

# EPFL

# *Physics of Materials*

## Chapter 5: Diffusion

Dr. Thomas LaGrange

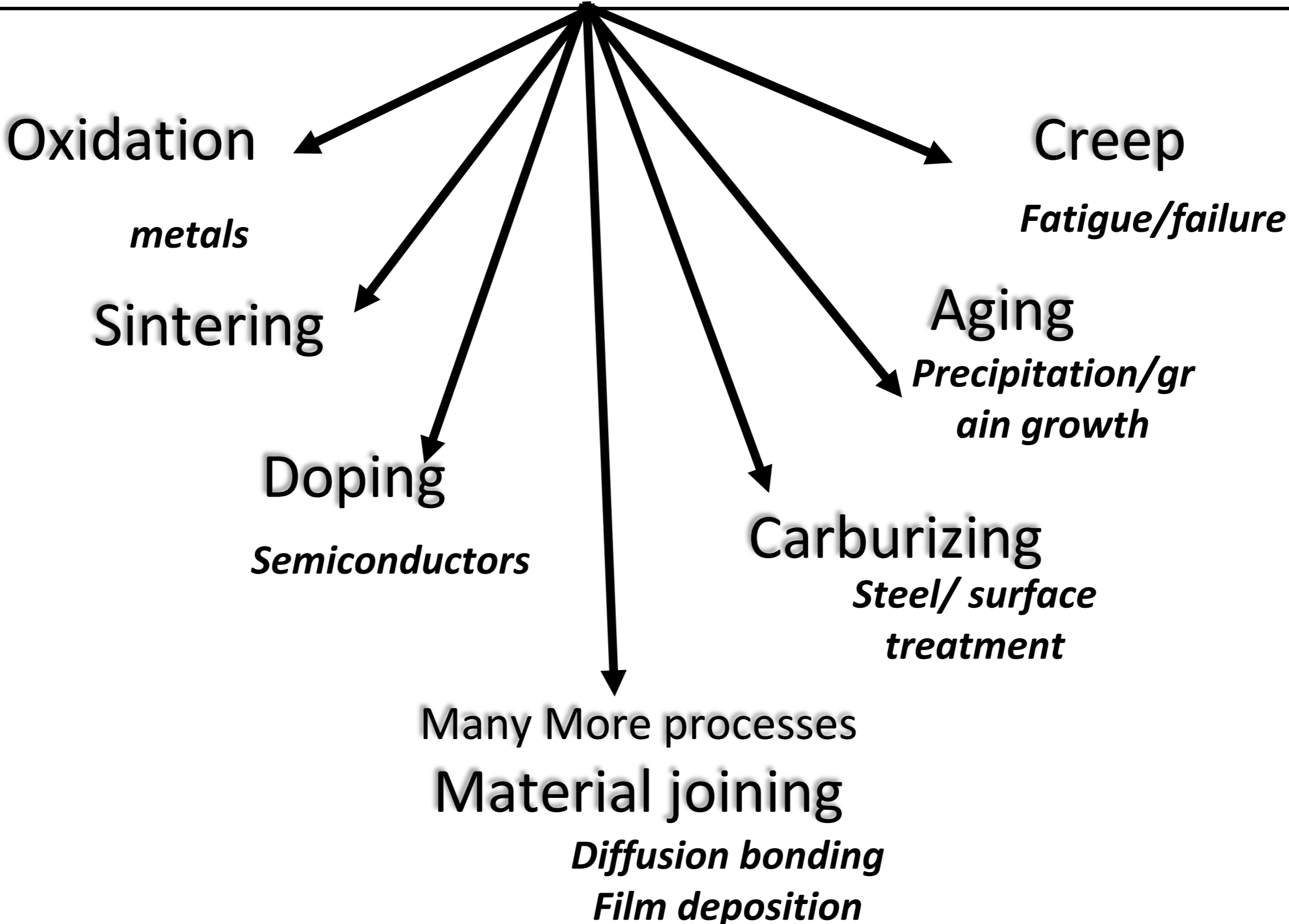
LUMES



**Masters Course PHYS-307**

**Fall 2025**




# 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

Yao Zhang <sup>1,2</sup> David Cortie,<sup>3,4</sup> Thomas LaGrange,<sup>5</sup> Waitung Lee,<sup>4</sup> Tane Butler <sup>1</sup>  
Bart Ludbrook <sup>1</sup> and Simon Granville<sup>1,2,\*</sup>


<sup>1</sup>Robinson Research Institute, Victoria University of Wellington, Wellington 6140, New Zealand

<sup>2</sup>MacDiarmid Institute for Advanced Materials and Nanotechnology, Wellington 6011, New Zealand

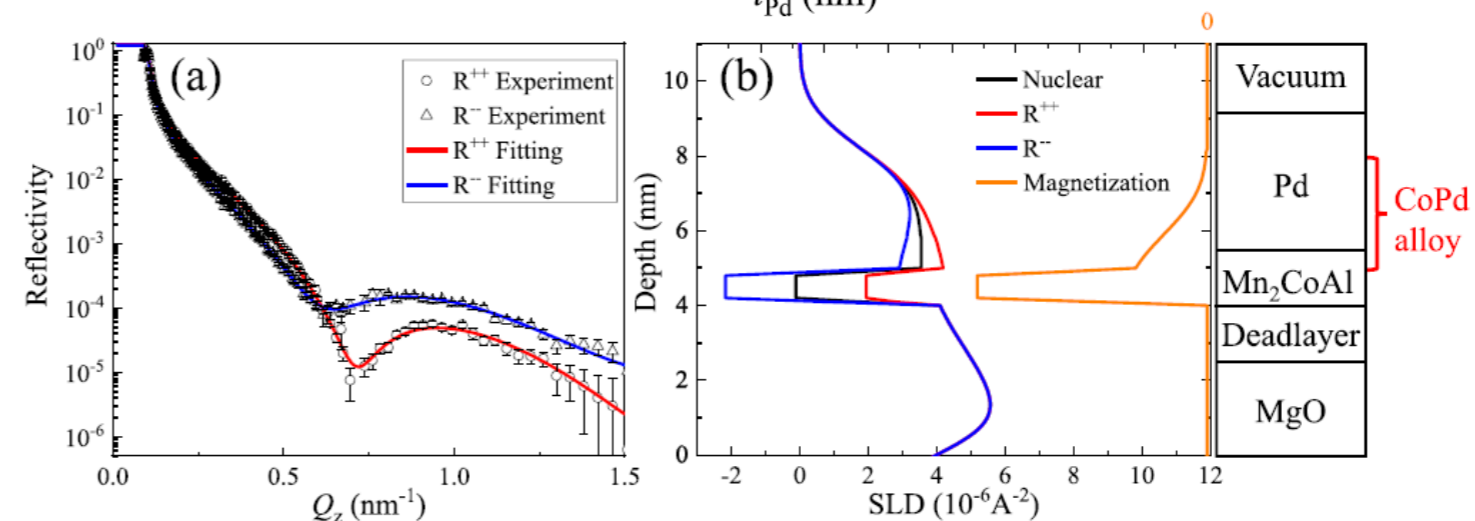
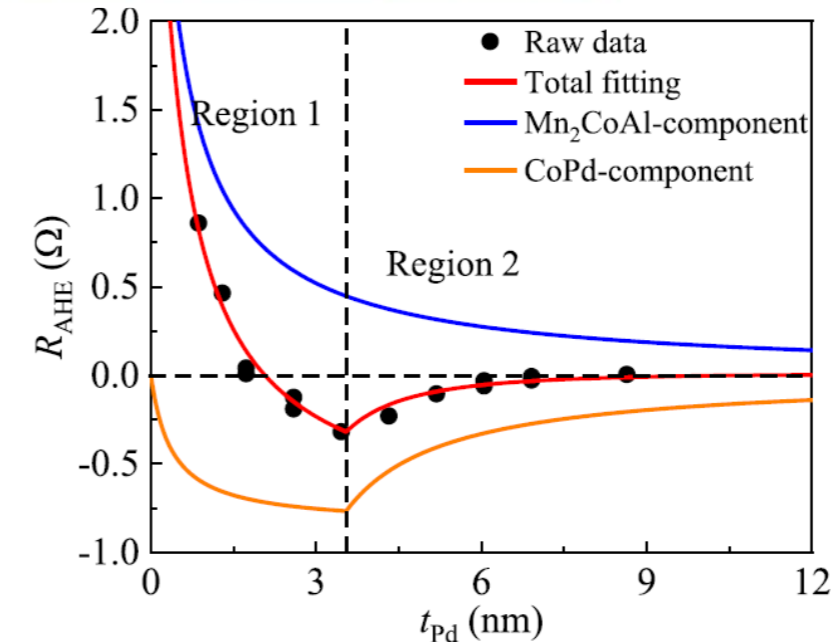
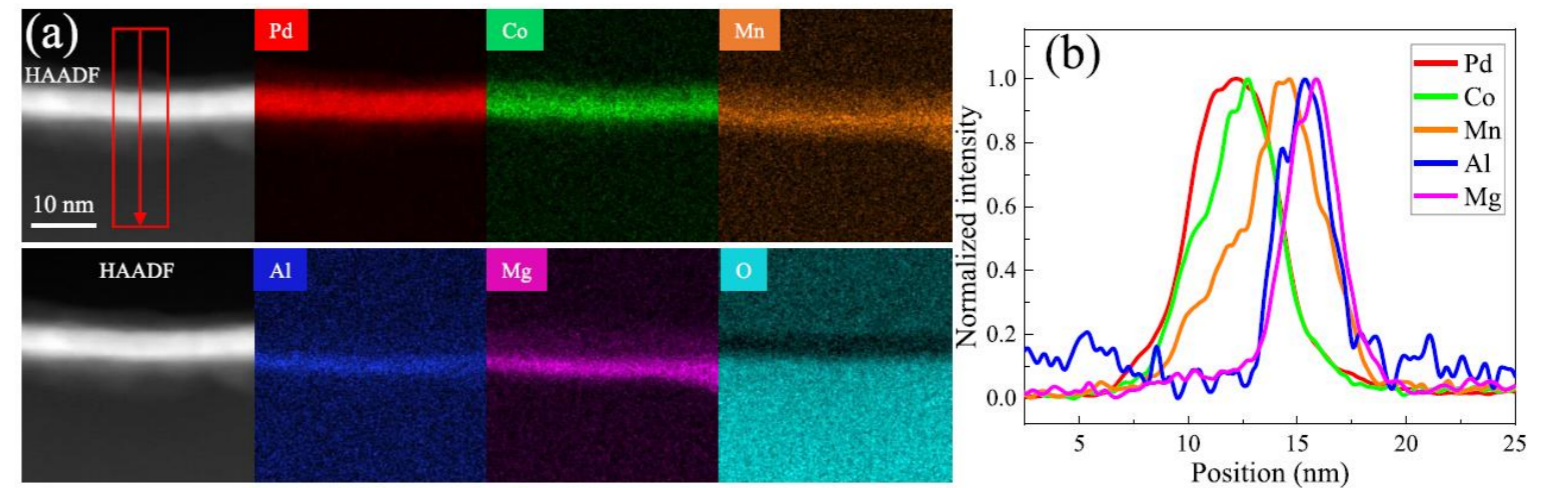
<sup>3</sup>Institute for Superconducting and Electronic Materials, University of Wollongong, Wollongong, NSW 2500, Australia

<sup>4</sup>The Australian Nuclear Science and Technology Organisation, Lucas Heights, NSW 2232, Australia

