# Physics of Materials

## Chapter 5: Diffusion

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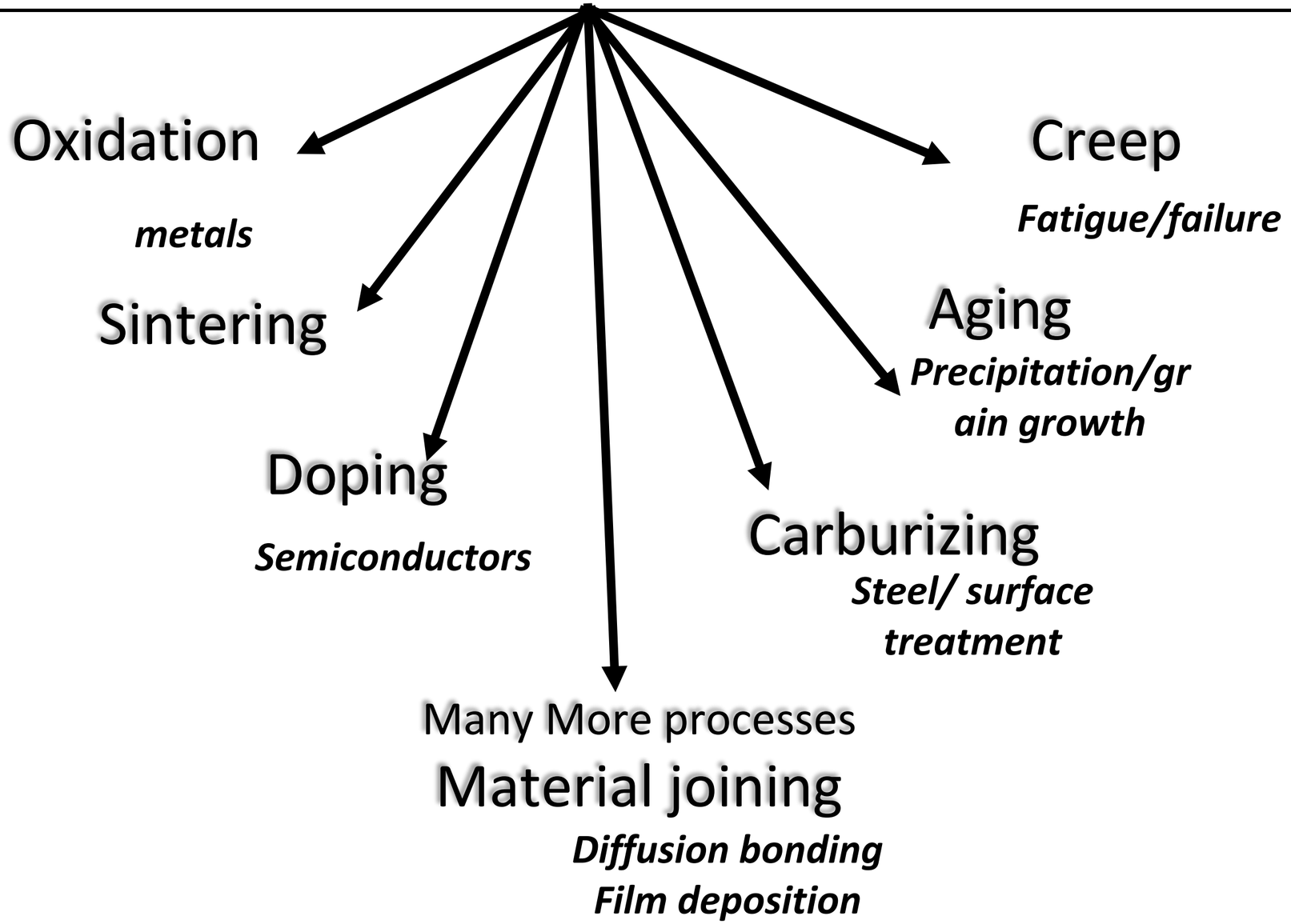
**Masters Course PHYS-307**

**Fall 2024**

# Roles of Diffusion



# Controlling diffusion is essential for fabricating Novel Spintronic and Quantum nanomaterials

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## Unraveling the sign reversal of the anomalous Hall effect in ferromagnet/heavy-metal ultrathin films

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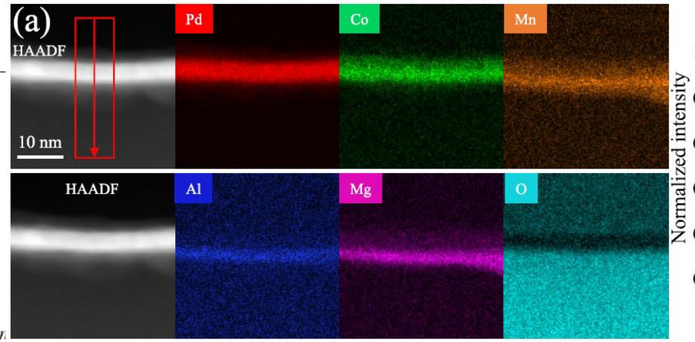
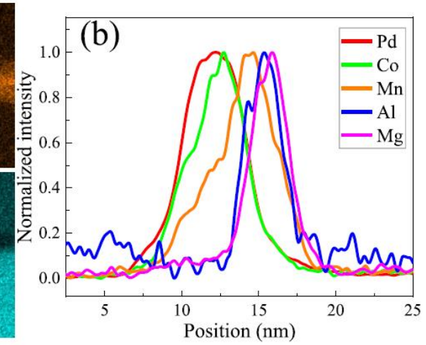
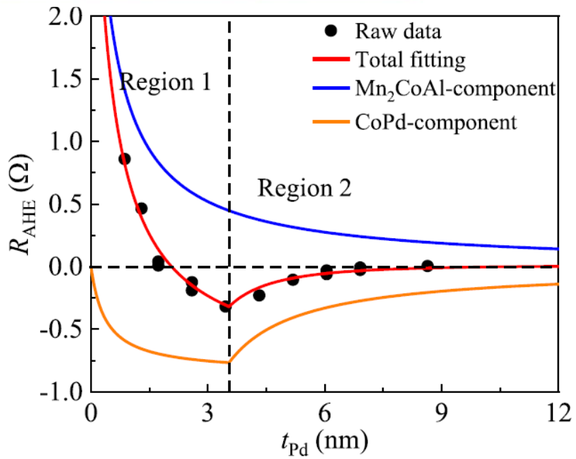
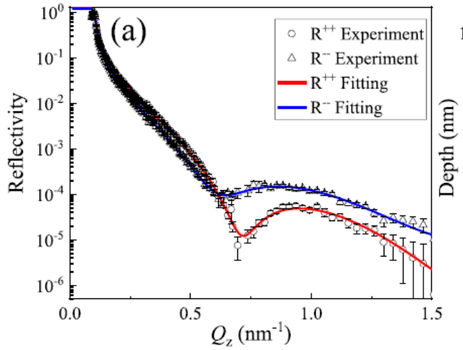
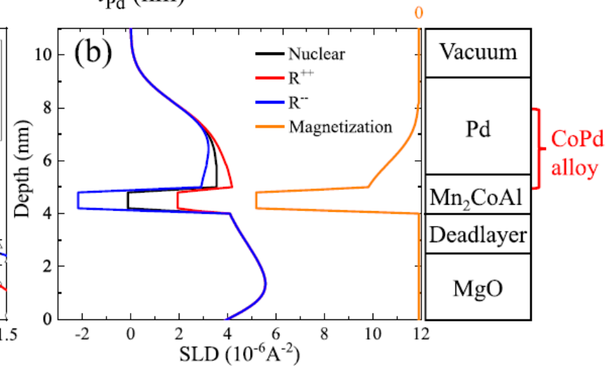
The sign reversal in the anomalous Hall effect (AHE) that occurs for material offers great prospects for AHE-based spintronic devices design. However, the mechanisms are still controversial in ultrathin ferromagnetic/heavy metal thin film systems due to the complicatedly interfacial effects. Here, we investigate the AHE sign reversal in ultrathin ferromagnetic $Mn_2CoAl$/Pd films, a system which has shown unusual AHE, significant spin-orbit coupling, and magnetic texturing. Element-sensitive cross-sectional STEM imaging and the depth-resolved magnetization profile from polarized neutron reflectometry identifies the presence of a second ferromagnetic layer from intermixed Co-Pd. To quantitatively explain the sign reversal of the AHE, we build a model based on two contributions, ferromagnetic $Mn_2CoAl$ and the intermixed CoPd layer. We also clarify that contributions to the AHE from magnetic proximity and spin Hall effect are negligible. Our work demonstrates that interfacial alloying can be a critical factor and provides insightful methods to determine the origins of the AHE in ferromagnet/heavy-metal thin film systems.



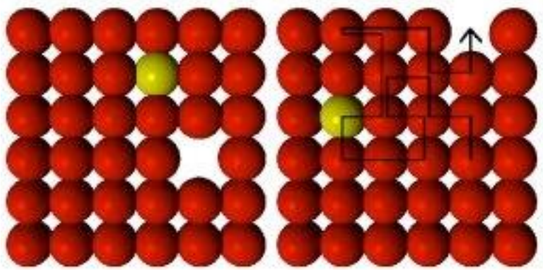



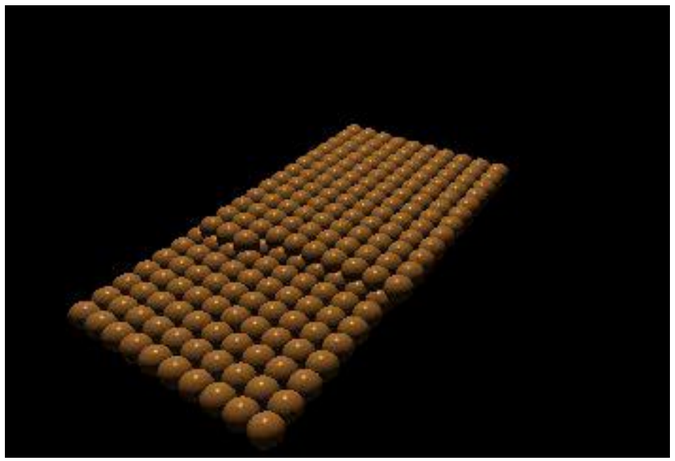



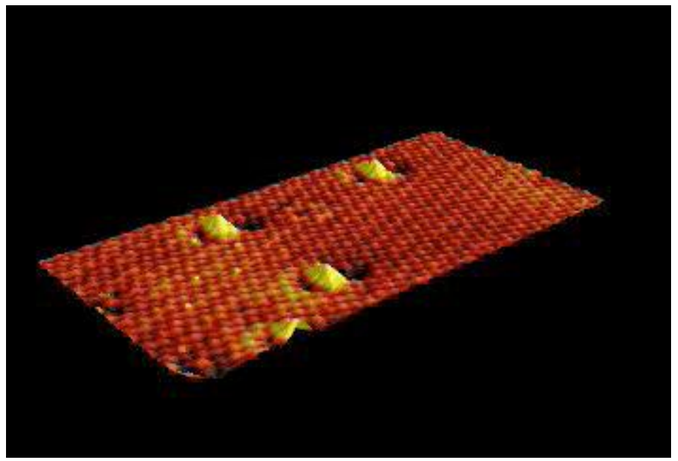



# The puzzle







vacancies

# Fundamental equations of diffusion

## Fick's laws

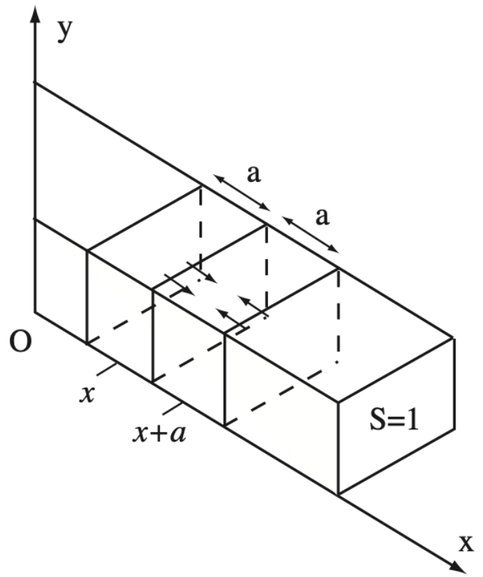
$$\vec{J}_A = -D_A \overrightarrow{grad} C_A$$ 1st law (steady state)

