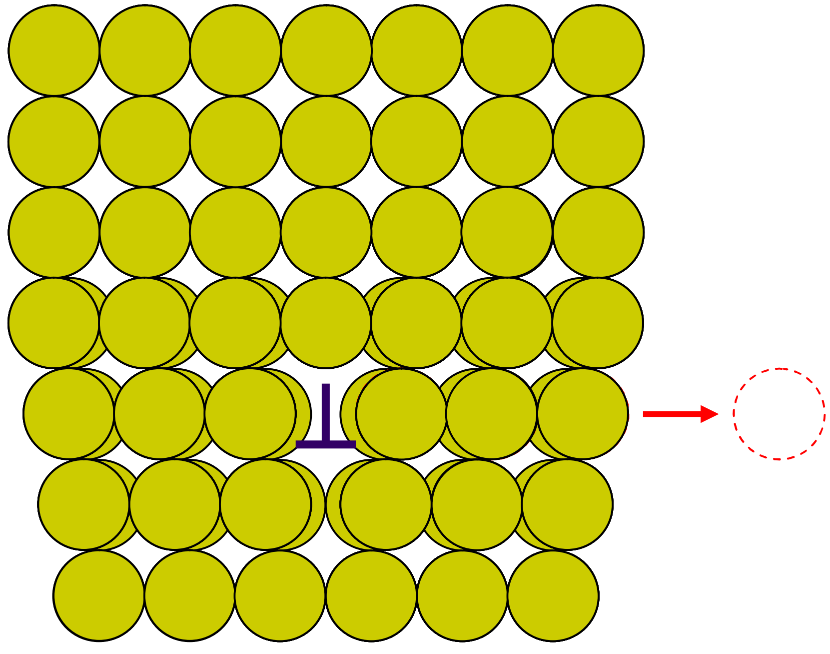


Difusão de Substitucionais

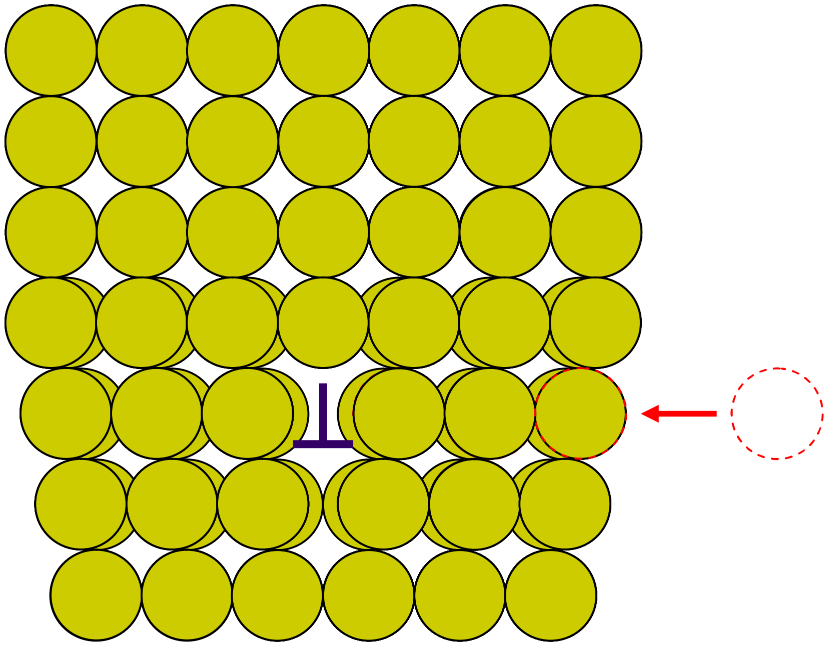


$$J_v = (D_A - D_B)\frac{\partial C_A}{\partial x}$$

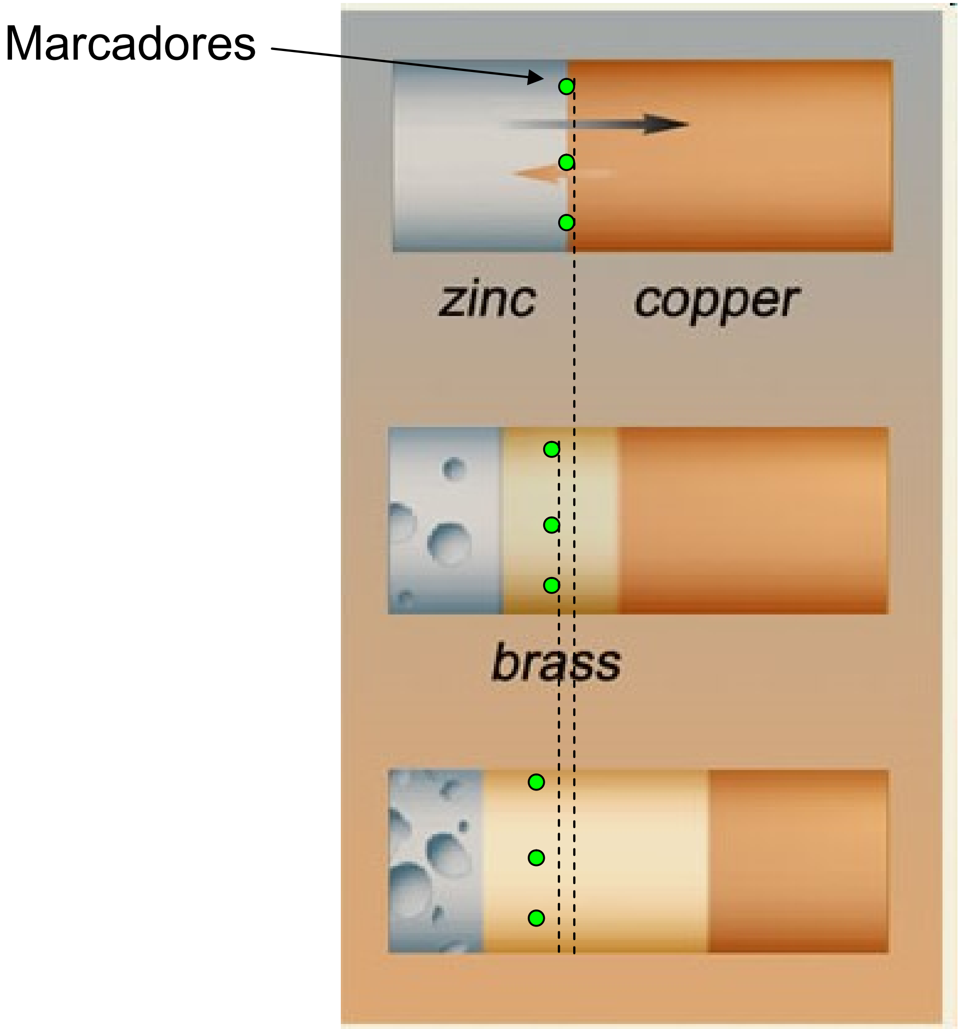
Criação de Vacâncias



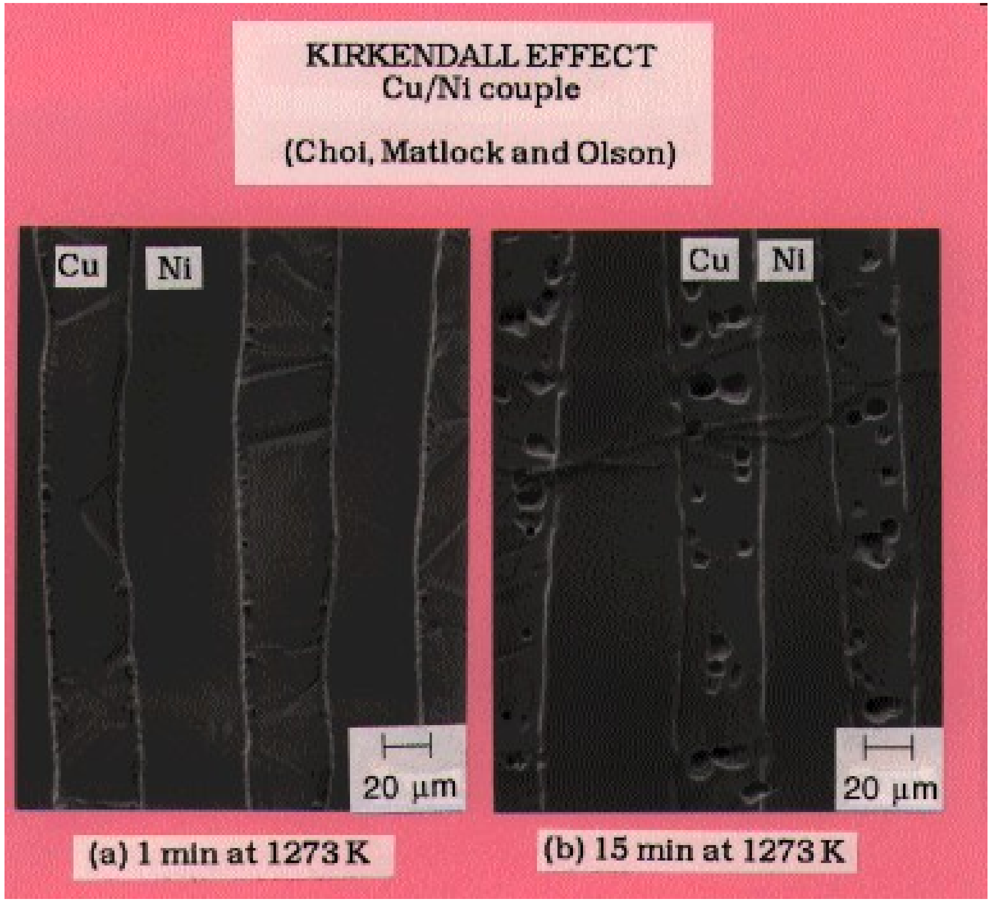