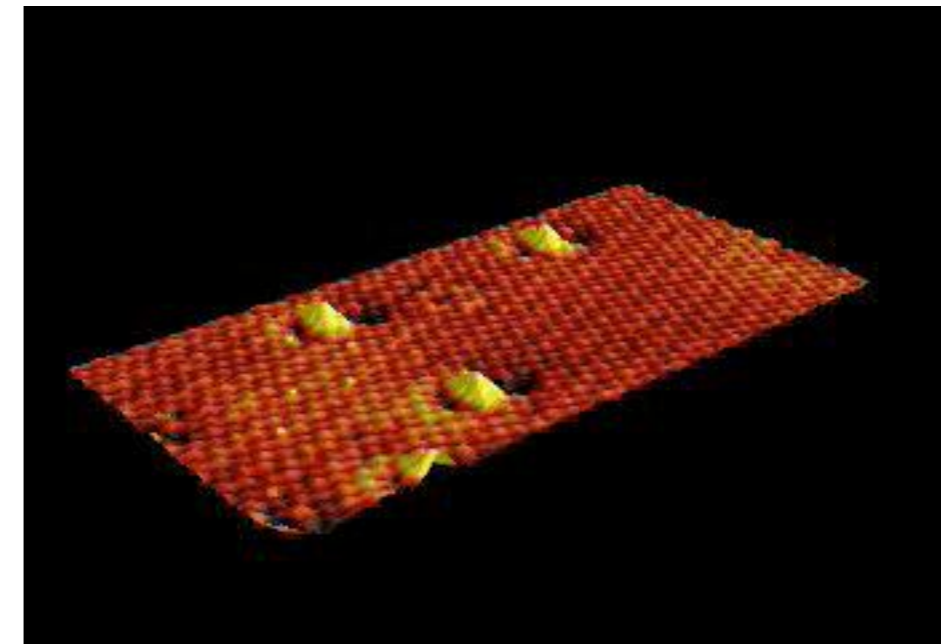
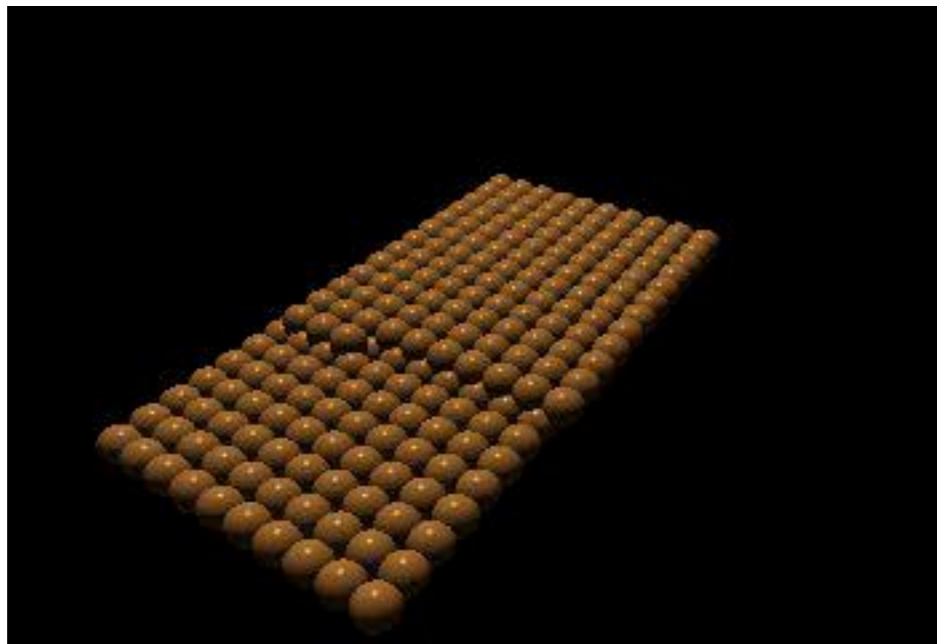
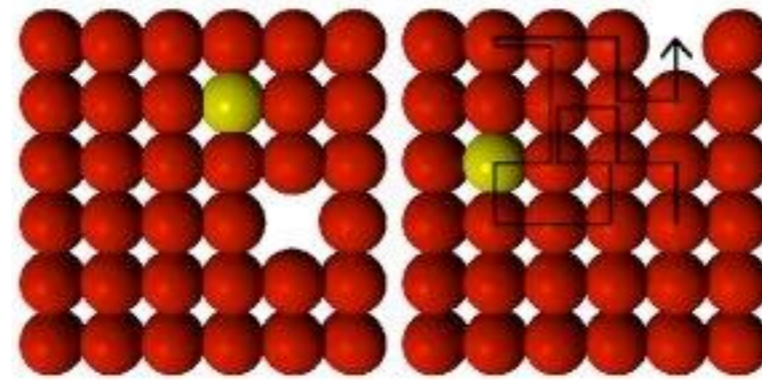
<sup>5</sup>Laboratory of Ultrafast Microscopy and Electron Scattering, École Polytechnique Fédérale de Lausanne EPFL, Lausanne 1015, Switzerland

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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<sub>2</sub>CoAl/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<sub>2</sub>CoAl 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

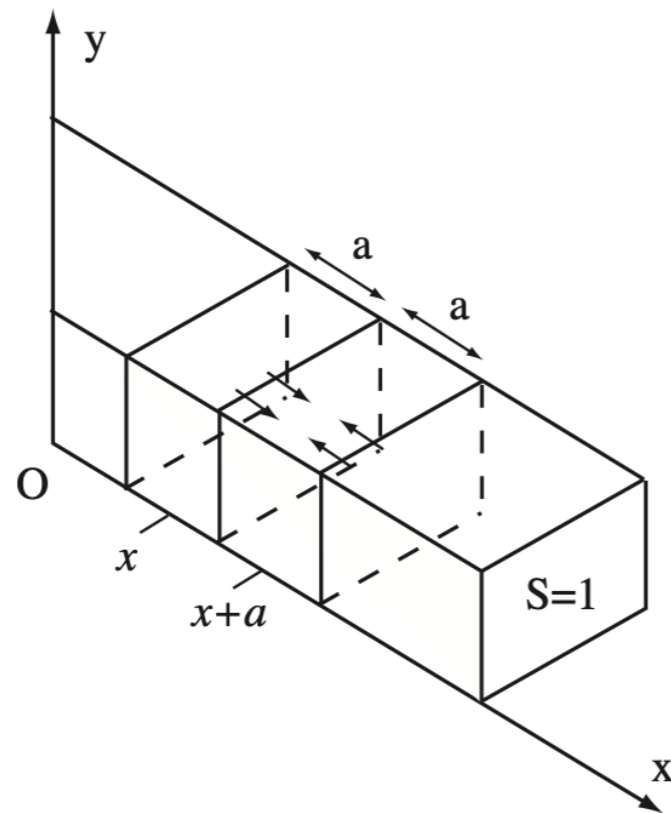
$$\vec{J}_A = -D_A \overrightarrow{\text{grad}} C_A \quad \text{1st law (steady state)}$$

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



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

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

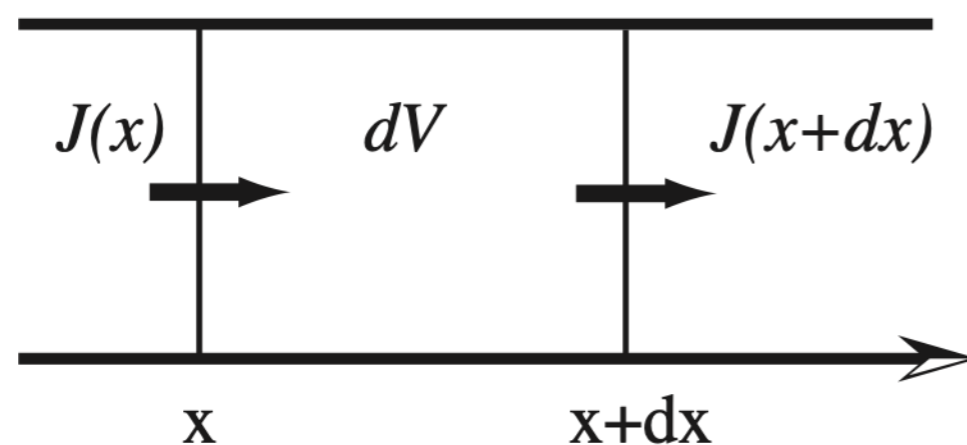


$$J_A = \frac{1}{2} \Gamma C_A(x) a - \frac{1}{2} \Gamma C_A(x+a) a$$

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

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

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



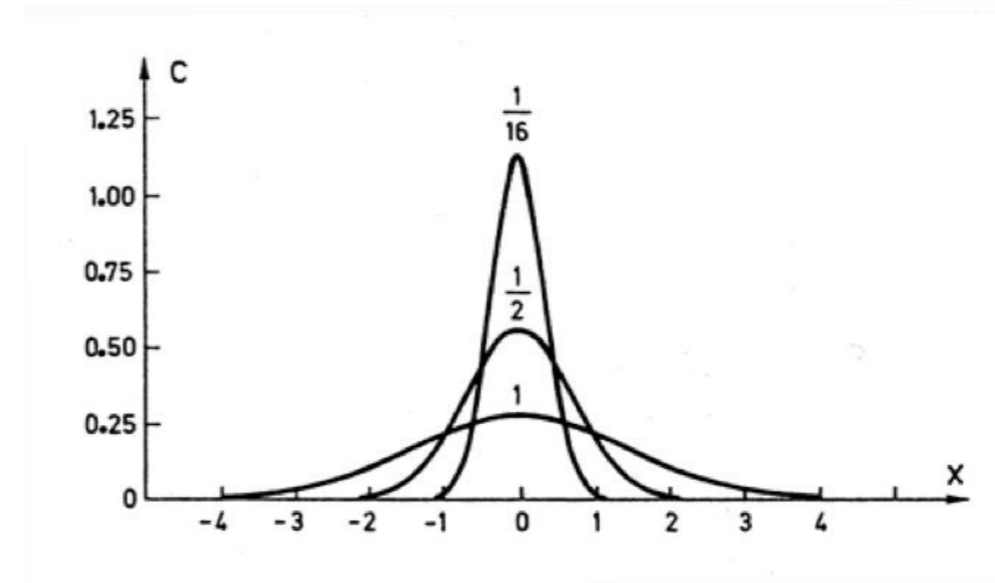
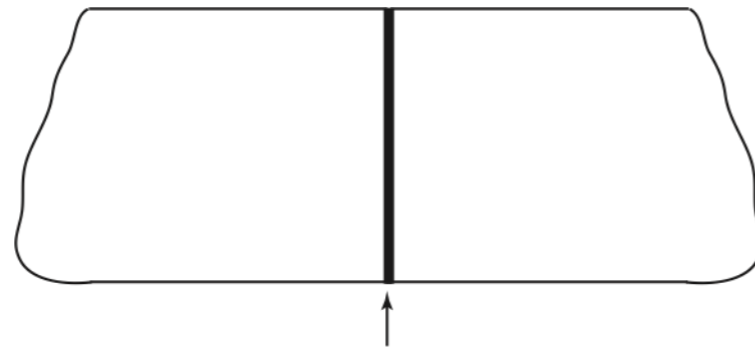
$$dV = S dx$$

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

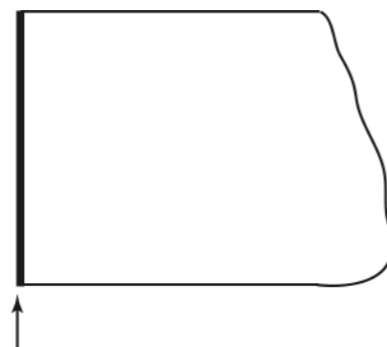
$$\frac{1}{dV} \frac{dn}{dt} = \frac{dC}{dt} = -\frac{dJ}{dx} \quad \text{in 3D:} \quad \frac{dC}{dt} = -\text{div} \vec{J}$$