$$\frac{\partial C_A}{\partial t} = -div\vec{J}_A$$ 2nd law(non-steady state)

$$\downarrow$$

$$\frac{\partial C_A}{\partial t} = D_A \Delta C_A$$

# Demonstration of the 1st law in a one-dimensional system

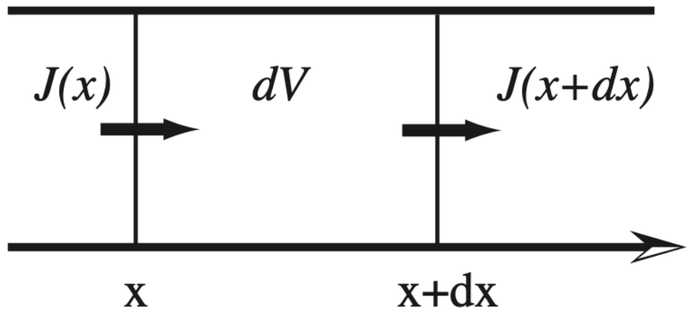



$$J_A = \frac{1}{2}\Gamma C_A(x)a - \frac{1}{2}\Gamma C_A(x+a)a$$

$$J_A = \frac{1}{2}\Gamma a\left[C_A(x) - C_A(x+a)\right] = -\frac{1}{2}\Gamma a^2 \frac{\partial C_A}{\partial x}$$

thus $D_A = \frac{1}{2}\Gamma a^2$

# Demonstration of the 2nd law in a one-dimensional system



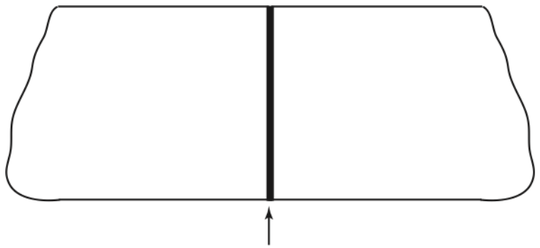

$$dV = Sdx$$

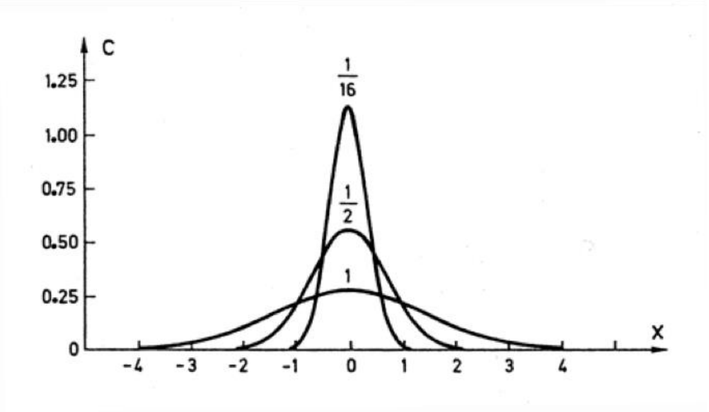
$$\frac{dn}{dt} = \left(J(x) - J(x+dx)\right)S = -S\frac{\partial J}{\partial x}dx = -\frac{\partial J}{\partial x}dV$$

$$\frac{1}{dV}\frac{dn}{dt} = \frac{dC}{dt} = -\frac{dJ}{dx}$$ in 3D: $$\frac{dC}{dt} = -div\vec{J}$$

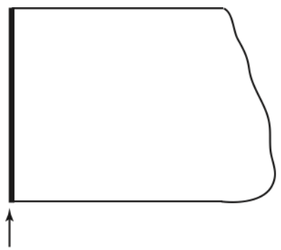
# Solutions of the Fick's second law: C(x,t)

Thin layer of an element B fully soluble in A





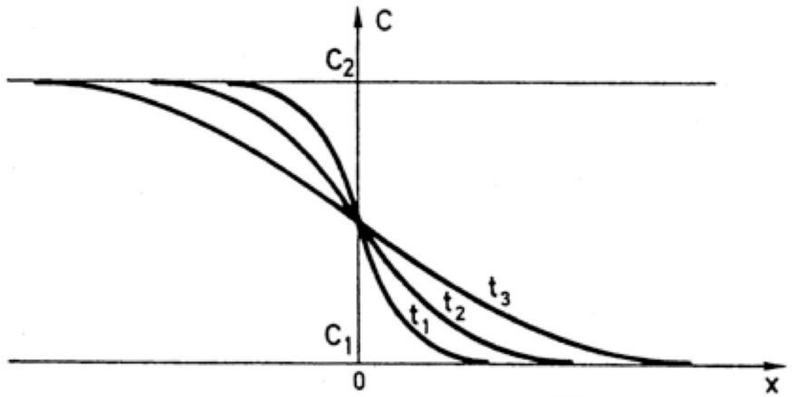

Surface layer: same solution



$$C(x,t) = \frac{M}{2\sqrt{\pi Dt}} e^{-\frac{x^2}{4Dt}}$$

# Solutions of the 2nd Fick equation: C(x,t)

## Interdiffusion



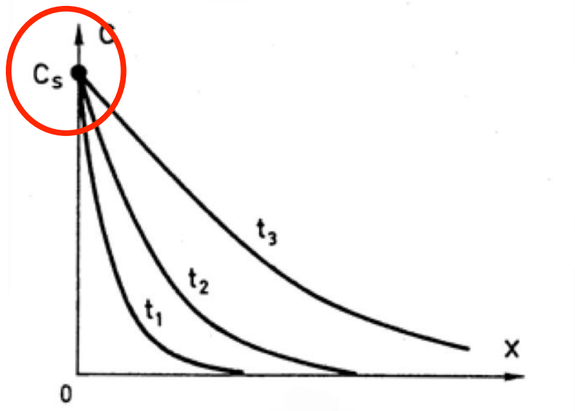

At $t=0$, $C=C_0$ for $-\infty < x < 0$

$C=0$ for $0 < x < \infty$

$$C(x,t) = \frac{C_0}{2}\left(1-\theta\left(\frac{x}{2\sqrt{Dt}}\right)\right)$$

$$\theta(y) = \frac{2}{\sqrt{\pi}}\int_0^y e^{-z^2}\,dz$$ is the error function

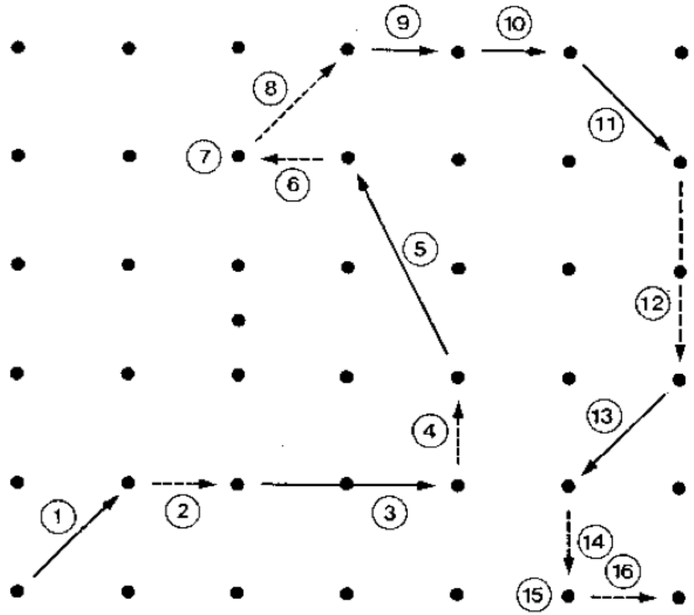
## Diffusion from a surface at constant concentration




$$\frac{C(x,t)-C_0}{C_s-C_0} = \left(1-\theta\left(\frac{x}{2\sqrt{Dt}}\right)\right)$$

# Diffusion coefficient and random walk

migration along vectors $\vec{\delta l}$ corresponding to dense directions




$$\vec{L} = \sum_i \vec{\delta l_i} \qquad \langle \vec{L} \rangle = 0 \qquad \langle \vec{L}^2 \rangle \neq 0$$

$$\langle \vec{L}^2 \rangle = \left\langle \sum_i \vec{\delta l}_i^2 \right\rangle + \left\langle \sum_{ij} \vec{\delta l}_i \vec{\delta l}_j \right\rangle$$

$$\langle \vec{L}^2 \rangle = \left\langle \sum_{i=1}^{n} \vec{\delta l}_i^2 \right\rangle = n\vec{\delta l}^2 = \Gamma t \vec{\delta l}^2$$

$$\vec{L}^2 = x^2 + y^2 + z^2 \Rightarrow \langle x^2 \rangle = \frac{1}{3}\langle \vec{L}^2 \rangle = \frac{1}{3}\Gamma t \delta l^2$$