Aniquilação de Vacâncias



Efeito Kirkendall



Efeito Kirkendall

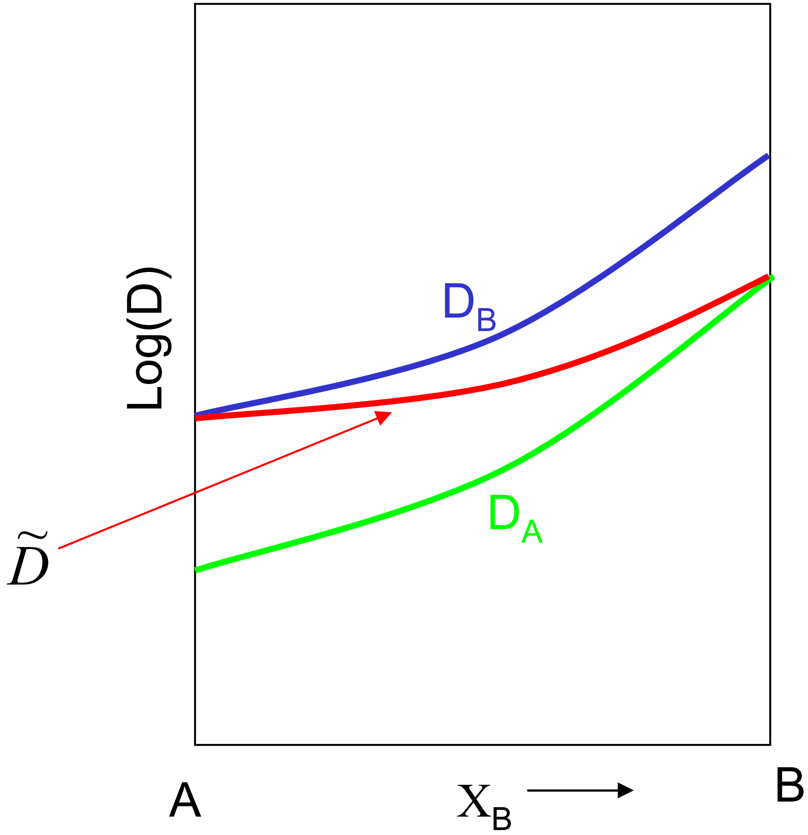


Equações de Darken

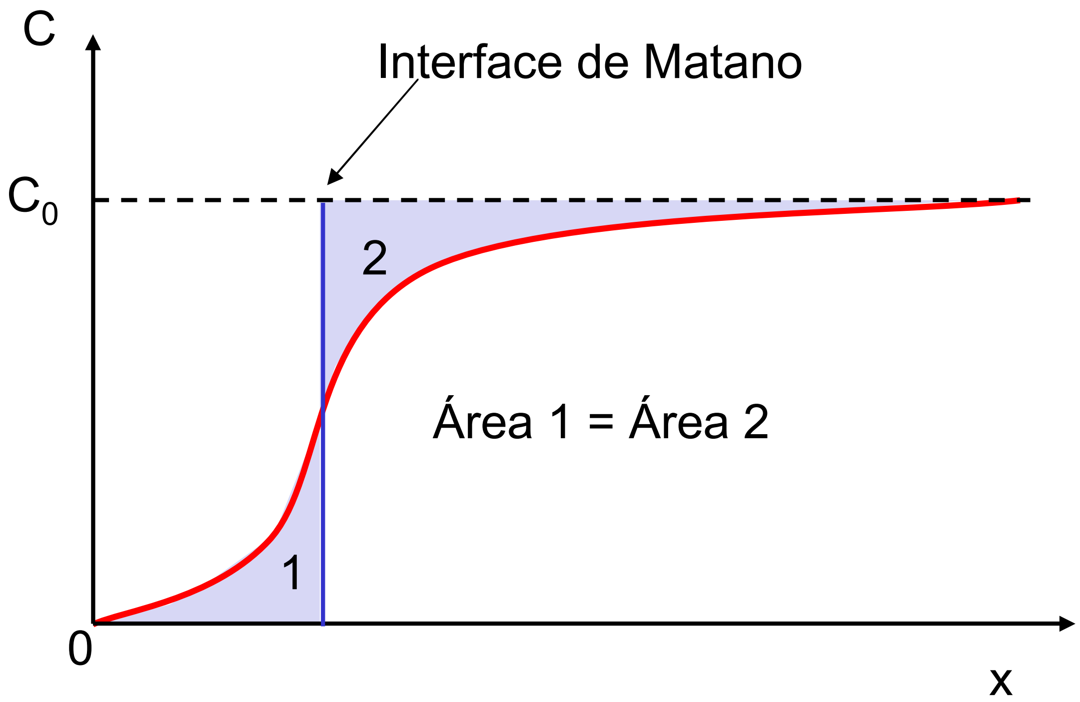
$$J_A = -(\chi_A D_A + \chi_B D_B)\frac{\partial C_A}{\partial x}$$

$$J_A = -\tilde{D}\frac{\partial C_A}{\partial x}$$