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

Thin layer of an element B fully soluble in A



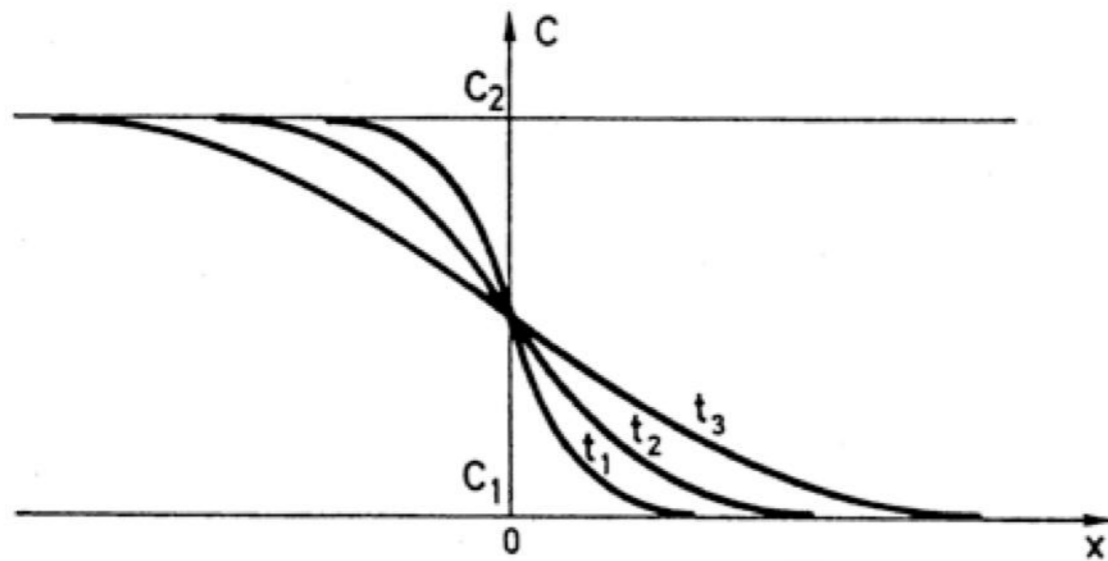
Surface layer: same solution



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

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

## Interdiffusion

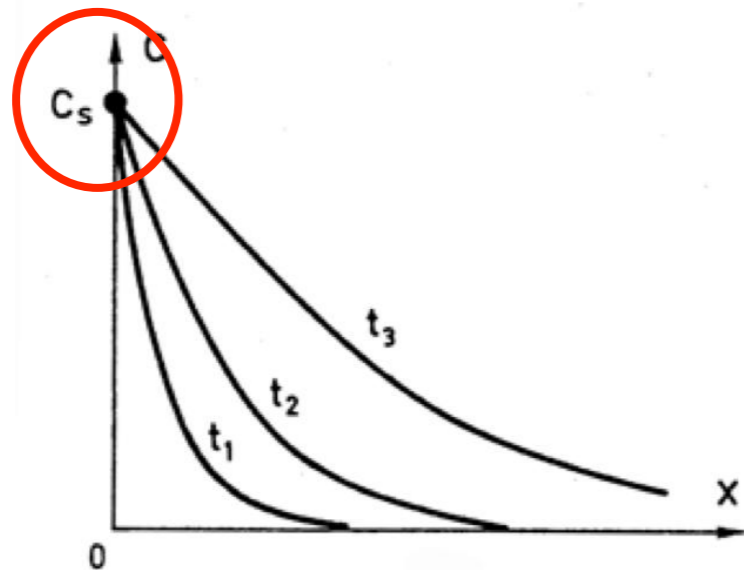


At  $t=0$ ,  $C=C_0$  for  $-\infty < x < 0$   
 $C=0$  for  $0 < x < \infty$

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

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

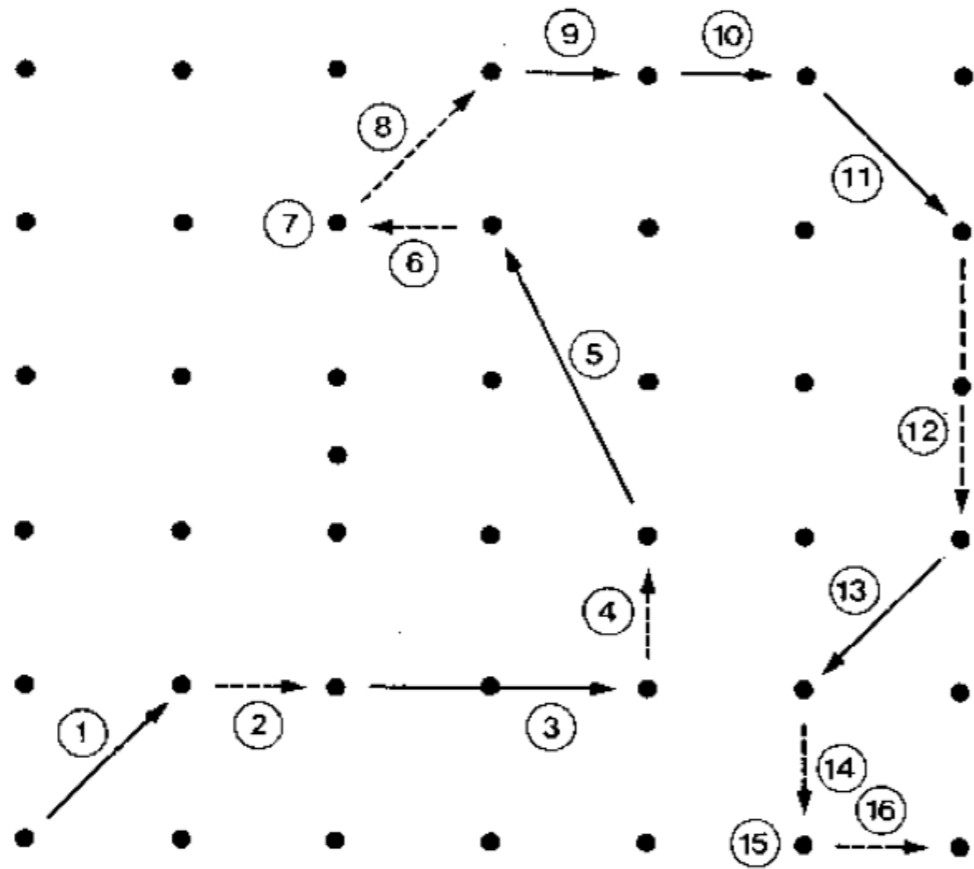
## Diffusion from a surface at constant concentration



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

# Diffusion coefficient and random walk

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



$$\vec{L} = \sum_i \vec{\delta l}_i \quad \langle \vec{L} \rangle = 0$$

$$\langle \vec{L}^2 \rangle \neq 0$$

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

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

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

# Particle flux through a surface S

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

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

$$D = \frac{1}{\textcircled{6}} \Gamma \delta l^2$$

simple cubic

coordination number

$$D = \frac{1}{\textcircled{8}} \Gamma \delta l^2$$

body-centered cubic

$$D = \frac{1}{\textcircled{12}} \Gamma \delta l^2$$

face-centered cubic

# Dependence with respect to temperature

$$D=D(T) \text{ since } \Gamma = \Gamma(T)$$

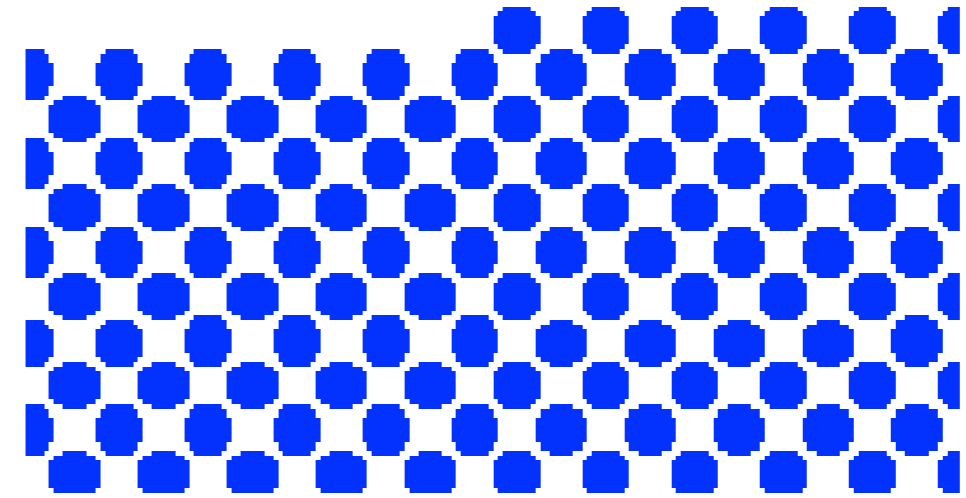
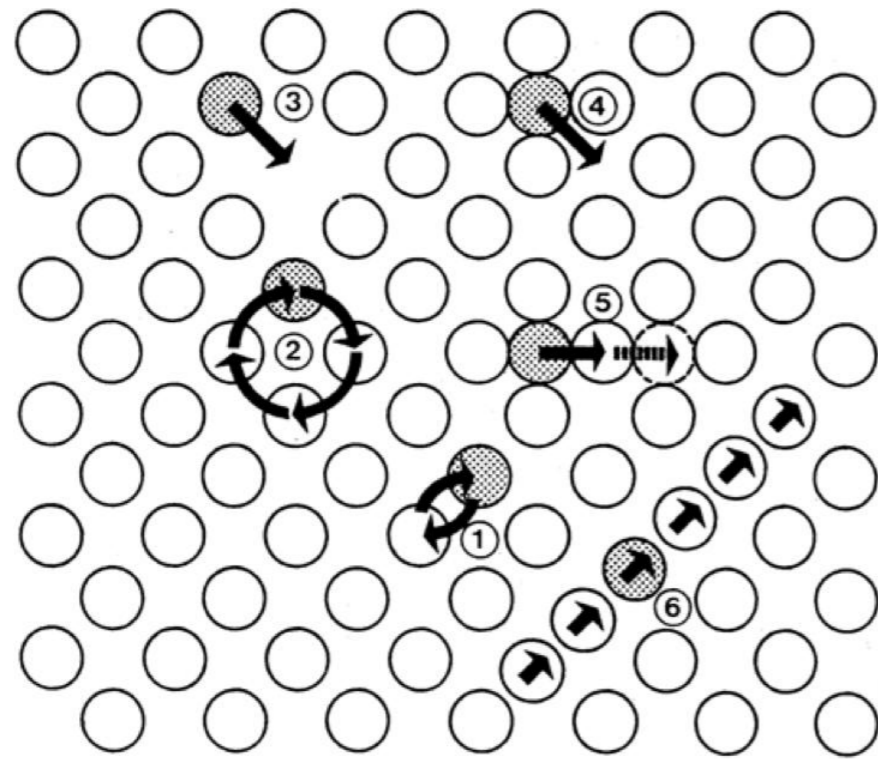
$$\Gamma = \nu_D P$$

$\nu_D$  is the Debye vibration frequency  $\sim 10^{13}$  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

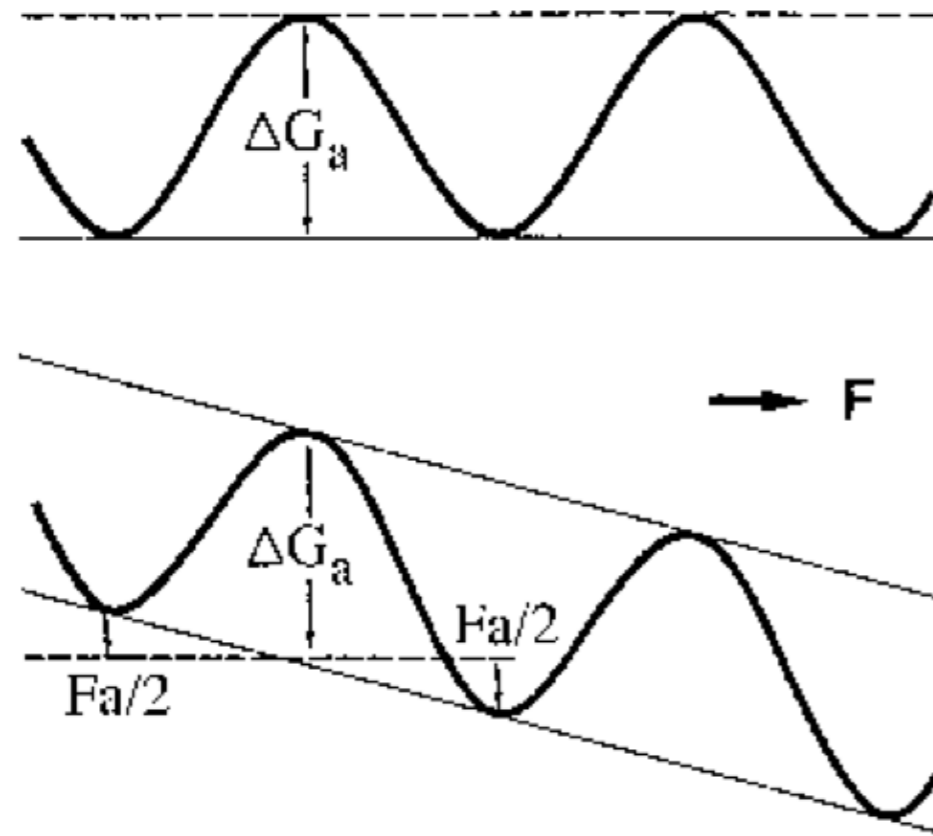
$$\Gamma = z\nu_D C_V \exp(-\Delta G_V^m / kT) = z\nu_D \exp(-(\Delta G_V^m + \Delta G_V^F) / kT)$$

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

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

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

# Force applied to a diffusing particle: Einstein equation



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

$$\Gamma^+ = v_0 e^{-\frac{\Delta G - \frac{a}{2}F}{kT}}$$

$$\Gamma^- = v_0 e^{-\frac{\Delta G + \frac{a}{2}F}{kT}}$$

$$\bar{v} = \frac{1}{2}av_0 e^{-\frac{\Delta G}{kT}} \left( e^{\frac{Fa}{2kT}} - e^{-\frac{Fa}{2kT}} \right) \approx \frac{1}{2}a^2 v_0 e^{-\frac{\Delta G}{kT}} \frac{F}{kT}$$

$$D_A = \frac{1}{2}a^2 v_0 e^{-\frac{\Delta G}{kT}}$$

and

$$v = \frac{D_A F}{kT}$$

Einstein equation

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

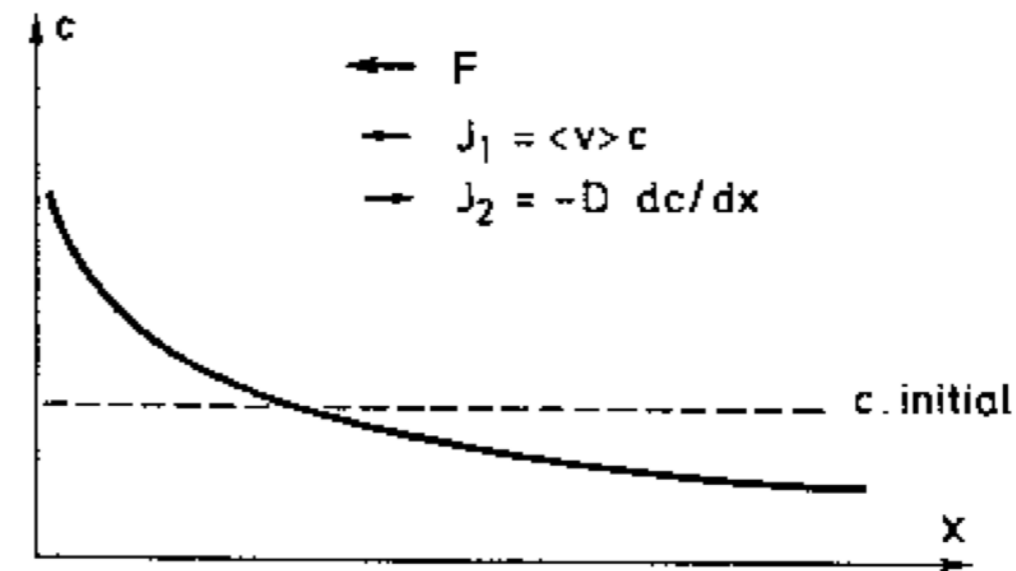
Particle flux

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

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

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

# Darcken equation

For instance

$$\vec{F} = -\overrightarrow{\text{grad}}\mu_A \quad \mu_A \text{ is the chemical potential}$$