# Particle flux though a surface S

$$\Phi = Jt = \frac{1}{2}C(x)\Delta - \frac{1}{2}C_A(x+\Delta)\Delta$$

$$J = -\frac{1}{2}\frac{\Delta^2}{t}\frac{\partial C(x)}{\partial x} = -\frac{1}{2}\frac{\langle x^2 \rangle}{t}\frac{\partial C(x)}{\partial x} \Rightarrow \boxed{D = \frac{1}{2}\frac{\langle x^2 \rangle}{t}} \text{ or } \langle x^2 \rangle = 2Dt$$

coordination number

$$\boxed{D = \frac{1}{6}\Gamma\delta l^2}$$ simple cubic

$$\boxed{D = \frac{1}{8}\Gamma\delta l^2}$$ body-centered cubic

$$\boxed{D = \frac{1}{12}\Gamma\delta l^2}$$ face-centered cubic

# Dependence with respect to temperature

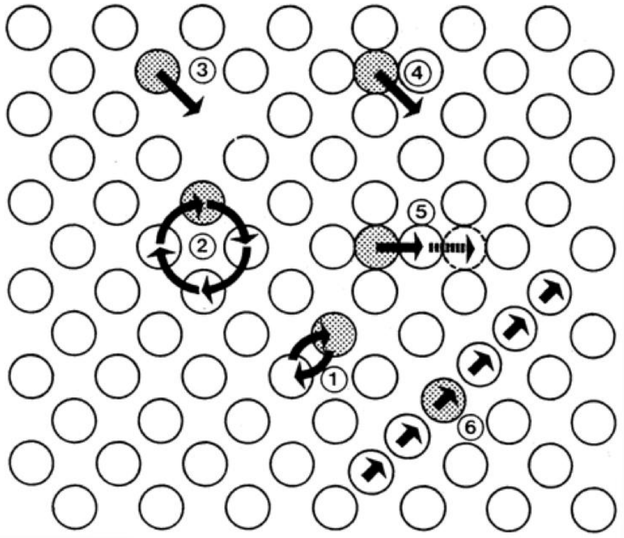
$D=D(T)$ since $\Gamma = \Gamma(T)$

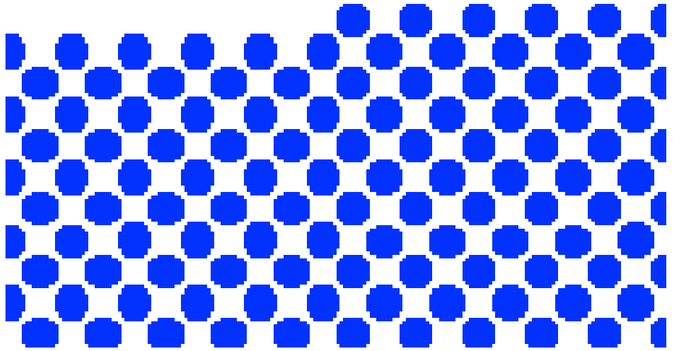
$$\Gamma = \nu_D P$$

$\nu_D$ is the Debye vibration frequency ~ $10^{13}$ Hz
Also known as the phonon frequency

$P \sim e^{-\frac{\Delta G}{kT}}$ is the probability that the atom has a sufficient energy to jump from one site to another

# Self-diffusion



vacancy mechanism

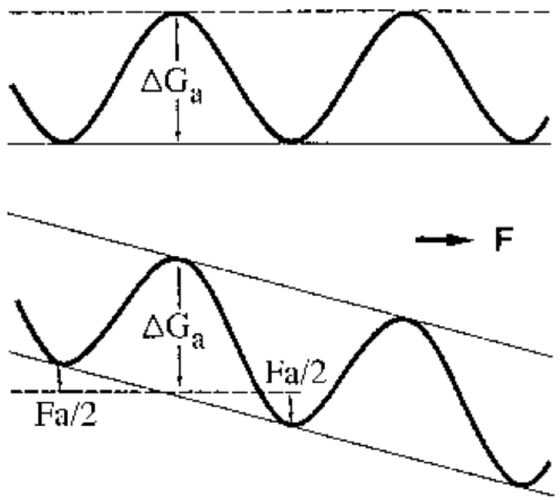
$$\Gamma = z\nu_D C_V \exp\left(-\Delta G_V^m / kT\right) = z\nu_D \exp\left(-\left(\Delta G_V^m + \Delta G_V^F\right)/kT\right)$$

$$D = \frac{1}{6}a^2 z\nu_D \exp\left(-\left(\Delta G_V^m + \Delta G_V^F\right)/kT\right)$$

$$D = \frac{1}{6}a^2 z\nu_D \exp\left(\left(\Delta S_V^m + \Delta S_V^F\right)/k\right)\exp\left(-\left(\Delta H_V^m + \Delta H_V^F\right)/kT\right) = D_0 \exp\left(-Q_{SD}/kT\right)$$

$$D_0 = \frac{1}{6}a^2 z\nu_D \exp\left(\left(\Delta S_V^m + \Delta S_V^F\right)/k\right)$$

# Force applied to a diffusing particle: Einstein equation




$$v = \frac{1}{2} a \left( \Gamma^{+} - \Gamma^{-} \right)$$

$$\Gamma^{+} = \nu_0 e^{-\frac{\Delta G - \frac{a}{2}F}{kT}} \qquad \Gamma^{-} = \nu_0 e^{-\frac{\Delta G + \frac{a}{2}F}{kT}}$$

$$\bar{v} = \frac{1}{2} a \nu_0 e^{-\frac{\Delta G}{kT}} \left( e^{\frac{Fa}{2kT}} - e^{-\frac{Fa}{2kT}} \right) \approx \frac{1}{2} a^2 \nu_0 e^{-\frac{\Delta G}{kT}} \frac{F}{kT}$$

$$D_A = \frac{1}{2} a^2 \nu_0 e^{-\frac{\Delta G}{kT}} \qquad \text{and} \qquad \boxed{v = \frac{D_A F}{kT}}$$

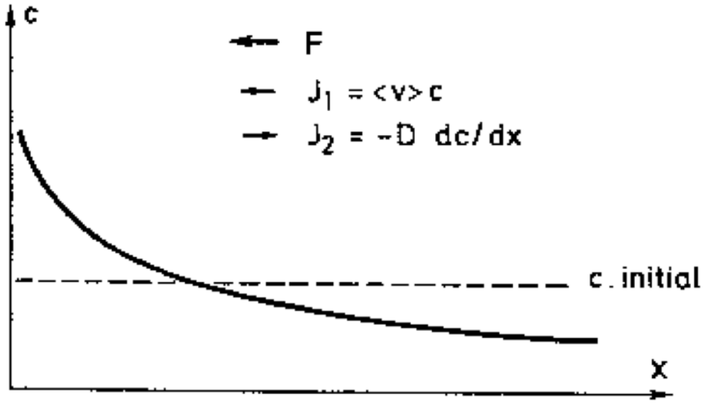
Einstein equation

# Demonstration in the case where the force derives from a potential

Particle flux $J_1 = \langle v \rangle C$

Concentration gradient $J_2 = -D\frac{dC}{dx}$

$$J = 0 \Rightarrow D\frac{dC}{dx} = \langle v \rangle C$$




If $F$ derives from a potential $F = -\frac{d\Phi}{dx}$

We suppose $C(x) = C_0 \exp(-\Phi(x)/kT)$

$$\frac{dC}{dx} = -\frac{C}{kT}\frac{d\Phi}{dx} = \frac{CF}{kT} \Rightarrow \langle v \rangle = \frac{FD}{kT}$$

# Darken equation

For instance

$$\vec{F} = -\overrightarrow{grad}\mu_A$$

$\mu_A$ is the chemical potential

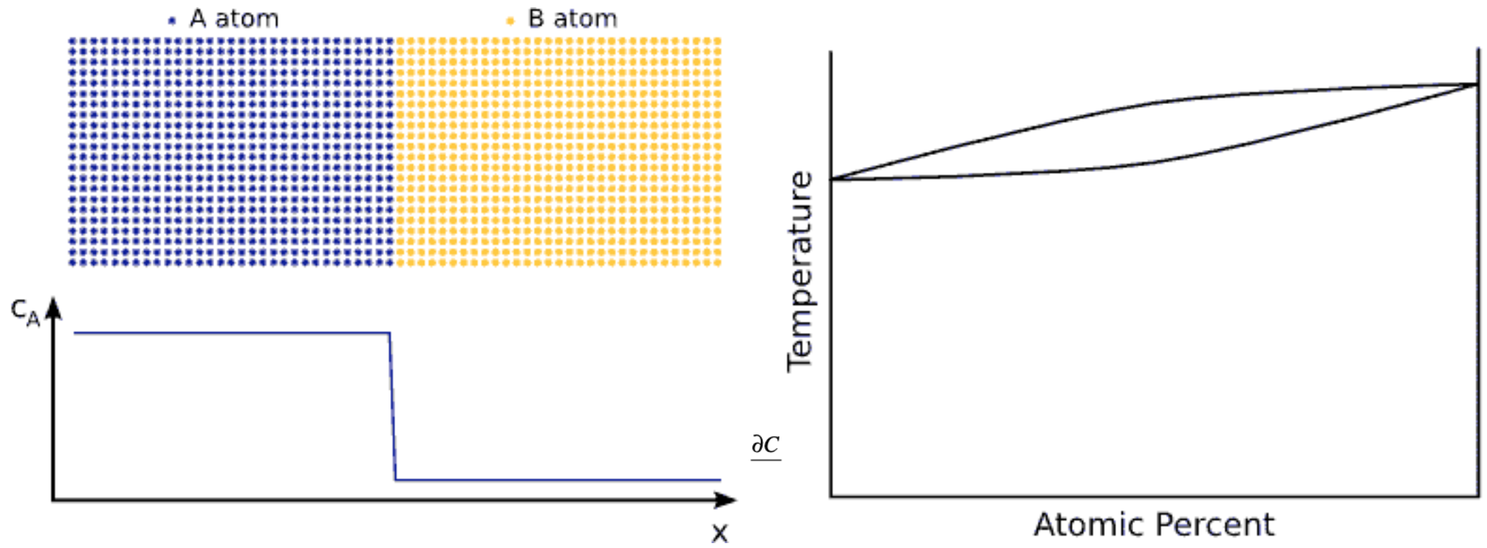
$$\mu_A = kT \ln C_A \Rightarrow F = -\frac{kT}{C_A}\frac{dC_A}{dx}$$

$$\vec{J}_A = C_A \vec{v}_A = -\frac{C_A D_A}{kT}\overrightarrow{grad}\mu_A = -\frac{C_A D_A}{kT}\frac{\partial \mu_A}{\partial C_A}\overrightarrow{grad}C_A = -D_A^* \cdot \overrightarrow{grad}C_A$$

$$D_A^* = \frac{C_A D_A}{kT}\frac{\partial \mu_A}{\partial C_A}$$

$$\frac{\partial C_A}{\partial t} = div\left(D_A^* \cdot \overrightarrow{grad}C_A\right)$$

# Interdiffusion : Boltzmann-Matano method




We must solve the one dimensional Fick equation

$$\frac{\partial C_A}{\partial t} = \frac{\partial}{\partial x}\left( D_A^* \cdot \frac{\partial C_A}{\partial x} \right)$$

# Reminder on scaling laws

$$\ddot{\vec{x}}_1(t) = -\frac{GM}{\left|\vec{x}_1(t)\right|^3}\vec{x}_1(t) \qquad t' = \tau t \quad \vec{x}'_1 = \lambda \vec{x}_1$$

$$\ddot{\vec{x}}'_1(t) = -\frac{G'M\ \vec{x}'_1(t)}{\left|\vec{x}'_1\right|^3} \qquad \vec{x}'_1(t=0) = \lambda \vec{x}_1(t=0)$$

$$\ddot{\vec{x}}_1(t) = \frac{\tau^2}{\lambda^3} G' \frac{M\ \vec{x}_1(t)}{\left|\vec{x}_1\right|^3} \Rightarrow \frac{\tau^2}{\lambda^3} G' = G$$