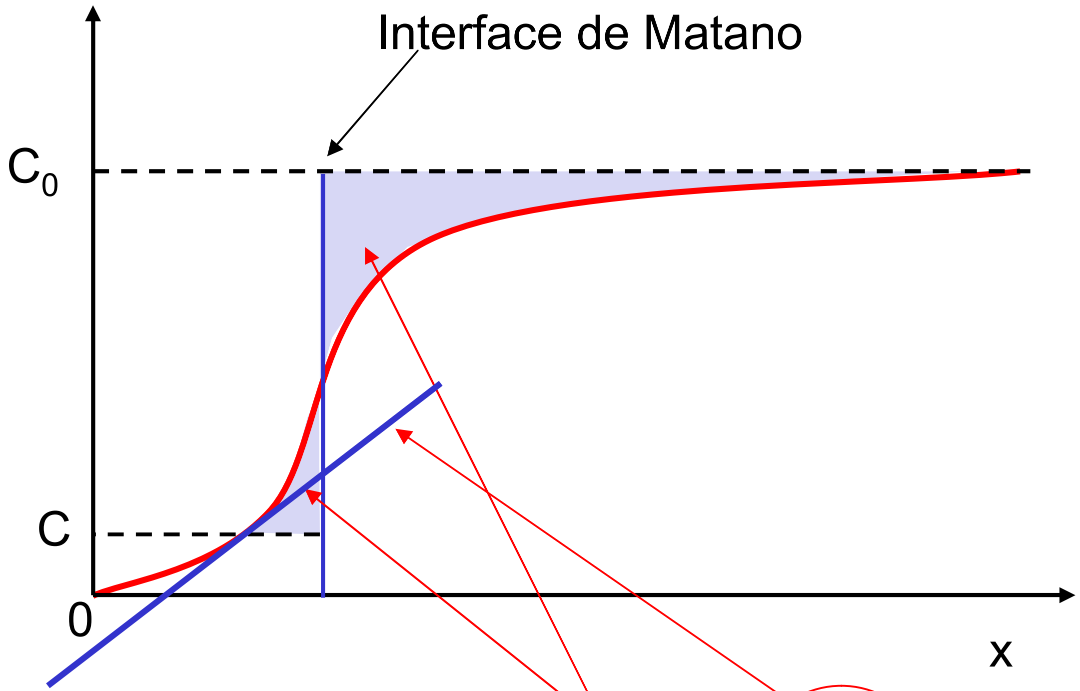
$$\frac{\partial C_A}{\partial t} = \frac{\partial}{\partial x}\left(\tilde{D}\frac{\partial C_A}{\partial x}\right)$$



Análise de Matano



Análise de Matano



$$\tilde{D} = -\frac{1}{2t}\int_{C_0}^{C} x\,dC \left(\frac{dx}{dC}\right)$$

Referências

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- Smallman, R.E. e Bishop, R.J. – Modern Physical Metallurgy and Materials Engineering, 6ª ed., Butterworth-Heinemann, 1999.
- Verhoeven, J.D. – Fundamentals of Physical Metallurgy, Wiley, 1989.