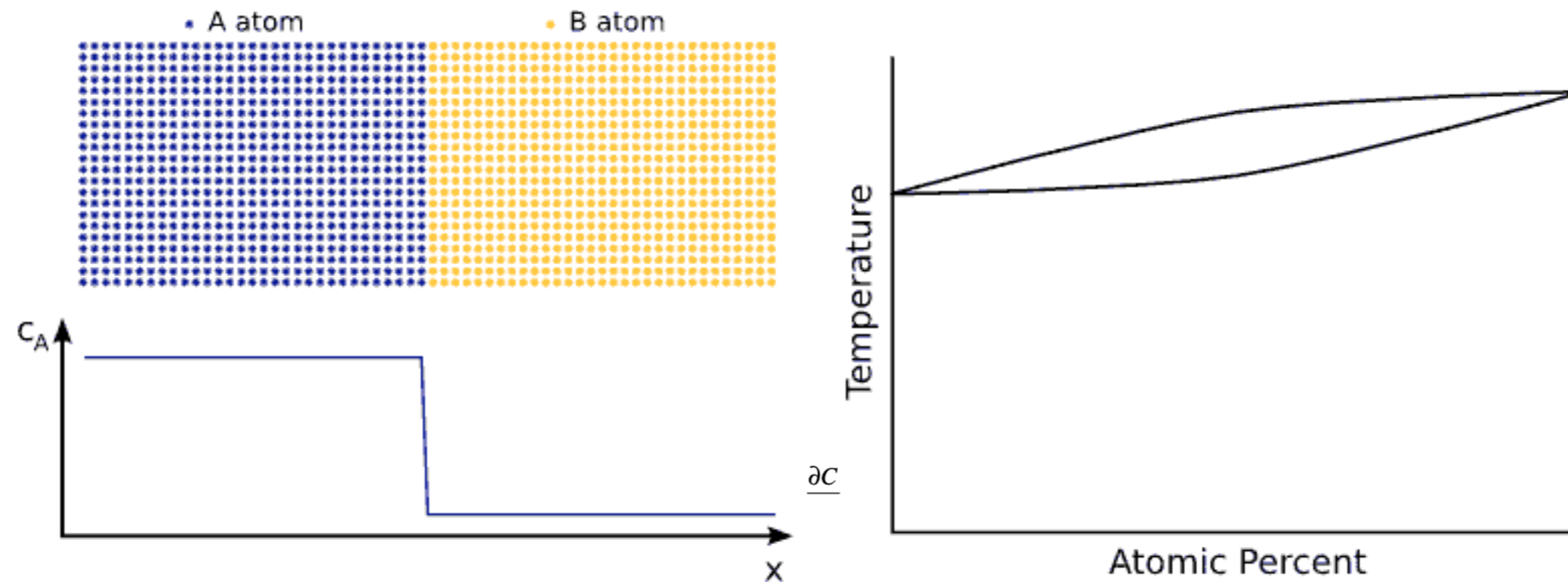
$$\mu_A = kT \ln C_A \Rightarrow F = -\frac{kT}{C_A} \frac{dC_A}{dx}$$

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

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

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

# 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

$$\ddot{\vec{x}}_1(t) = -\frac{GM}{|\vec{x}_1(t)|^3} \vec{x}_1(t)$$

$$t' = \tau t \quad \vec{x}'_1 = \lambda \vec{x}_1$$

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

$$\vec{x}'_1(t=0) = \lambda \vec{x}_1(t=0)$$

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

Consider another planet (2) characterized by:

$$\ddot{\vec{x}}_2(t) = -\frac{G'M \vec{x}_2(t)}{|\vec{x}_2(t)|^3}$$

$$\vec{x}_2(t=0) = \lambda \vec{x}_1(t=0)$$

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

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

# Scale changes in the diffusion equation

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

$$c_1(t=0) = c(x,0)$$

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

$$c'_1(t=0) = c(x',0)$$

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

$$t' = \tau t \quad x'_1 = \lambda x_1$$

New concentration profile

$$c_2(x,t)$$

$$\frac{\partial}{\partial t_2} c_2(x_2, t_2) = \frac{\partial}{\partial x_2} \left( D \frac{\partial}{\partial x_2} c_2(x_2, t_2) \right)$$

$$c_2(t=0) = c(\lambda x, 0)$$

$$\frac{\tau D'}{\lambda^2} = D$$

$$\frac{x}{\sqrt{t}} = \frac{x'}{\sqrt{t'}}$$

This can be deduced from the mean free path

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

# 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

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

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

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

We get

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

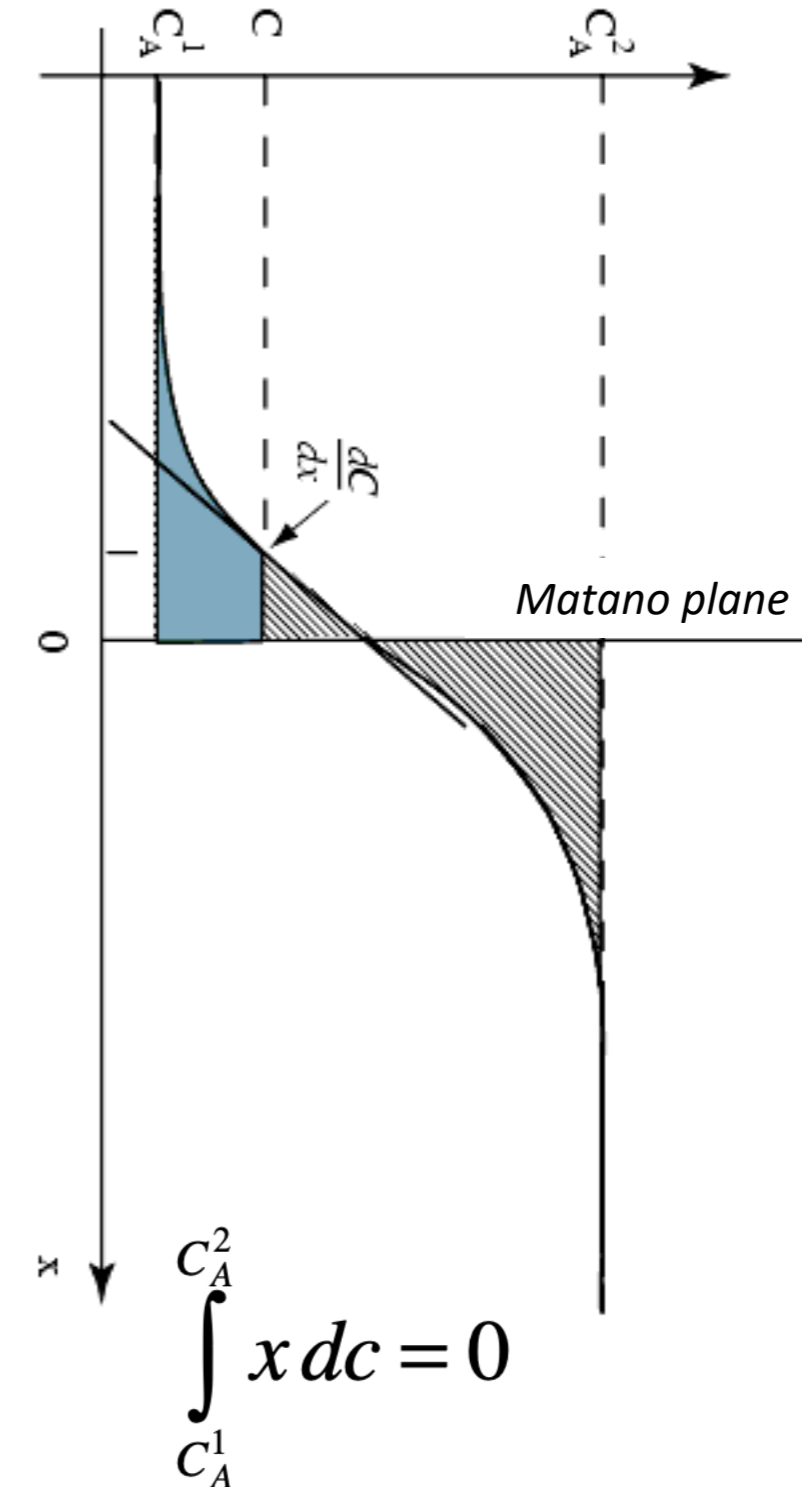
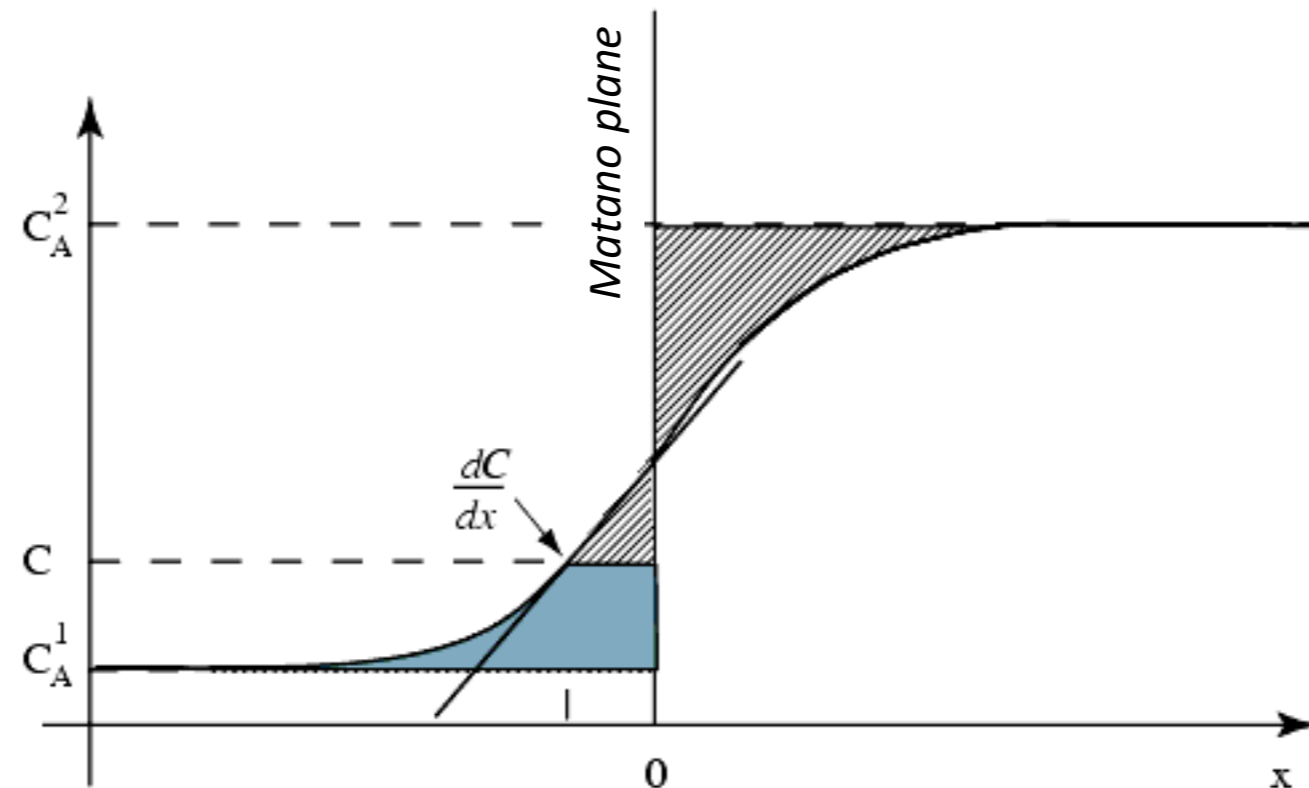
$$D_A^*(C) = -\frac{1}{2} \frac{\int_{C_A}^C \eta dC}{\left. \frac{dC_A}{d\eta} \right|_C}$$

# 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



# Solving the diffusion equation: Heaviside step distribution

$$C_A(x, t = 0) = \theta(x)$$

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

$$\lim_{t \rightarrow 0} \left. \frac{\partial C_A}{\partial x} \right|_t = \delta(x)$$

$$D_A^* = \text{constant}$$

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

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

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

$$\frac{d}{d\eta} (C_A(\eta)) = k e^{-\eta^2 / 4D_A^*}$$

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

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

# Solving the diffusion equation: Heaviside step distribution

$$C_A(x, t = 0) = \theta(x)$$

$$\lim_{t \rightarrow 0} \left. \frac{\partial C_A}{\partial x} \right|_t = \delta(x)$$