Consider another planet (2) characterized by:

$$\ddot{\vec{x}}_2(t) = -\frac{G'M\vec{x}_2(t)}{\left|\vec{x}_2(t)\right|^3} \qquad \vec{x}_2(t=0) = \lambda \vec{x}_1(t=0)$$

If $G = G' \Rightarrow \frac{\tau^2}{\lambda^3} = 1$ $\quad \vec{x}'_1(t')$ and $\vec{x}_2(t)$ same trajectories

$$\left(\frac{t'}{t}\right)^2 = \left(\frac{x'_1}{x_1}\right)^3 = \left(\frac{x_2}{x_1}\right)^3$$ Kepler's 3rd law

# Scale changes in the diffusion equation

$$\frac{\partial}{\partial t}c_1(x,t)=\frac{\partial}{\partial x}\left(D\frac{\partial}{\partial x}c_1(x,t)\right) \qquad c_1(t=0)=c(x,0)$$

$$\frac{\partial}{\partial t'}c'_1(x',t')=\frac{\partial}{\partial x'}\left(D'\frac{\partial}{\partial x'}c'_1(x',t')\right) \qquad c'_1(t=0)=c(x',0)$$

$$\frac{\partial}{\partial t}c'_1(\lambda x,\tau t)=\frac{\partial}{\partial x}\left(\frac{\tau D'}{\lambda^2}\frac{\partial}{\partial x}c'_1(\lambda x,\tau t)\right) \qquad t'=\tau t \quad x'_1=\lambda x_1$$

New concentration profile $c_2(x,t)$

$$\frac{\partial}{\partial t_2}c_2(x_2,t_2)=\frac{\partial}{\partial x_2}\left(D\frac{\partial}{\partial x_2}c_2(x_2,t_2)\right) \qquad c_2(t=0)=c(\lambda x,0)$$

$$\frac{\tau D'}{\lambda^2}=D \qquad \frac{x}{\sqrt{t}}=\frac{x'}{\sqrt{t'}}$$

This can be deduced from the mean free path

$$2D'=\frac{\vec{x}'^2}{t'}=\frac{\lambda^2}{\tau}\frac{\vec{x}^2}{t}=2D\frac{\lambda^2}{\tau} \Rightarrow D'=\frac{D\lambda^2}{\tau}$$

# Solution of the diffusion equation

$$\frac{\partial C_A}{\partial t} = \frac{\partial}{\partial x}\left( D_A^* \cdot \frac{\partial C_A}{\partial x} \right)$$

Variable change $\boxed{\eta = \frac{x}{\sqrt{t}}}$

$$\frac{\partial}{\partial t} = \frac{\partial \eta}{\partial t}\frac{\partial}{\partial \eta} = -\frac{x}{2t^{3/2}}\frac{\partial}{\partial \eta}$$

$$\frac{\partial}{\partial x} = \frac{\partial \eta}{\partial x}\frac{\partial}{\partial \eta} = \frac{1}{\sqrt{t}}\frac{\partial}{\partial \eta}$$

We get

$$-\frac{\eta}{2}\frac{dC_A}{d\eta} = \frac{d}{d\eta}\left( D*_A \frac{dC_A}{d\eta} \right)$$

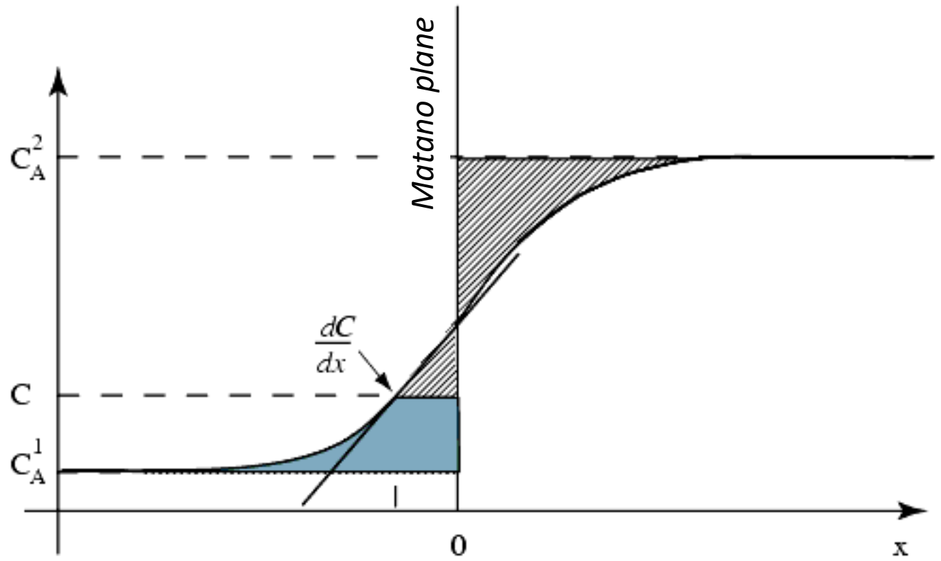
$$D*_A(C) = -\frac{1}{2}\frac{\int_{C_A}^{C} \eta\, dC}{\left.\frac{dC_A}{d\eta}\right|_C}$$

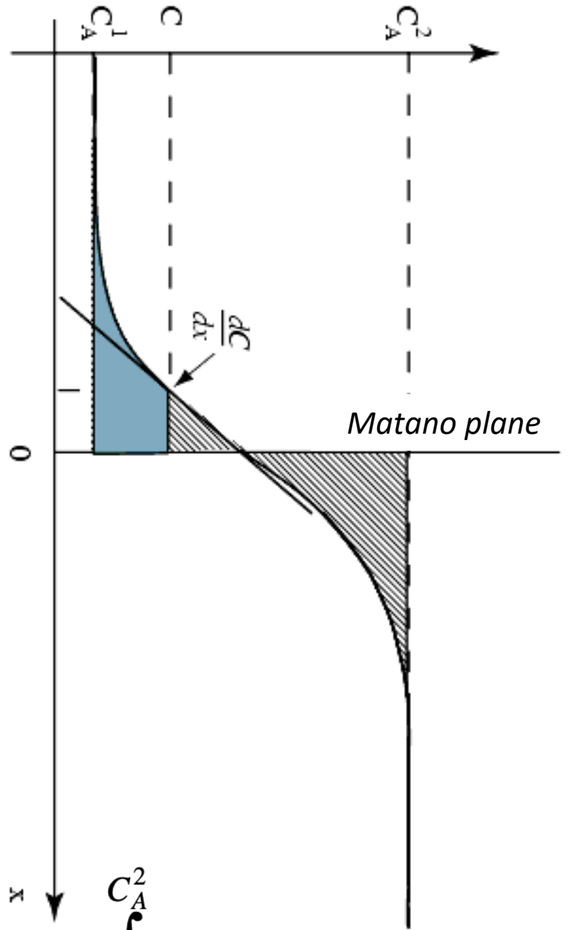
# Solving the diffusion equation: Boltzmann-Matano method

In terms of variables $x$ and $t$

$$D^*_A(C) = -\frac{1}{2}\frac{\int_{C_A^1}^{C} x\,dC}{\left.\frac{dC_A}{dx}\right|_C}$$

experimental method




$$\int_{C_A^1}^{C_A^2} x\,dc = 0$$

# Solving the diffusion equation: Heaviside step distribution

$$C_A(x,t=0)=\theta(x) \qquad C_B(x,t=0)=\theta(-x)$$

$$\lim_{t\to 0}\left.\frac{\partial C_A}{\partial x}\right|_t=\delta(x) \qquad D^*_A=constant$$

$$\frac{\partial C_A}{\partial t}=\frac{\partial}{\partial x}\left(D_A^*\cdot\frac{\partial C_A}{\partial x}\right)$$

$$-\frac{\eta}{2}\frac{dC_A}{d\eta}=D^*_A\frac{d^2}{d\eta^2}C_A$$

Consider a reduced variable $\eta=\frac{x}{\sqrt{t}}$

$$\frac{d}{d\eta}\left(C_A(\eta)\right)=ke^{-\eta^2/4D^*_A}$$

$$\left.\frac{\partial c}{\partial x}\right)_t=\frac{\partial c}{\partial \eta}\frac{\partial \eta}{\partial x}=\frac{1}{\sqrt{t}}\frac{\partial c}{\partial \eta}$$

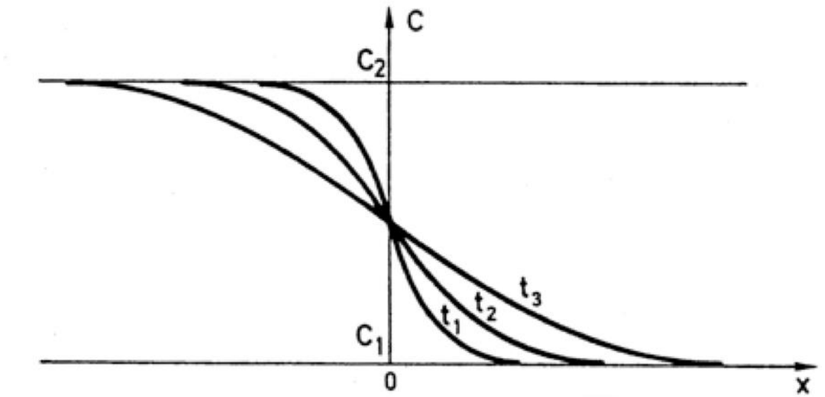
$$\Rightarrow \quad \lim_{t\to 0}\left(\frac{k}{\sqrt{t}}e^{-\eta^2/4D^*_A}\right)=\delta(x) \;\Rightarrow\; k=\frac{1}{\sqrt{4D^*_A\pi}}$$

# Solving the diffusion equation: Heaviside step distribution

$$C_A(x,t=0)=\theta(x) \qquad C_B(x,t=0)=\theta(-x)$$

$$\lim_{t\to 0}\left.\frac{\partial C_A}{\partial x}\right|_t=\delta(x) \qquad D^*_A = constant$$

$$\frac{\partial C_A}{\partial t}=\frac{\partial}{\partial x}\left(D_A^*\cdot\frac{\partial C_A}{\partial x}\right)$$

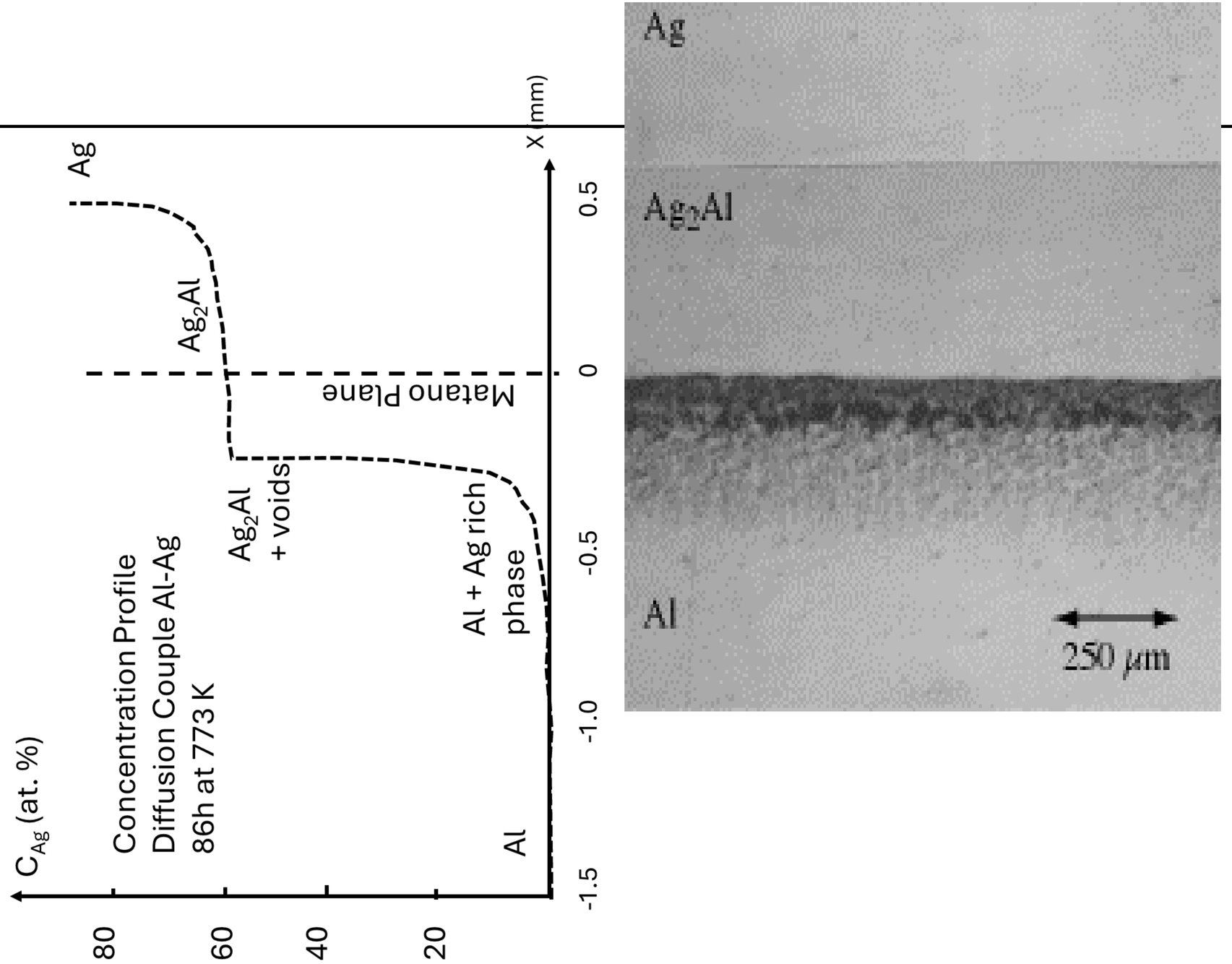


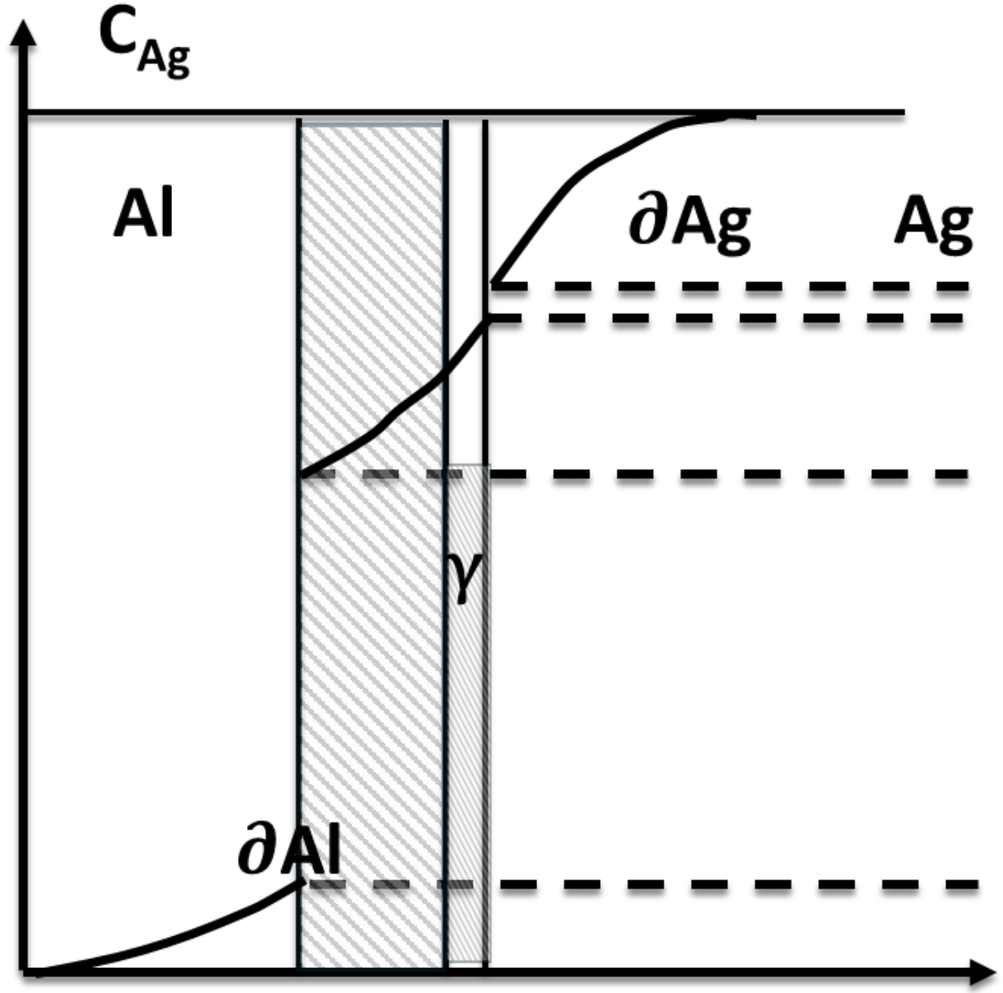

$$\frac{d}{d\eta}C_A=\frac{1}{\sqrt{4\pi D^*_A}}\exp\left[-\eta^2/4D^*_A\right]$$

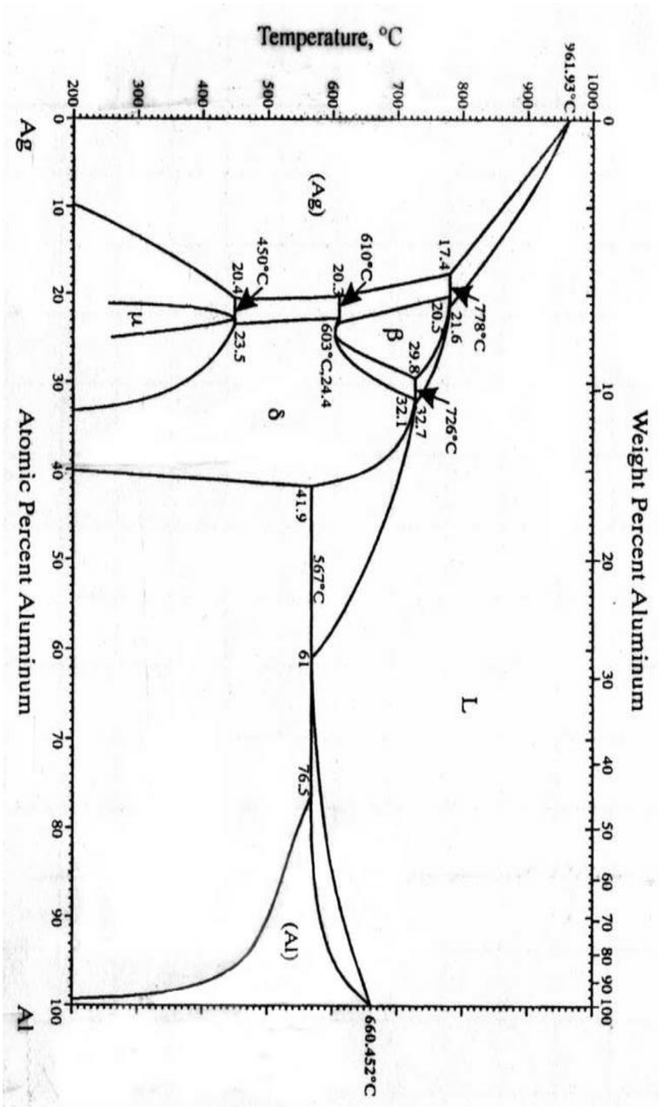
$$\frac{\partial C_A}{\partial x}=\frac{1}{\sqrt{4\pi D^*_A\, t}}\exp\left[-x^2/4D^*_A\, t\right]$$

$$C_A(x)=C_0 erf\left(x/2\sqrt{D^*_A t}\right) \qquad erf(x)=\frac{2}{\sqrt{\pi}}\int_0^x e^{-z^2}\,dz$$

In reality, the situation is actually different.....

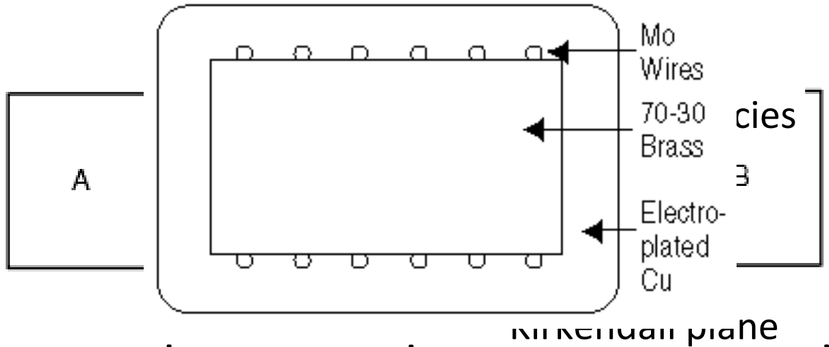



$C_{Ag}$
Al
∂Ag
Ag
γ
∂Al


Temperature, °C
961.93°C
Ag
(Ag)
450°C
610°C
778°C
726°C
567°C
660.452°C
μ
β
δ
L
(Al)
Atomic Percent Aluminum
Weight Percent Aluminum
Al

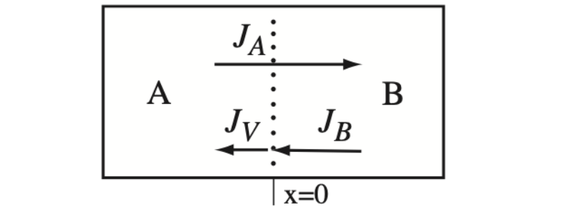
# Kirkendall effect

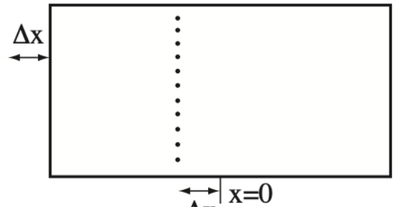
Original experiment (1947)