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

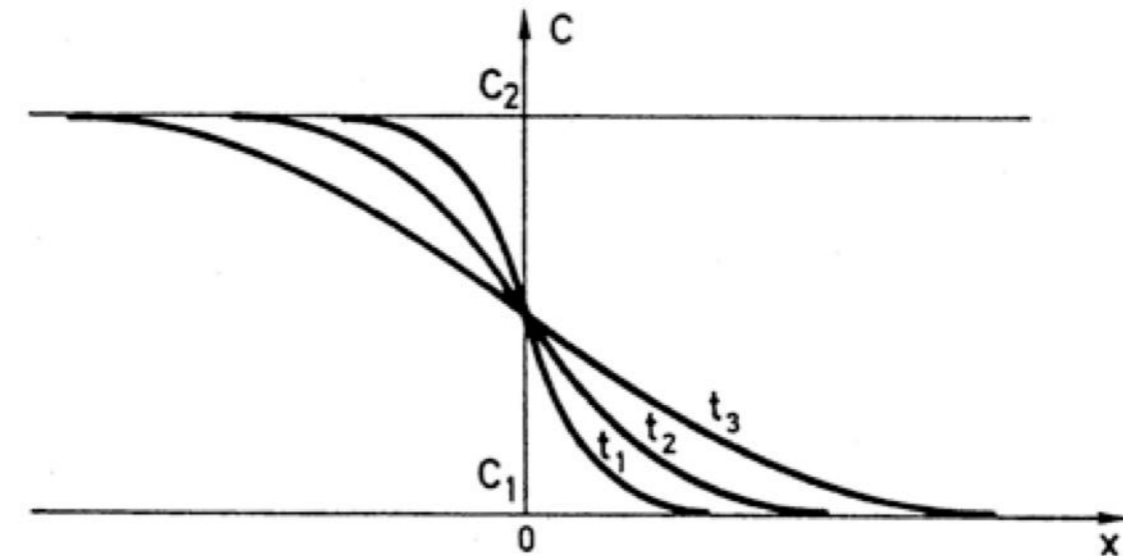
$$\frac{d}{d\eta} C_A = \frac{1}{\sqrt{4\pi D_A^*}} \exp\left[-\eta^2 / 4D_A^*\right]$$

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

$$C_A(x) = C_0 \operatorname{erf}\left(x / 2\sqrt{D_A^* t}\right)$$

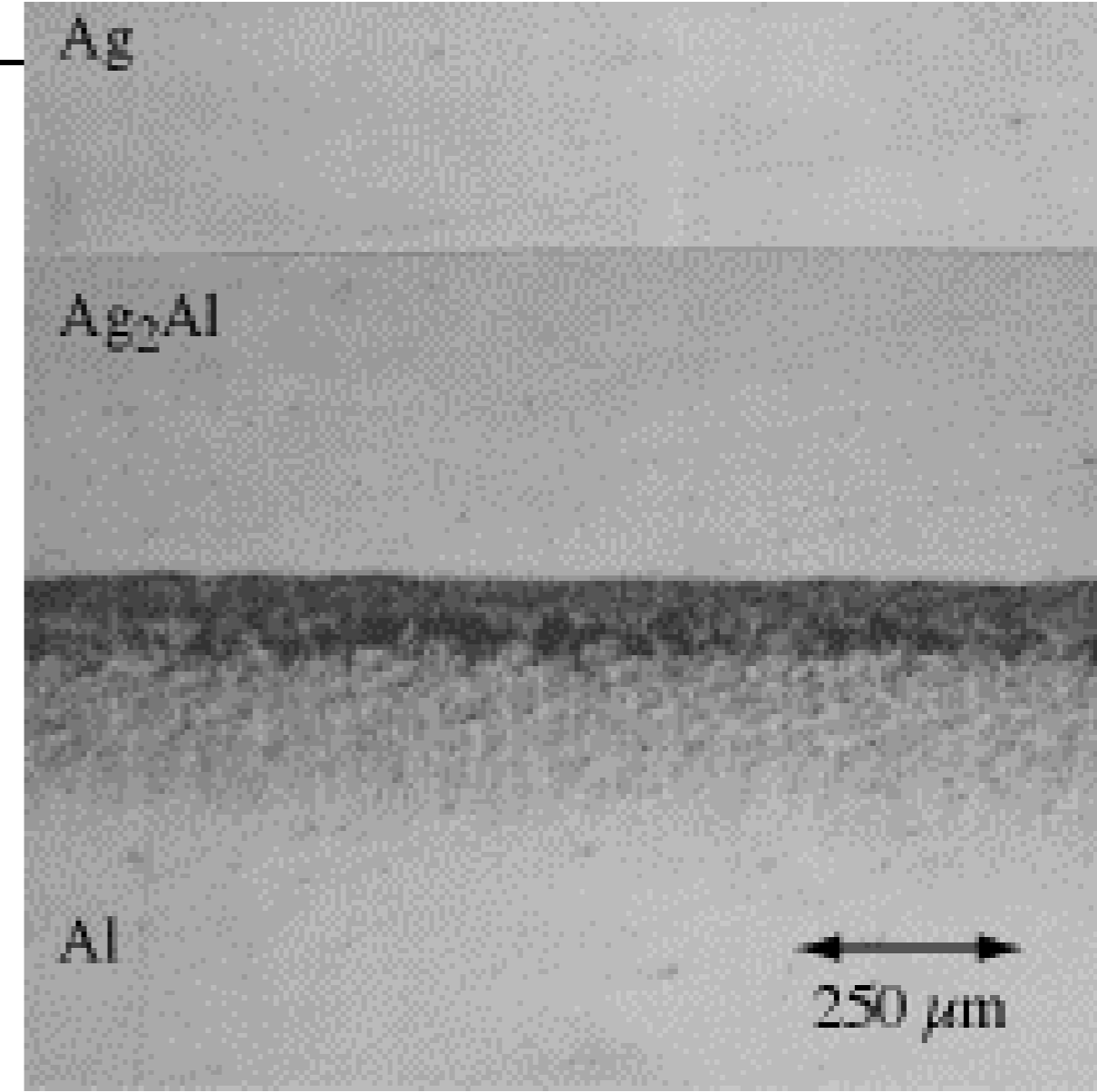
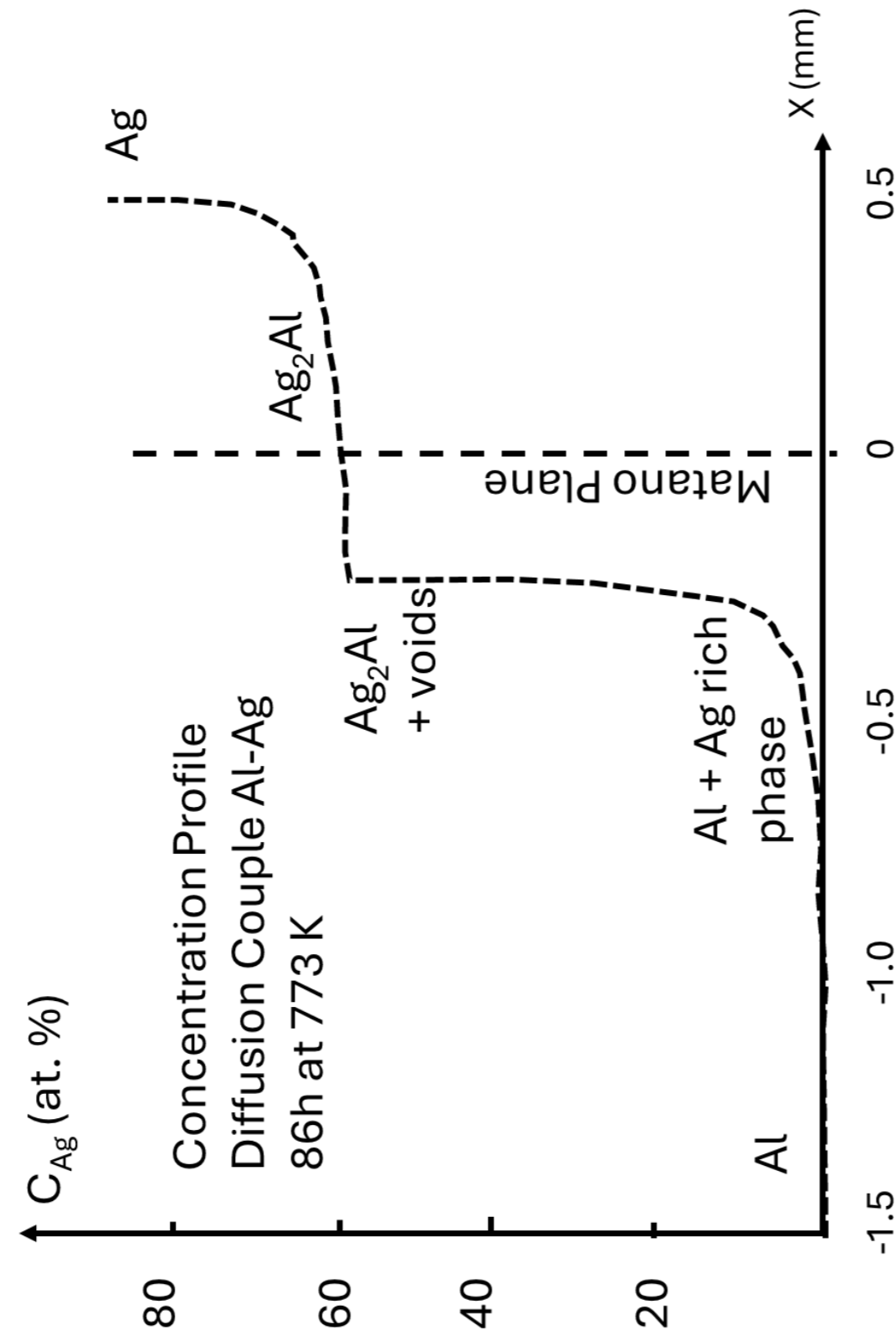
$$C_B(x, t = 0) = \theta(-x)$$