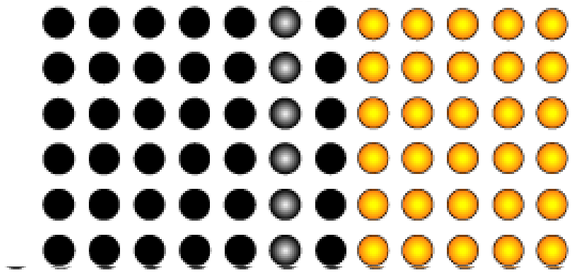



Da Silva, Mehl configuration (1951)

Explanation: the sample moves depending on the lab reference frame



# Kirkendall effect: solving of the problem

$$J_v + J_A + J_B = 0$$ Fixed reference (lab)

$$J_A = -D_A^* \frac{\partial C_A}{\partial x} \qquad J_B = -D_B^* \frac{\partial C_B}{\partial x}$$

Velocity of vacancies

$$v_v = J_v \Omega \qquad v_v = -(J_A + J_B)\Omega$$

Moving reference (sample) $\Rightarrow J_A^0 + J_B^0 = 0$ $C_A + C_B = const.$

$$\frac{\partial C_A}{\partial x} = -\frac{\partial C_B}{\partial x} \qquad v_v = (D_A^* - D_B^*)\frac{\partial X_A}{\partial x} \qquad X_A = C_A \cdot \Omega$$

$$J_A^0 = -\tilde{D}\frac{\partial C_A}{\partial x} \qquad J_B^0 = -\tilde{D}\frac{\partial C_B}{\partial x}$$

# Kirkendall effect: solving the problem

$$J_A^0 = J_A + v_v C_A = -D_A^* \frac{\partial C_A}{\partial x} + v_v C_A \qquad J_B^0 = J_B + v_v C_B = -D_B^* \frac{\partial C_A}{\partial x} + v_v C_B$$

$$J_A^0 == -D_A^* \frac{\partial C_A}{\partial x} + \left(D_A^* - D_B^*\right)\frac{\partial C_A}{\partial x} X_A = -\left(D_A^* - X_A D_A^* + X_A D_B^*\right)\frac{\partial C_A}{\partial x}$$

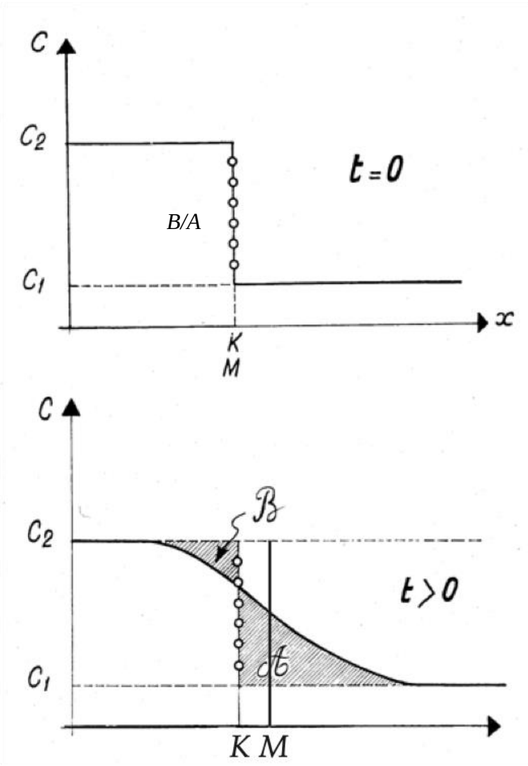
$$\tilde{D} = X_B D_A^* + X_A D_B^*$$

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

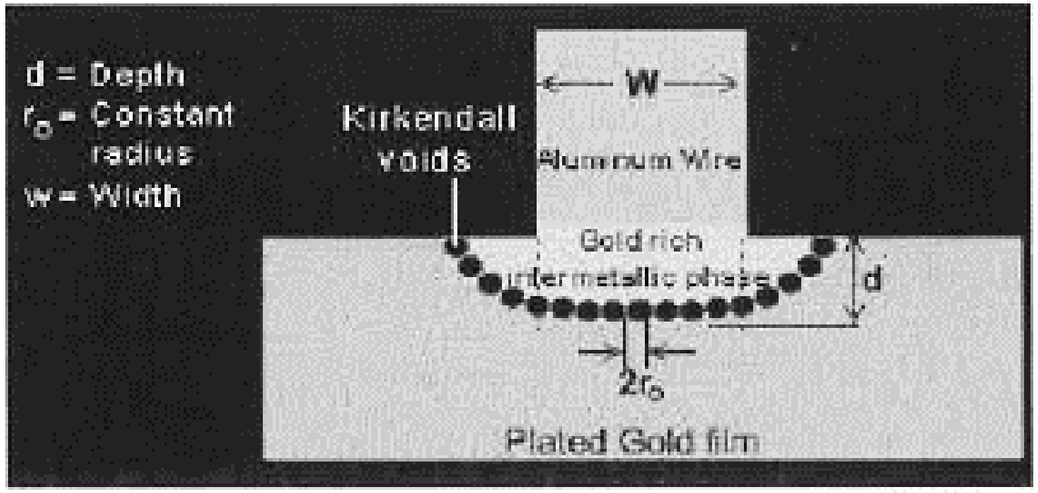
We get $\tilde{D}$ by the B-M method

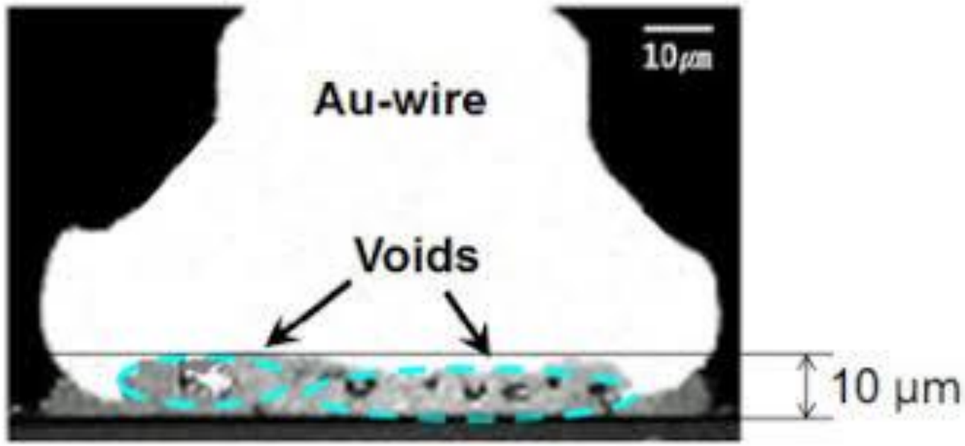
velocity of Kirkendall plane $v_v = (D_A^* - D_B^*)\frac{\partial X_A}{\partial x}$

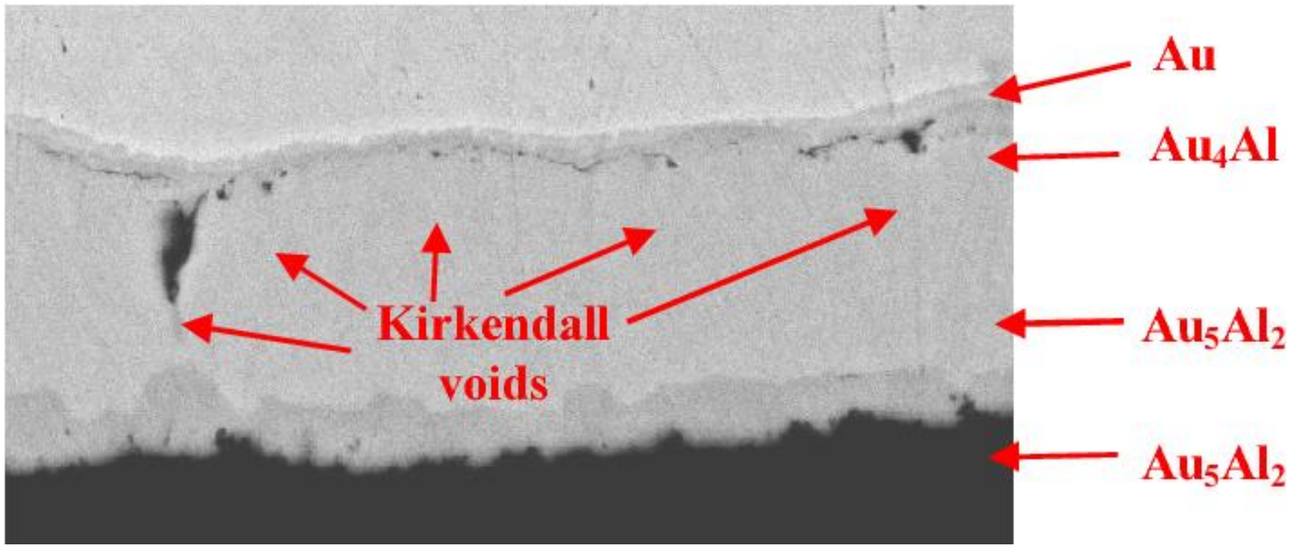
$D^\star_B / D^\star_A = B/A$



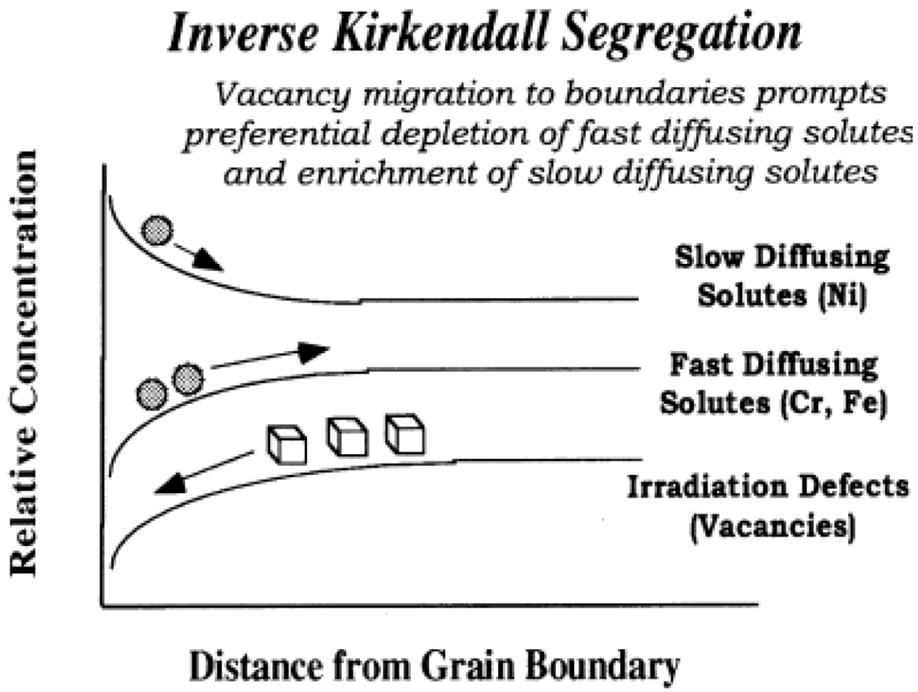
# Example of the Kirkendall effect: Wire Bonding

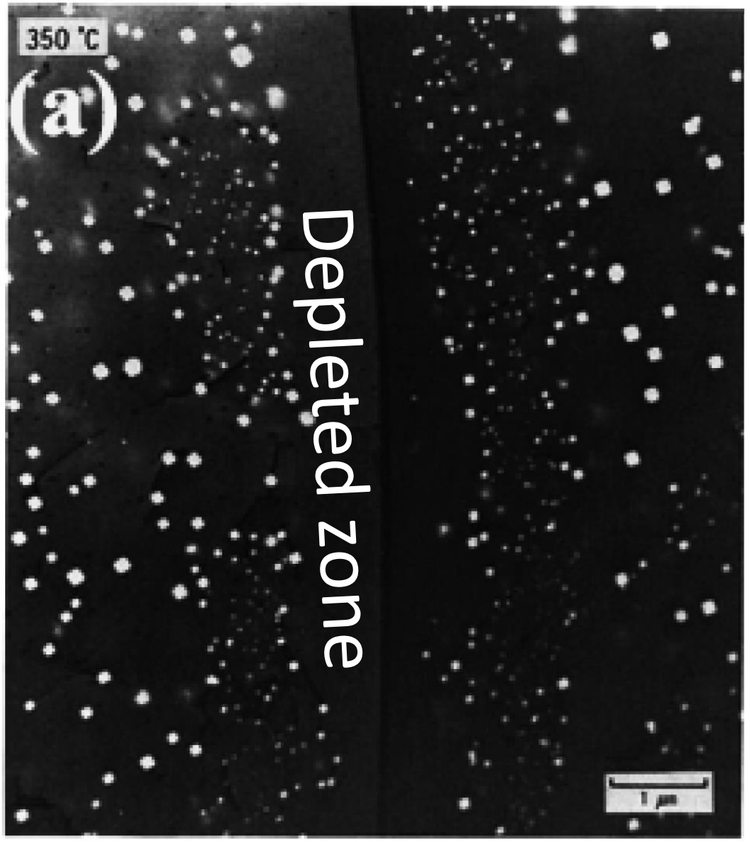


# Inverse Kirkendall effect during Neutron Irradiation



# Some examples of diffusion coefficients: Fick's equations

## Self diffusion

13–10 *Diffusion in metals*

**Table 13.1** SELF-DIFFUSION IN SOLID ELEMENTS—*continued*

| Element | $A$ $cm^2 s^{-1}$ | $Q$ $kJ\ mol^{-1}$ | Temp. range K |
|---|---|---|---|
| *Group IIB* | | | |
| Zn | ∥c 0.13 | 91.7 | 513–691 |
| | ⊥c 0.18 | 96.3 | |
| Cd | ∥c 0.118 | 77.92 | 420 600 |
| | ⊥c 0.183 | 82.02 | |
| *Group IIIA and rare earths* | | | |
| Y | ∥c 0.82 | 252.5 | 1 173-1 573 |
| | ⊥c 5.2 | 280.9 | |
| β-La | 1.5 | 188.8 | 933 1 113 |
| γ-La | 0.013 | 102.6 | 1 140 -1 170 |
| | 0.11 | 125.2 | 1 151 -1 183 |
| γ-Ce | 0.55 | 153.2 | 801–965 |
| δ-Ce | 0.012 | 90.0 | 992–1 044 |
| β-Pr | 0.087 | 123.1 | 1 323-1.473 |
| Er | ∥c 3.71 | 301.66 | 1 479–1 684 |
| | ⊥c 4.51 | 302.58 | |
| Eu | 1.0 | 144.4 | 771 -1 072 |
| β-Gd | 0.01 | 136.9 | 1 549–1 581 |
| α-Yb | 0.034 | 146.79 | 823- 983 |
| γ-Yb | 0.12 | 121.0 | 1 031 -1 083 |
| *Group IIIB* | | | |
| Al | 1.71 | 142.4 | 723 923 |
| | 2.25 | 144.4 | 573–923 |
| | 0.137 | 123.5 | 298 581[a] |
| | 0.176 | 126.4 | 358 482 |
| Ga | $D=5.3\ 10^{-13}$ | | 282.8 |
| | $D=5.3\ 10^{-13}$ | | 293.0 |
| | $D=7.8\ 10^{-13}$ | | 298.0 |
| | $D=9.3\ 10^{-13}$ | | 300.5 |
| | $D=42\ 10^{-13}$ | | 302.7 |
| In | ∥c 2.7 | 78.3 | 317 417 |
| | ⊥c 3.7 | 78.3 | |
| α-Tl | ∥c 0.4 | 95.9 | 423 498 |
| | ⊥c 0.4 | 94.6 | |
| β-Tl | 0.42 | 80.18 | 513 573 |

## Diffusion at low concentration

**Table 13.2** TRACER IMPURITY DIFFUSION COEFFICIENTS

*In Ag*

| Element | $A$ $cm^2 s^{-1}$ | $Q$ $kJ\ mol^{-1}$ | Temp. range K | Method | Ref. |
|---|---|---|---|---|---|
| Cu | 1.23 | 193.0 | 990–1 218 | IVa(i), s.c., $Cu^{64}$, 99.99% | 13 |
| | 0.029 | 164.1 | 699–897 | IVa(iii) (SIMS), s.c., 99.99% | 258 |
| Au | 0.85 | 202.1 | 991 -1 198 | IVa(i), s.c., $Au^{195}$, 99.99% | 18 |
| Zn | 0.54 | 174.6 | 916–1 197 | IVa(i), s.c., $Zn^{65}$, 99.99% | 14 |
| | 0.532 | 174.6 | 970–1 225 | IVa(i), s.c., $Zn^{65}$, 9.999% | 259 |
| Cd | 0.44 | 174.6 | 866–1 210 | IVa(i), s.c., $Cd^{111}$, 99.99% | 10 |
| Hg | 0.079 | 159.5 | 926–1 1221 | IVa(i), s.c., $Hg^{203}$, 99.99% | 13 |
| Al | 0.13 | 159.5 | 873–1 223 | IIb (X-ray), p.c., | 211 |
| Ga | 0.42 | 162.9 | 873 1 213 | IIb (X-ray), p.c., — | 260 |
| In | 0.41 | 170.1 | 886–1 209 | IVa(i), s.c., $In^{114}$, 99.99% | 10 |
| | 0.36 | 169.0 | 553–838 | IVa(i), s.c., $In^{114}$, 99.999% | 261 |
| Tl | 0.15 | 158.7 | 918 -1 073 | IVa(i), p.c., $Tl^{204}$, — | 15 |
| Ge | 0.084 | 152.8 | 943–1 123 | IVa(i)m p.c., $Ge^{71}$, — | 15 |
| Sn | 0.25 | 165.0 | 865–1 1210 | IVa(i), s.c., $Sn^{113}$, 99.99% | 10 |
| Pb | 0.22 | 159.5 | 973–1 098 | IVa(i), p.c., $Pb^{210}$, | 19 |
| As | 0.42 | 149.6 | 915 -1 213 | IVa(iii) (EMPA), p.c., 99.98% | 107 |
| Sb | 0.169 | 160.4 | 743 1 215 | IVa(i), s.c., $Sb^{124}$, 99.99% | 11 |
| S | 1.65 | 167.5 | 873–1 173 | IVb, s.c., $S^{35}$, 99.999% | 108 |
| Se | 0.285 | 157.4 | 759- 1 109 | IVa(i) (ion impl), s.c., $Se^{75}$, 99.999% | 262 |
| Te | 0.21 | 154.7 | 650 1 169 | IVa(i), s.c., $Te^{121}$, 99.999% | 109 |
| Ti | 1.33 | 198 | 1 051- 1 220 | IIa(ii) (EMPA), p.c., 99.999% | 263 |
| V | 2.72 | 209 | 1 012 1 218 | IVb, p.c., $V^{48}$, 99.999% | 263 |
| Cr | 3.29 | 210 | 1 023 1 215 | IVb, p.c., $Cr^{51}$, 99.999% | 263 |
| | 1.07 | 192.6 | 976–1 231 | IVa(i), s.c., $Cr^{51}$, 99.9999% | 264 |
| Mn | 4.29 | 196 | 883 1 212 | IVb, p.c., $Mn^{54}$, 99.999% | 263 |
| Fe | 2.6 | 205.2 | 1 073–1 205 | IVa(i), s.c., $Fe^{59}$, 99.999% | 106 |
| Ru | 180 | 275.5 | 1 066–1 219 | IVa(i), s.c., $Ru^{103+106}$, 99.99% | 12 |
| Co | 1.9 | 204.1 | 973–1 214 | IVa(i), s.c., $Co^{60}$, 99.999% | 106 |

# Some examples of diffusion coefficients: chemical diffusion

## Chemical diffusion

**Table 13.4 CHEMICAL DIFFUSION COEFFICIENT MEASUREMENTS—*continued***

| *Element 1* At.% | *Element2* At.% | *A* $cm^2 s^{-1}$ | *Q* $kJ\,mol^{-1}$ | *D* $cm^2 s^{-1}$ | *Temp. range* K |
|---|---|---|---|---|---|
| Mo | Pd | | | | |
| | 61 | $5.5 \times 10^{-5}$ | 188.4 | | |
| | 66 | $4.0 \times 10^{-5}$ | 165.4 | $(D_{Pd} \approx {}^{(a)} 10\text{–}20 \times D_{Mo})$ | |
| | 71 | $5.0 \times 10^{-5}$ | 177.9 | | |
| | 75 | $2.4 \times 10^{-4}$ | 200.5 | — | |
| | 80 | $1.6 \times 10^{-3}$ | 218.6 | — | 1 273–1 873 |
| | 85 | $1.6 \times 10^{-2}$ | 253.3 | — | |
| | 90 | $9.0 \times 10^{-1}$ | 293.1 | — | |
| | 95 | $1.4 \times 10^{-1}$ | 282.6 | — | |

(a) At the original composition in pure Mo/pure Nb couples.

| | | | | | |
|---|---|---|---|---|---|
| Mo | Ta | | | | |
| | 'Ta rich' | $4.68 \times 10^{-5}$ | 251.2 | — | 2 175–2 573 |
| | 'Mo rich' | $4.16 \times 10^{-5}$ | 234.5 | — | |
| Mo | Ti | | | | |
| 0 | | $\sim 2 \times 10^{-2}$ | 196.8 | — | |
| 10 | | $\sim 2 \times 10^{-2}$ | 209.3 | $D_{Ti}/D_{Mo}$ | |
| 20 | ($\beta$) | $\sim 1 \times 10^{-2}$ | 217.7 | ~3 at 1 600° | 1 483–1 873 |
| | | | | ~13 at 820° | |
| 30 | | $\sim 10^{-2}$ | 263.8 | — | |
| 40 | | $\sim 10^{-2}$ | 255.4 | — | |
| (a) | | | | | |
| 0–10 | ($\beta$) | $1.3 \times 10^{-4}$ | 138.6 | — | 1 173–1 573 |
| Sol. soln range | ($\alpha$) | $3.5 \times 10^{-8}$ | 118.9 | — | 873–1 073 |