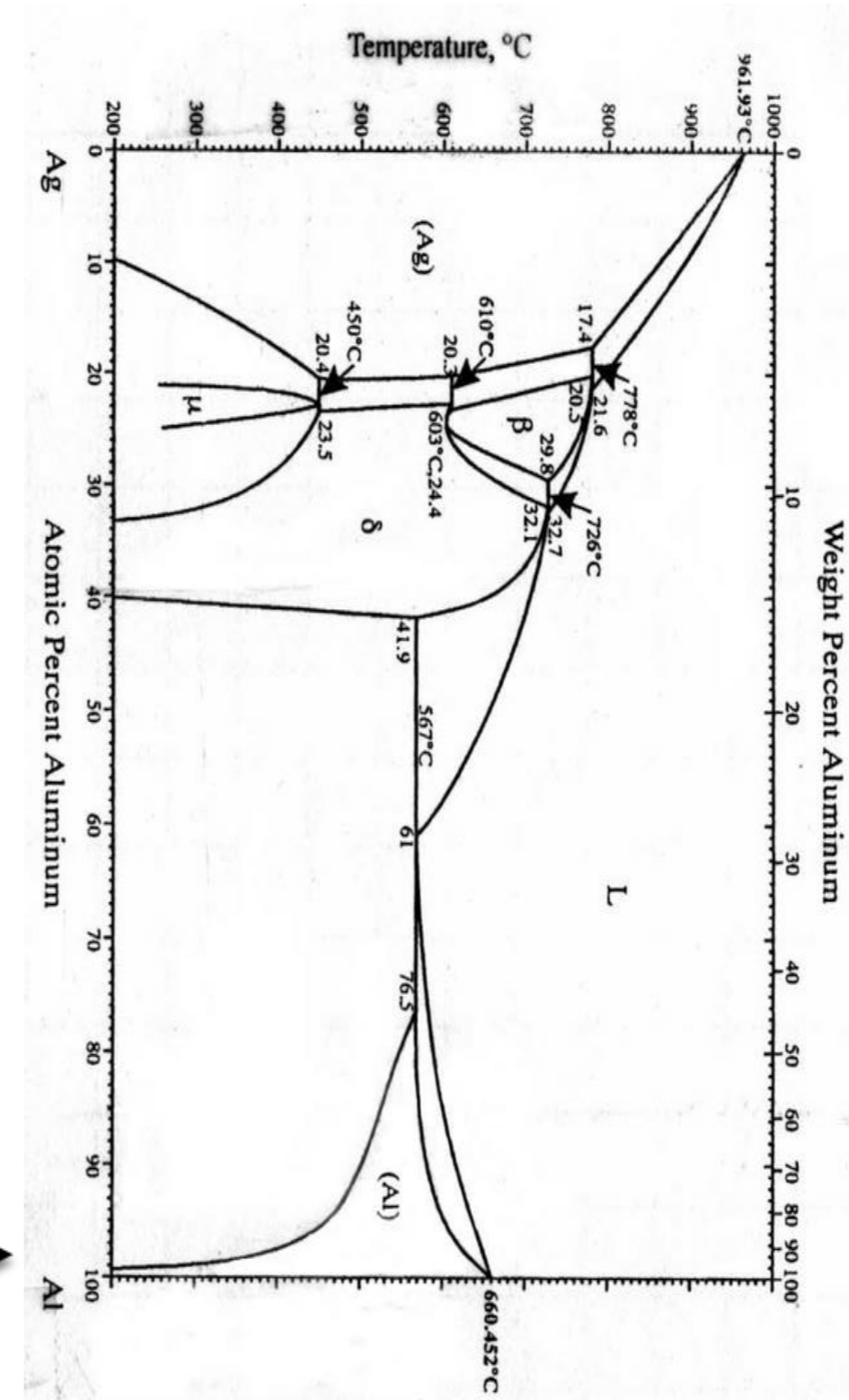
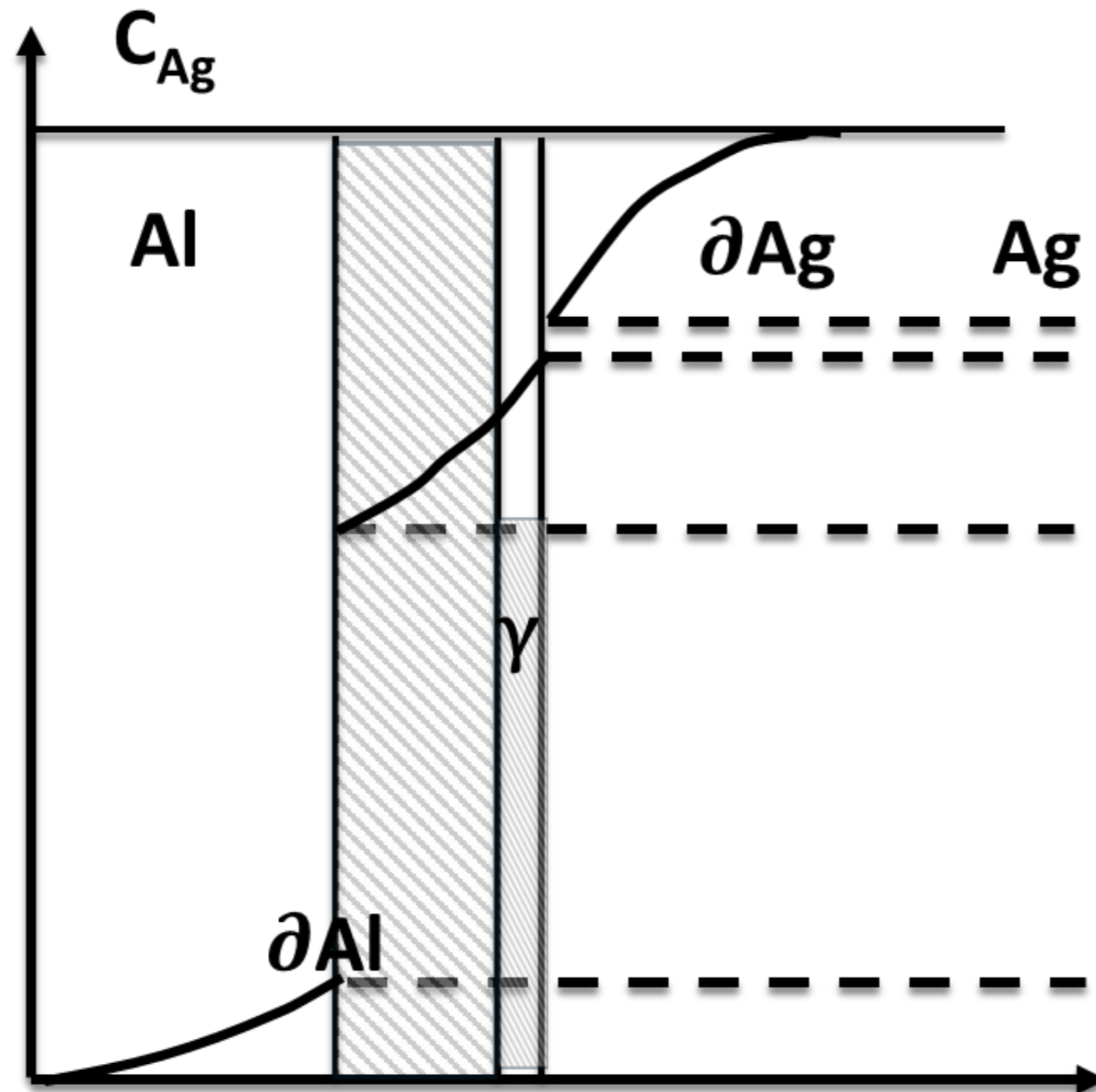
$$D_A^* = \text{constant}$$



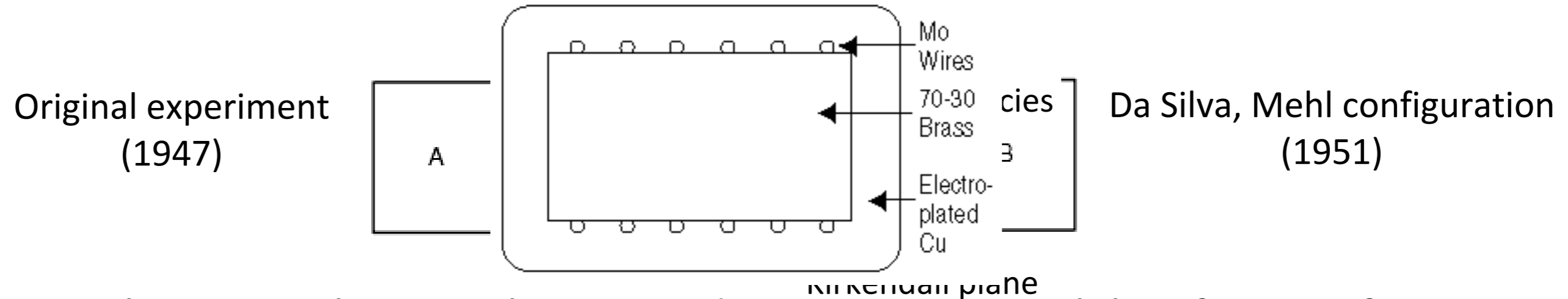
$$\operatorname{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-z^2} dz$$

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

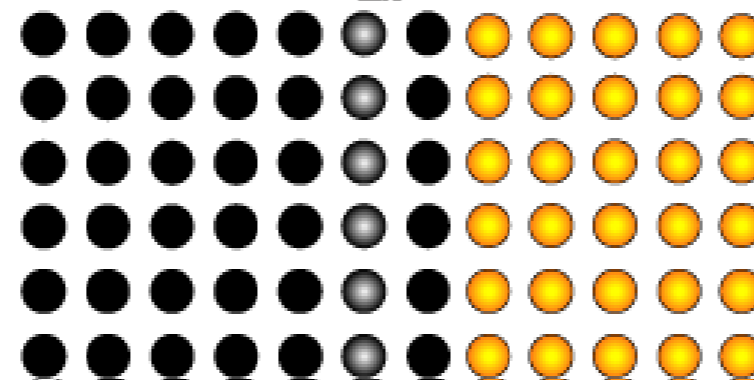
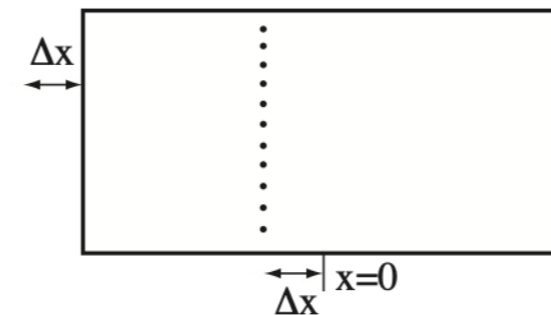
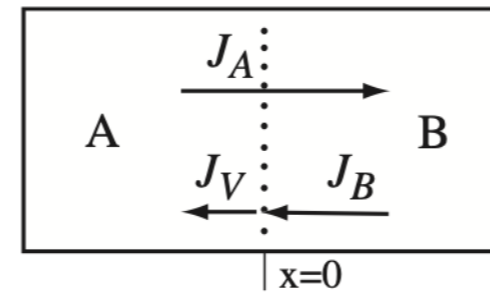




# Kirkendall effect



Explanation: the sample moves depending on the lab reference frame



# Kirkendall effect: solving of the problem

$$J_v + J_A + J_B = 0 \quad \text{Fixed reference (lab)}$$

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

Velocity of vacancies

$$v_v = J_v \Omega$$

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

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

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

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

# Kirkendall effect: solving the problem

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

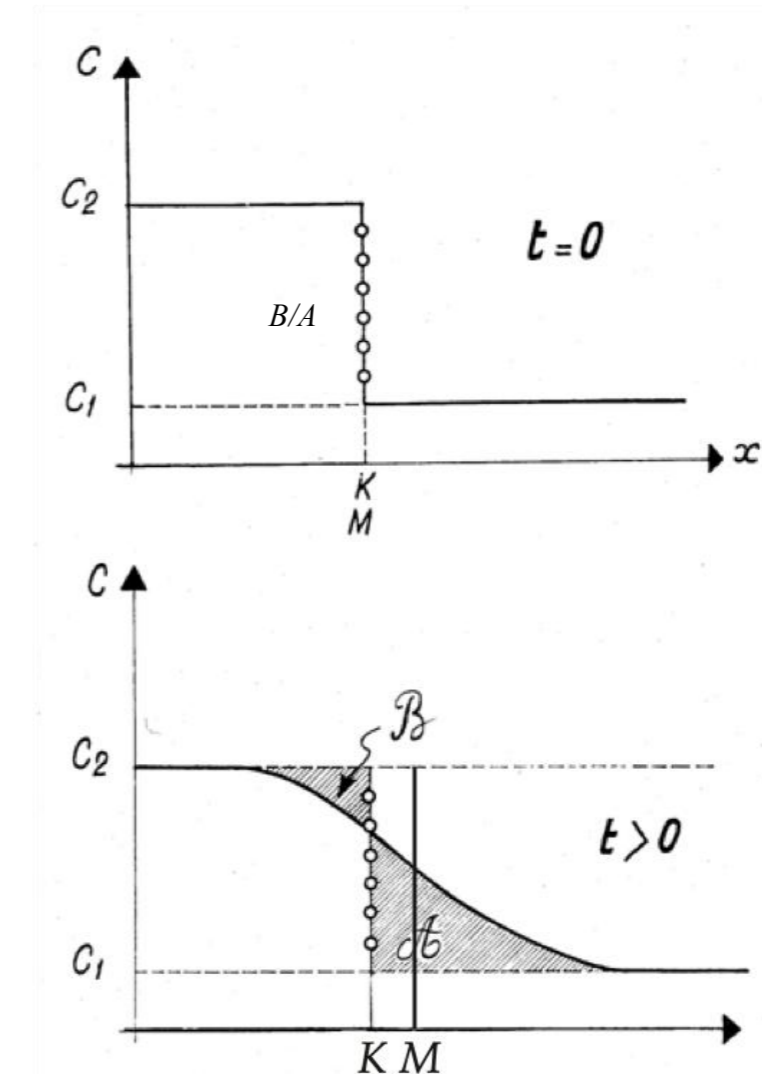
$$J_A^0 = -D_A^* \frac{\partial C_A}{\partial x} + (D_A^* - D_B^*) \frac{\partial C_A}{\partial x} X_A = - (D_A^* - X_A D_A^* + X_A D_B^*) \frac{\partial C_A}{\partial x}$$

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

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

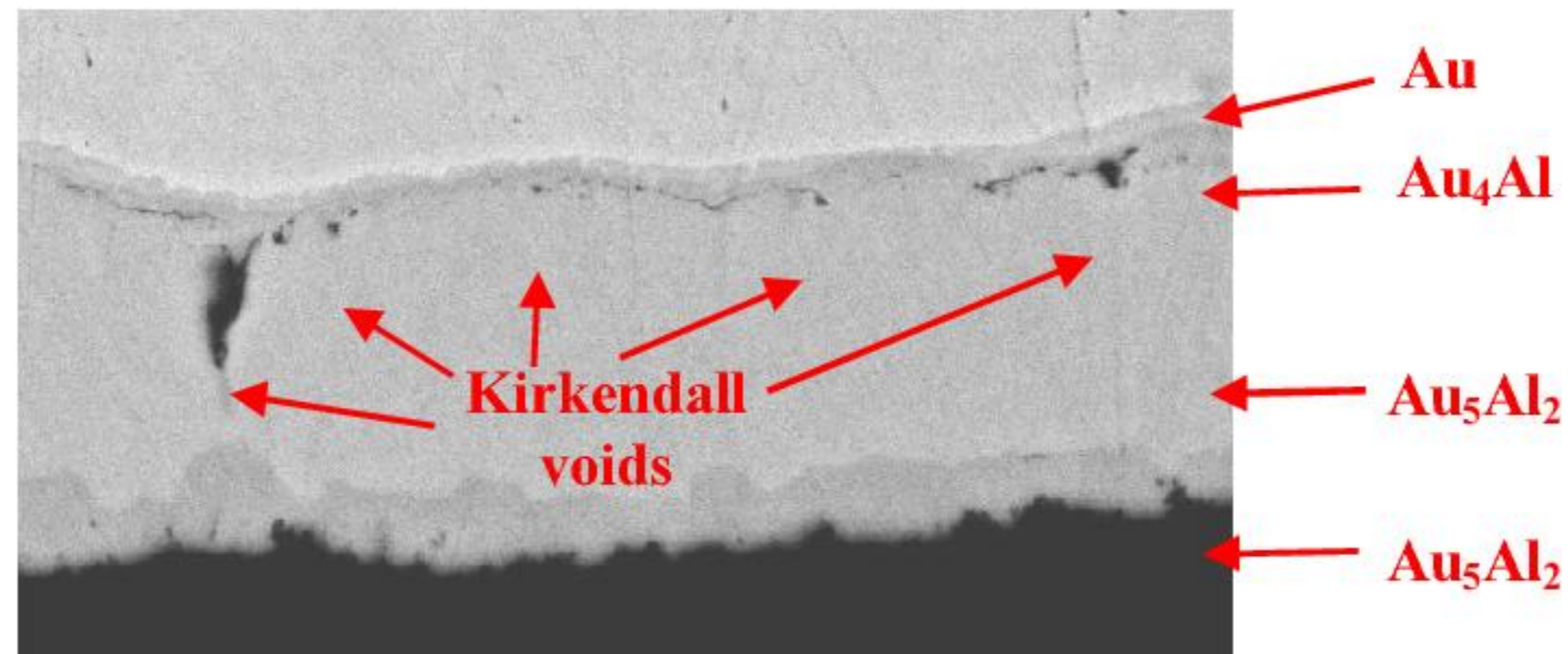
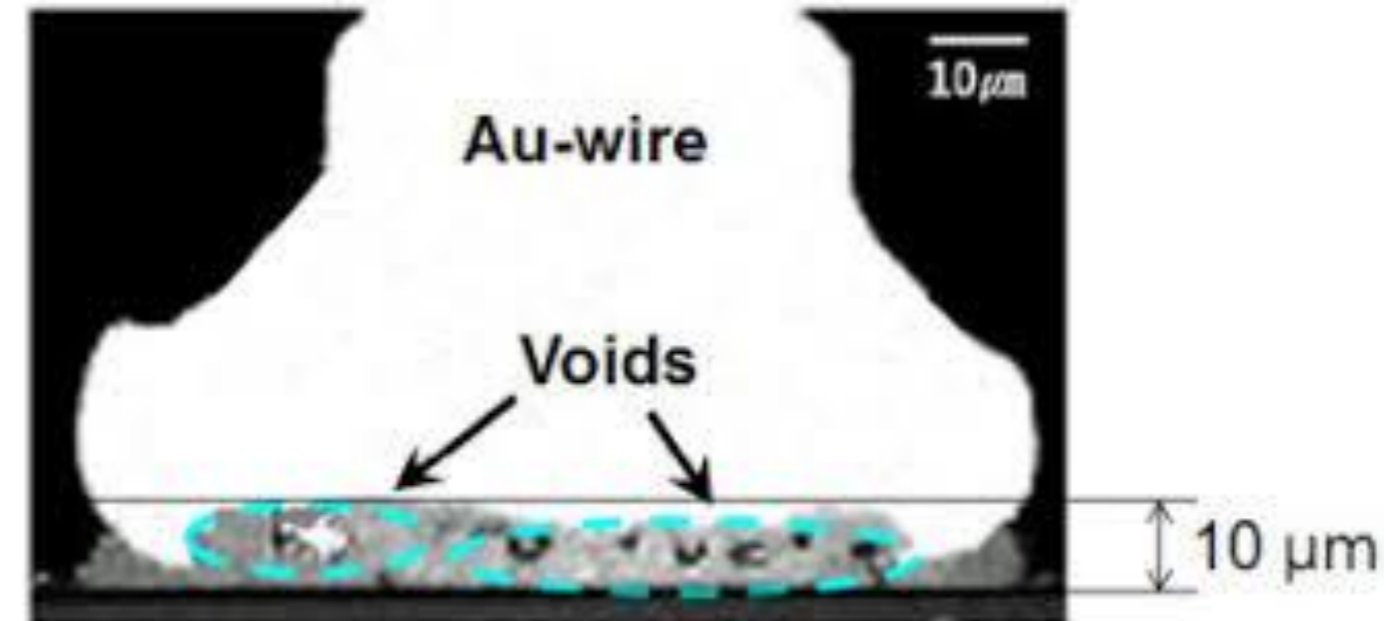
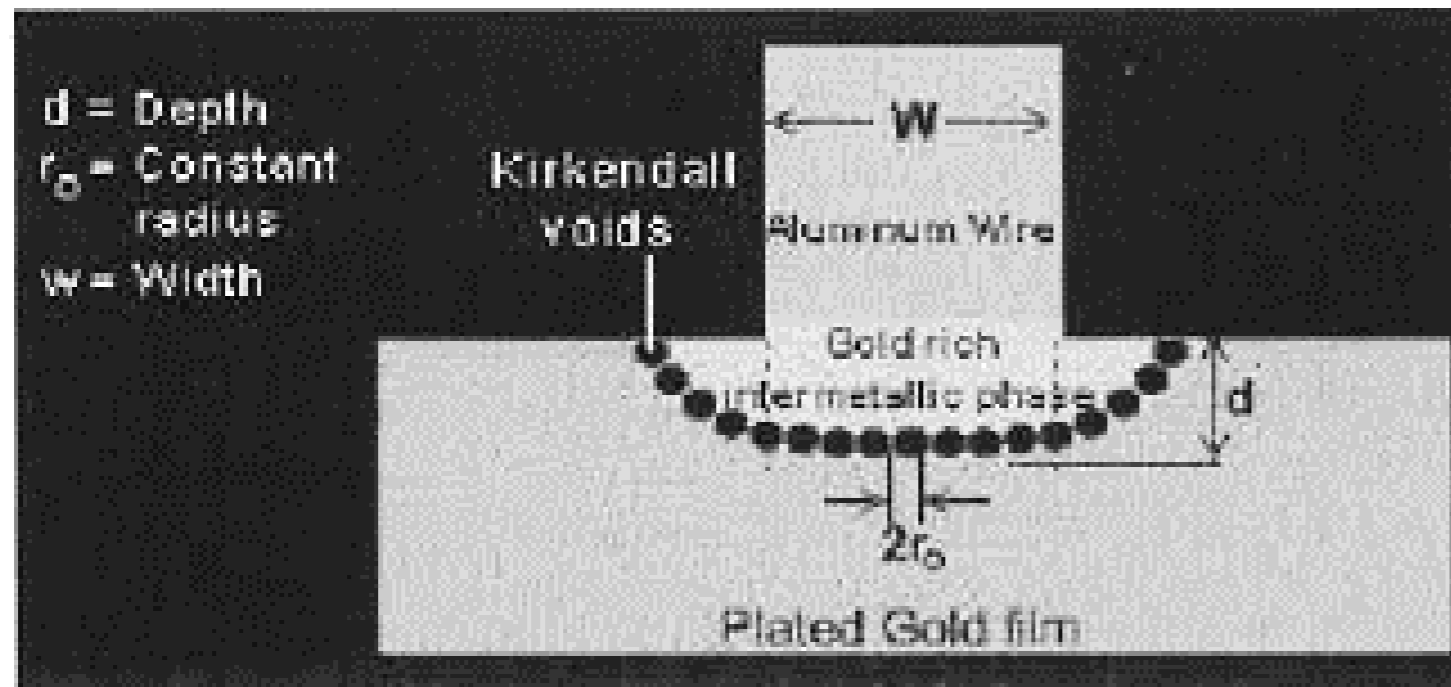
We get  $\tilde{D}$  by the B-M method

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

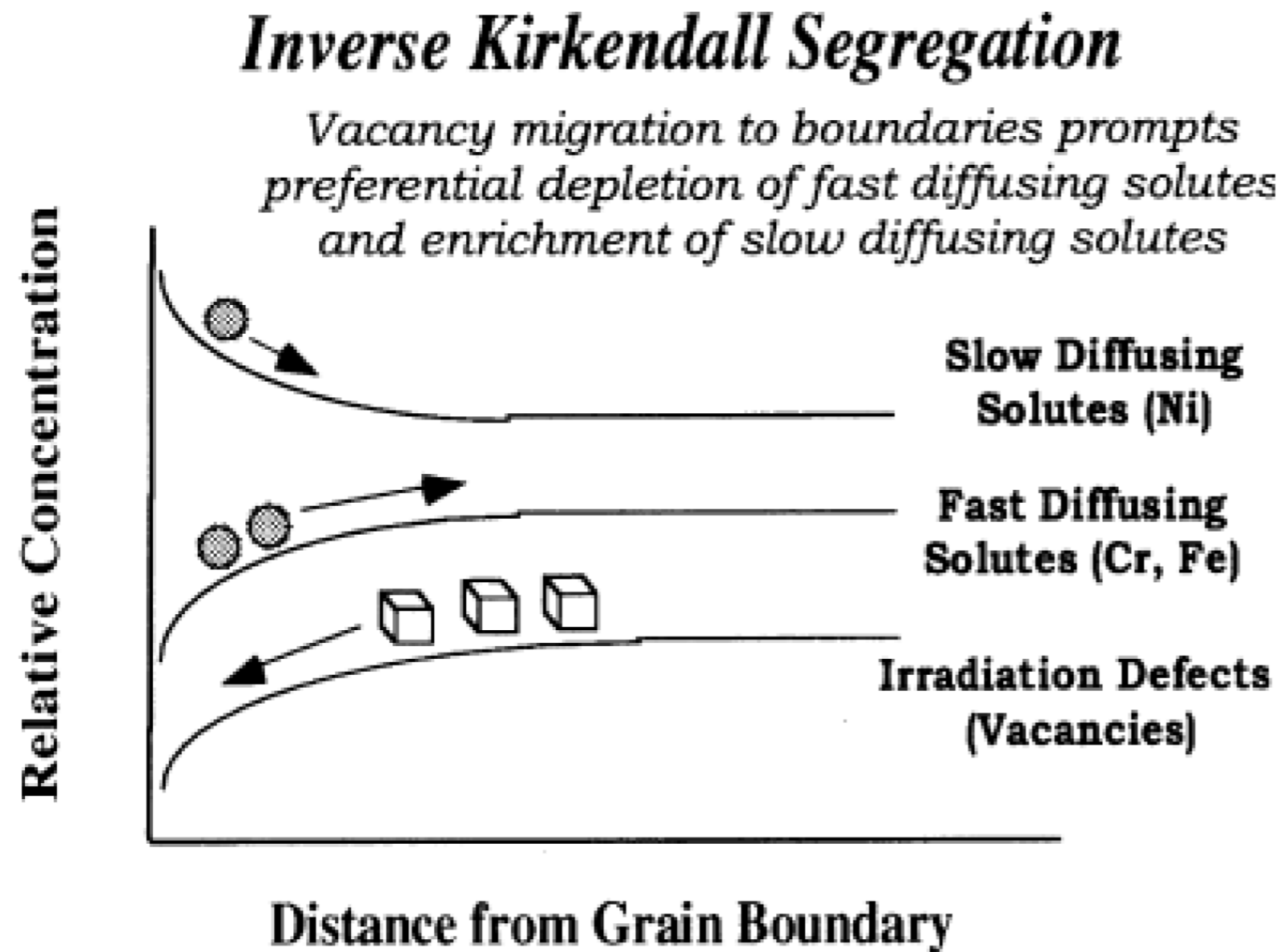


$$D_B^* / D_A^* = B/A$$

# 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	$A$ $\text{cm}^2\text{s}^{-1}$	$Q$ $\text{kJ mol}^{-1}$	Temp. range K
<b>Group IIB</b>			
Zn	c 0.13 1c 0.18	91.7 } 96.3 }	513-691
Cd	c 0.118 1c 0.183	77.92 } 82.02 }	
<b>Group IIIA and rare earths</b>			
Y	1c 0.32 1c 5.2	252.5 } 280.9 }	1173-1573
$\beta$ -La	1.5	188.8	
$\gamma$ -La	0.013	102.6	1140-1170
	0.11	125.2	1151-1183
$\gamma$ -Ce	0.55	153.2	901-965
$\delta$ -Ce	0.012	90.0	992-1044
$\beta$ -Pr	0.087	123.1	1323-1473
Er	c 3.71 1c 4.51	301.66 } 302.58 }	1479-1684
Eu	1.0	144.4	
$\beta$ -Gd	0.01	136.9	1549-1581
$\alpha$ -Yb	0.034	146.79	823-983
$\gamma$ -Yb	0.12	121.0	1031-1083
<b>Group IIIB</b>			
Al	1.71	142.4	723-923
	2.25	144.4	573-923
	0.137	123.5	298-581 <sup>141</sup>
	0.176	126.4	358-482
Ga	$D=5.3 \cdot 10^{-13}$		282.8
	$D=5.3 \cdot 10^{-13}$		293.0
	$D=7.8 \cdot 10^{-13}$		298.0
	$D=9.3 \cdot 10^{-13}$		300.5
	$D=42 \cdot 10^{-13}$		302.7
In	1c 2.7 1c 3.7	78.3 } 78.3 }	317-417
	1c 0.4 1c 0.4	95.9 } 94.6 }	
$\alpha$ -Ti	0.42	80.18	513-573