## Diffusion in binary alloys

**Table 13.3 DIFFUSION IN HOMOGENEOUS ALLOYS—*continued***

| *Element 1* (purity) At.% | *Element 2* (purity At.% | *A*† $cm^2 s^{-1}$ | *Q*† $kJ\,mol^{-1}$ | *A*† $cm^2 s^{-1}$ | *Q*† $kJ\,mol^{-1}$ | *Temp. range* K | *Ref.* |
|---|---|---|---|---|---|---|---|
| Co | Cr | | | | | | |
| (--) | (—) | | IVb | p.c. | | | |
| | 4 | 0.67 | 275.5 | — | — | 1 373–1 623 | 33 |
| | 7 | 56.3 | 332.0 | — | -- | | |
| Co | Cr Ni | | | | | | |
| ( ) | (—) (--) | | IVb | p.c. | | | |
| | 9 26 | 6.3 | 301.9 | | -- | 1 373–1 623 | 33 |
| | 18 26 | 0.4 | 268.8 | -- | — | | |
| Co | Cu Si | | | | | | |
| (99.99) | (99.99) ( ) | | | IVa(i), p.c., $Co^{58}$ | | | |
| 0–2 68 | 0.54 | | $B_1 \sim -9$ | | | 1 325 | 158 |
| Co | Fe | | | | | | |
| ( ) | ( ) | | IVa(i) | p.c. | | | |
| | | 1.33 | 290.6 | 1.26 | 286.8 | 1 285–1 437($\gamma$) | |
| 50 | 50 | 2.0 | 251.2 | 0.25 | 230.3 | 1 068–1218($\alpha$) | 34 |
| | | | 556.8 | | 556.8 | 928–995(CsCl) | |
| ( ) | ( ) | | IVb | p.c. | | | |
| — | 21 | 0.54 | 272.1 | — | — | 1 373–1 573 | 33 |
| ( ) | ( ) | | IVa(iii) | p.c. | | | |
| | 0 | | Diffusion of Ni $D_{Ni} = 13.10^{-12}$ | | | | |
| | 30.2 | | = 11.5 | | | | |
| -- | 68.5 | | ≈8–8.8 | | | 1 409 | 82 |
| -- | 88.3 | | ~5 | | | | |
| — | 100 | | ≈6 | | | | |
| ( ) | ( ) | | IVb | p.c. | (F = Ferromagnetic) | | |
| 0 | (bcc) | 1.83 | 234.0 | — | | 1 073–1 172 | |
| | (fcc) | 0.77) | 265.0 | | — | 1 223–1 633 | |
| 3 | (bcc) | 9.17 | 266.3 | — | — | 903–1 023(F) | |
| 6.8 | (bcc) | 0.469 | 187.1 | — | -- | 903–1 073(F) | |
| | | $5.72 \times 10^{-5}$ | 146.5 | -- | — | 1 153–1 193 | |
| | (fcc) | 0.109 | 326.2 | — | - - | 1 283–1 583 | |
| 28.6 | (bcc) | $1.25 \times 10^{-3}$ | 198.0 | - | — | 903–1 083(F) | |
| | (fcc) | $3.36 \times 10^{-2}$ | 266.3 | — | — | 1 333–1 583 | 107 |
| 49.6 | (bcc) | $6.59 \times 10^{-2}$ | 247.0 | - | — | 1 023–1 123(F) | |
| | (fcc) | 0.154 | 349.6 | -- | — | 1 333–1 583 | |
| 67.2 | (bcc) | $6.04 \times 10^{-3}$ | 190.9 | — | -- | 903–1 153(F) | |
| | (fcc) | $3.15 \times 10^{-2}$ | 265.0 | — | - | 1 333–1 583 | |
| 89.6 | (fcc) | $6.44 \times 10^{-2}$ | 251.2 | -- | — | 1 073–1 283(F) | |
| | | $1.61 \times 10^{-2}$ | 234.0 | — | — | 1 333–1 153 | |
| 100 | (fcc) | 0.50 | 273.8 | - | — | 1 045–1 321(F) | |
| | | 0.17 | 260.4 | — | — | 1 465–1 570 | |
| (99.8) | (99.9) | IVb | p.c. | $Co^{60}$ | | | |
| 0 | | 0.029 | 247.4 | -- | — | | |
| 8 | | 20.54 | 321.5 | — | — | | |
| 10 | | 15.65 | 369.0 | — | — | 1 233–1 493 | 131 |
| 15 | | 1.98 | 289.7 | — | — | | |
| 20 | | 0.31 | 261.7 | — | — | | |
| Co | Fe | | | | | | |
| ( ) | ( ) | IVb, s.c., $Fe^{59}$ | | | | | |
| | 6 | — | — | 0.58 | 273.3 | 1 081–$T_c$ | |
| - | 6 | — | — | 0.15 | 261.7 | $T_c$–1 573 | 176 |
| - | 10 | — | — | 0.68 | 279.3 | 1 081–$T_c$ | |
| -- | 10 | — | — | 0.18 | 263.3 | $T_c$–1 573 | |

# Some examples of diffusion coefficients: interdiffusion

| Co | Fe | | | |
|---|---|---|---|---|
| ( ) | ( ) | | IVa(i) | p.c. |
| | | 1.33 | 290.6 | 1.26 |
| 50 | 50 | 2.0 | 251.2 | 0.25 |
| | | | 556.8 | |
| ( ) | ( ) | | IVb | p.c. |
| — | 21 | 0.54 | 272.1 | — |
| ( ) | ( ) | | IVa(iii) | p.c. |
| | 0 | Diffusion of Ni | | |
| | 30.2 | $D_{Ni} = 13.10^{-12}$ | | |
| — | 68.5 | = 11.5 | | |
| — | 88.3 | ~8–8.8 | | |
| — | 100 | ~5 | | |
| | | ~6 | | |
| ( ) | ( ) | | IVb | p.c. |
| 0 | (bcc) | 1.83 | 234.0 | — |
| | (fcc) | 0.77) | 265.0 | — |
| 3 | (bcc) | 9.17 | 266.3 | — |
| 6.8 | (bcc) | 0.469 | 187.1 | — |
| | | $5.72 \times 10^{-5}$ | 146.5 | — |
| | (fcc) | 0.109 | 326.2 | — |
| 28.6 | (bcc) | $1.25 \times 10^{-3}$ | 198.0 | — |
| | (fcc) | $3.36 \times 10^{-2}$ | 266.3 | — |
| 49.6 | (bcc) | $6.59 \times 10^{-2}$ | 247.0 | — |
| | (fcc) | 0.154 | 349.6 | — |
| 67.2 | (bcc) | $6.04 \times 10^{-3}$ | 190.9 | — |
| | (fcc) | $3.15 \times 10^{-2}$ | 265.0 | — |
| 89.6 | (fcc) | $6.44 \times 10^{-2}$ | 251.2 | — |
| | | $1.61 \times 10^{-2}$ | 234.0 | — |
| 100 | (fcc) | 0.50 | 273.8 | — |
| | | 0.17 | 260.4 | — |
| (99.8) | (99.9) | IVb | p.c. | $Co^{60}$ |
| 0 | | 0.029 | 247.4 | — |
| 8 | | 20.54 | 321.5 | — |
| 10 | | 15.65 | 369.0 | — |
| 15 | | 1.98 | 289.7 | — |
| 20 | | 0.31 | 261.7 | — |
| Co | Fe | | | |
| ( ) | ( ) | IVb, s.c., $Fe^{59}$ | | |
| | 6 | — | — | 0.58 |
| | 6 | — | — | 0.15 |
| | 10 | — | — | 0.68 |
| — | 10 | — | — | 0.18 |

## Interdiffusion coefficient

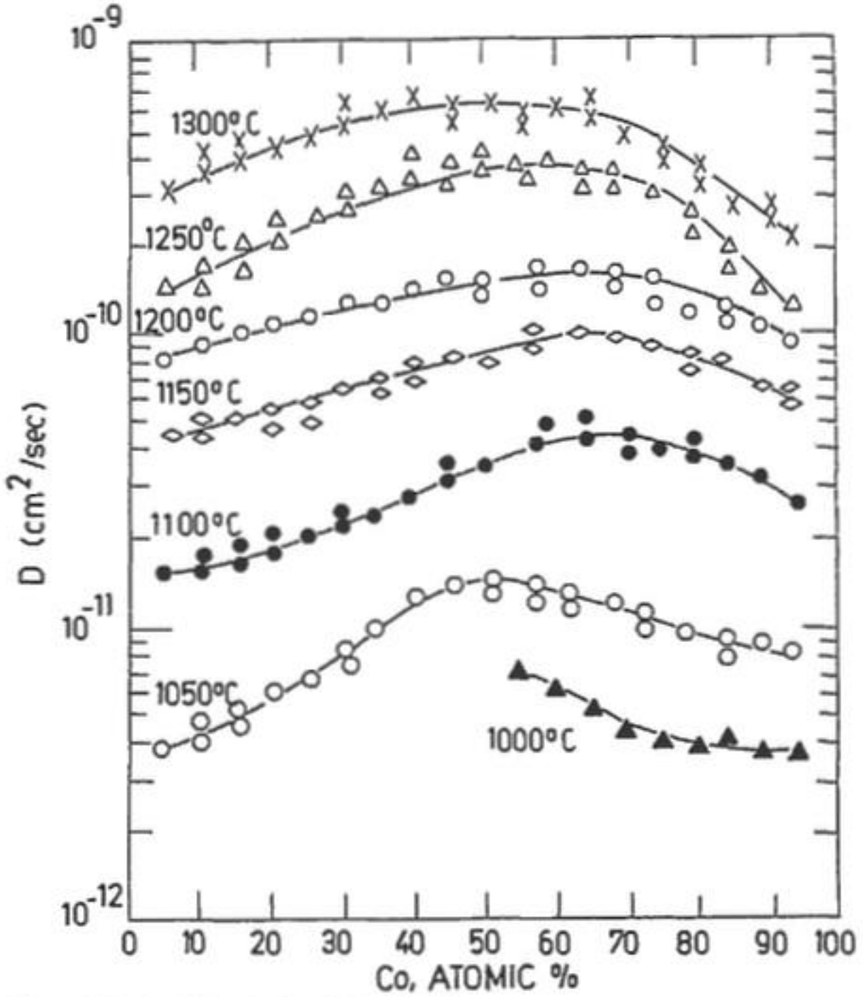



Figure 13.6b *Interdiffusion in f.c.c. FeCo alloys*[318]