## Diffusion at low concentration

Table 13.2 TRACER IMPURITY DIFFUSION COEFFICIENTS

Element	$A$ $\text{cm}^2\text{s}^{-1}$	$Q$ $\text{kJ mol}^{-1}$	Temp. range K	Method	Ref.
<i>In Ag</i>					
Cu	1.23	193.0	990-1218	IVa(i), s.c., Cu <sup>64</sup> , 99.99%	13
	0.029	164.1	699-897	IVa(iii) (SIMS), s.c., 99.99%	
Au	0.85	202.1	991-1198	IVa(i), s.c., Au <sup>199</sup> , 99.99%	18
Zn	0.54	174.6	916-1197	IVa(i), s.c., Zn <sup>65</sup> , 99.99%	14
	0.532	174.6	970-1225	IVa(i), s.c., Zn <sup>63</sup> , 9.999%	259
Cd	0.44	174.6	866-1210	IVa(i), s.c., Cd <sup>111</sup> , 99.99%	10
Hg	0.079	159.5	926-1221	IVa(i), s.c., Hg <sup>203</sup> , 99.99%	13
Al	0.13	159.5	873-1223	Ib (X-ray), p.c.,	211
Ga	0.42	162.9	873-1213	Ib (X-ray), p.c.,	260
In	0.41	170.1	886-1209	IVa(i), s.c., In <sup>115</sup> , 99.99%	10
	0.36	169.0	553-838	IVa(i), s.c., In <sup>113</sup> , 99.999%	261
Tl	0.15	158.7	918-1073	IVa(i), p.c., Tl <sup>204</sup> ,	15
Ge	0.084	152.8	943-1123	IVa(i)m p.c., Ge <sup>71</sup> ,	15
Sn	0.25	165.0	865-1210	IVa(i), s.c., Sn <sup>113</sup> , 99.99%	10
Pb	0.22	159.5	973-1098	IVa(i), p.c., Pb <sup>210</sup> ,	19
As	0.42	149.6	915-1213	IVa(iii) (EMPA), p.c., 99.98%	107
Sb	0.169	160.4	743-1215	IVa(i), s.c., Sb <sup>124</sup> , 99.99%	11
S	1.65	167.5	873-1173	IVb, s.c., S <sup>32</sup> , 99.999%	108
Se	0.285	157.4	759-1109	IVa(i) (ion impl), s.c., Se <sup>75</sup> , 99.999%	262
Te	0.21	154.7	650-1169	IVa(i), s.c., Te <sup>125</sup> , 99.999%	109
Ti	1.33	198	1051-1220	Ia(ii) (EMPA), p.c., 99.999%	263
V	2.72	209	1012-1218	IVb, p.c., V <sup>51</sup> , 99.999%	263
Cr	3.29	210	1023-1215	IVb, p.c., Cr <sup>51</sup> , 99.999%	263
	1.07	192.6	976-1231	IVa(i), s.c., Cr <sup>51</sup> , 99.9999%	264
Mn	4.29	196	883-1212	IVb, p.c., Mn <sup>54</sup> , 99.999%	263
Fe	2.6	205.2	1073-1205	IVa(i), s.c., Fe <sup>57</sup> , 99.999%	106
Ru	180	275.5	1066-1219	IVa(i), s.c., Ru <sup>101/100</sup> , 99.99%	12
Co	1.9	204.1	973-1214	IVa(i), s.c., Co <sup>60</sup> , 99.999%	106

# Some examples of diffusion coefficients: chemical diffusion

## Chemical diffusion

Table 13.4 CHEMICAL DIFFUSION COEFFICIENT MEASUREMENTS—continued

Element 1 At. %	Element 2 At. %	A cm <sup>2</sup> s <sup>-1</sup>	Q kJ mol <sup>-1</sup>	D cm <sup>2</sup> s <sup>-1</sup>	Temp. range K
Mo	Pd	61	188.4	$(D_{Pd} \approx {}^{(a)}_{10-20} \times D_{Mo})$	1273-1873
		66	165.4		
		71	177.9		
		75	200.5		
		80	218.6		
		85	253.3		
		90	293.1		
		95	282.6		

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

Mo	Ta	4.68 × 10 <sup>-3</sup>	251.2	—	2175-2573
	'Ta rich'				
	'Mo rich'	4.16 × 10 <sup>-3</sup>	234.5	—	
Mo	Ti	0	196.8	$D_{Ti}/D_{Mo}$	1483-1873
		10	209.3		
		20	217.7		
		30	263.8		
		40	255.4		
0-10	(β)	1.3 × 10 <sup>-4</sup>	138.6	—	1173-1573
Sol. soln range	(α)	3.5 × 10 <sup>-8</sup>	118.9	—	873-1073

## Diffusion in binary alloys

Table 13.3 DIFFUSION IN HOMOGENEOUS ALLOYS—continued

Element 1 (purity) At. %	Element 2 (purity) At. %	A† cm <sup>2</sup> s <sup>-1</sup>	Q† kJ mol <sup>-1</sup>	A† cm <sup>2</sup> s <sup>-1</sup>	Q† kJ mol <sup>-1</sup>	Temp. range K	Ref.
Co (—)	Cr (—)	4	275.5	p.c.	—	1373-1623	33
		7	332.0				
Co ( )	Cr Ni (—) (—)	9	301.9	p.c.	—	1373-1623	33
		18	268.8				
		26	0.4				
Co (99.99)	Cu Si (99.99) ( )	0.54	B <sub>1</sub> = -9	IVa(i), p.c., Co <sup>38</sup>	—	1325	158
Co ( )	Fe ( )	50	251.2	0.25	230.3	1068-1218(α)	34
		2.0	556.8		556.8	928-995(CrCl)	
( )	( )	0.54	272.1	p.c.	—	1373-1573	33
( )	( )		IVa(iii)	p.c.			
	0	Diffusion of Ni D <sub>Ni</sub> = 13.10 <sup>-12</sup>				1409	82
	30.2	= 11.5					
	68.5	= 8-8.8					
	88.3	= 5					
	100	= 6					
( )	( )	1.83	234.0	p.c.	—	1073-1172	107
0	(bcc)						
	(fcc)	0.77	265.0		—	1223-1633	
3	(bcc)	9.17	266.3		—	903-1023(F)	
6.8	(bcc)	0.469	187.1		—	903-1073(F)	
	(fcc)	5.72 × 10 <sup>-3</sup>	146.5		—	1153-1193	
28.6	(fcc)	0.109	326.2		—	1283-1583	
49.6	(bcc)	1.25 × 10 <sup>-3</sup>	198.0		—	903-1093(F)	
	(fcc)	3.36 × 10 <sup>-2</sup>	266.3		—	1333-1583	
67.2	(bcc)	6.59 × 10 <sup>-2</sup>	247.0		—	1023-1123(F)	
	(fcc)	0.154	349.6		—	1333-1583	
89.6	(bcc)	6.04 × 10 <sup>-3</sup>	190.9		—	903-1153(F)	
	(fcc)	3.15 × 10 <sup>-2</sup>	265.0		—	1333-1583	
	(fcc)	6.44 × 10 <sup>-2</sup>	251.2		—	1073-1283(F)	
	(fcc)	1.61 × 10 <sup>-2</sup>	234.0		—	1333-1153	
100	(fcc)	0.50	273.8		—	1045-1321(F)	
		0.17	260.4		—	1465-1570	
(99.8)	(99.9)	IVb	p.c.	Co <sup>40</sup>	—		
0		0.029	247.4		—		
8		20.54	321.5		—		
10		15.65	369.0		—	1233-1493	
15		1.98	289.7		—		
20		0.31	261.7		—		
Co ( )	Fe ( )	IVb, s.c., Fe <sup>39</sup>	—	0.58	273.3	1081-T <sub>c</sub>	176
	6	—	—	0.15	261.7	T <sub>c</sub> -1573	
	10	—	—	0.68	279.3	1081-T <sub>c</sub>	
	10	—	—	0.18	263.3	T <sub>c</sub> -1573	

# Some examples of diffusion coefficients: interdiffusion

Co (%)	Fe (%)		IVa(i)	p.c.
( )	( )	1.33	290.6	1.26
50	50		251.2	0.25
( )	( )		556.8	
( )	( )	0.54	IVb	p.c.
( )	( )		272.1	
( )	( )		IVa(iii)	p.c.
	0	Diffusion of Ni $D_{Ni} = 13.10^{-12}$ = 11.5 = 8-8.8 = 5 = 6		
	30.2			
	68.5			
	88.3			
	100			
( )	( )		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	
	(fcc)	$5.72 \times 10^{-3}$	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	
	(fcc)	$1.61 \times 10^{-2}$	234.0	
100	(fcc)	0.50	273.8	
		0.17	260.4	
(99.8)	(99.9)	IVb	p.c.	Co <sup>40</sup>
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 <sup>59</sup>		
( )	( )			0.58
	6			0.15
	6			0.68
	10			0.18
	10			

## Interdiffusion coefficient

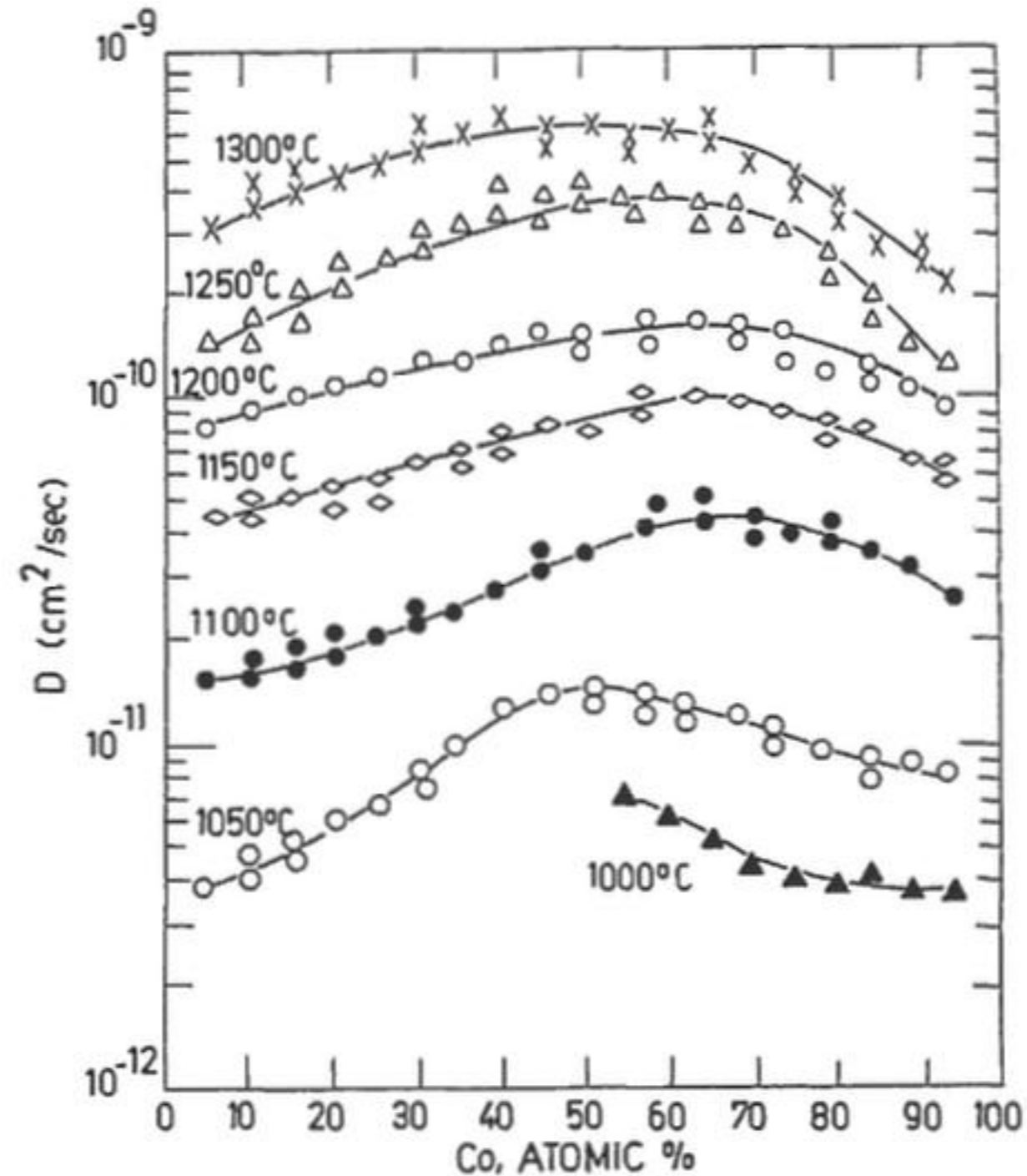


Figure 13.6b Interdiffusion in f.c.c. FeCo alloys<sup>218</sup>