DE LA RECHERCHE À L'INDUSTRIE

Computing transport coefficients from the atomic scale

Long-time multi-scale simulations of activated events: from theory to practice

T. Schuler

Coarse-graining ?

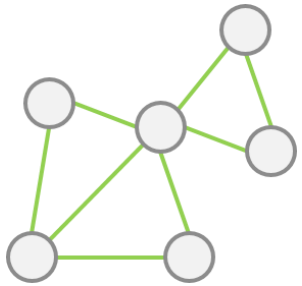
Assume we know our transitions and the associated rates :

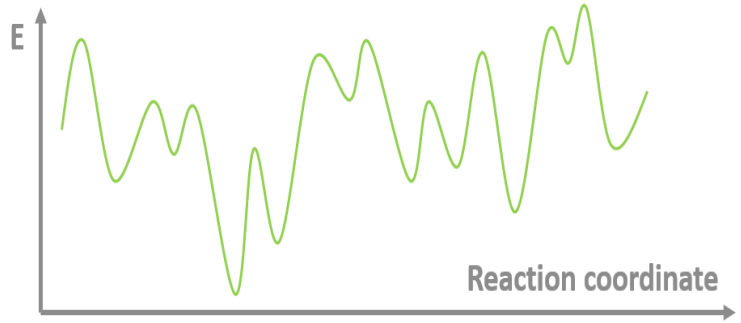
$$\omega_{nm} = \nu_{nm} \exp\left(-\frac{G^{mig}(n \to m)}{k_B T}\right)$$

?

How do I get physical insight at a higher scale from these transitions ?
e.g. diffusion coefficients

$$D_\alpha = D_\alpha^0 \exp\left(-\frac{Q_\alpha}{k_B T}\right)$$





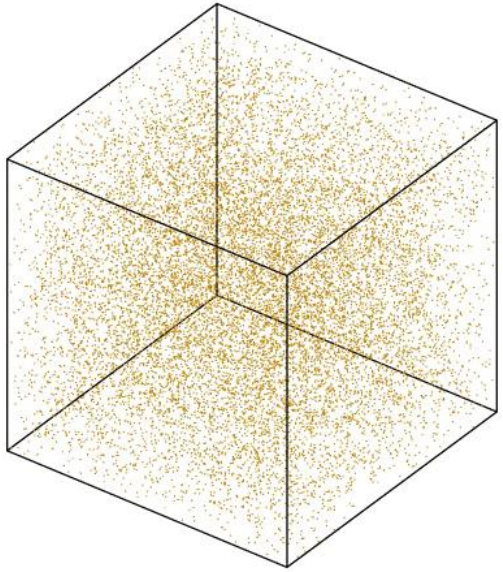
Such representation is not enough for diffusion coefficient.

➢ We need to add information about how atoms move in (real) space during each ransition.

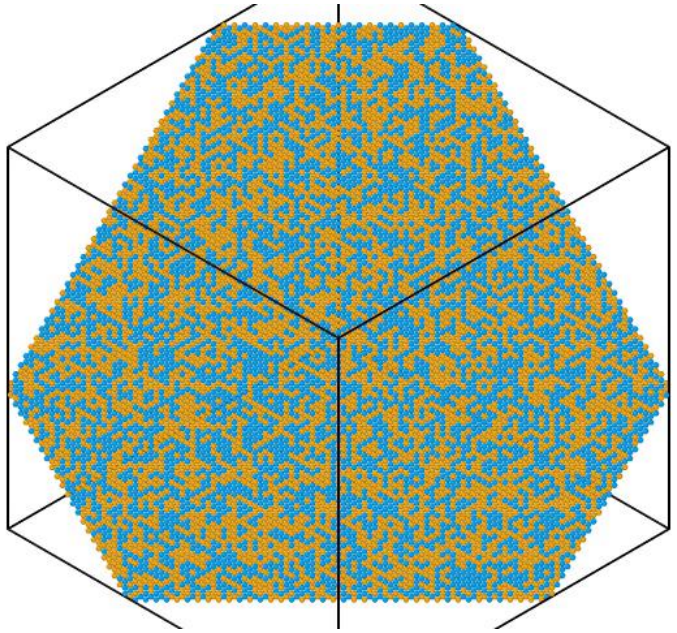
We will focus on crystals :

- easier to discretize (manageable number of configurations)
- defect mediated diffusion with rather small number defect concentrations (local events)
- yet this introduces the so-called « kinetic correlations »

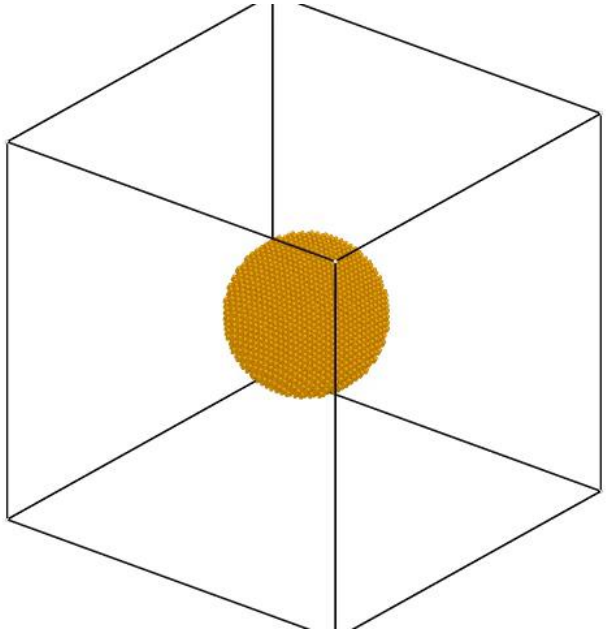
Why bother with diffusion/transport coefficients ?



Nucleation-Growth-Coalescence
(Classical theory of nucleation)



Spinodal decomposition
(Cahn-Hilliard equations)



Driven alloys
(Ballistic mixing under irradiation)

Other coarse-grain simulations where atom redistribution is of interest:

- **Object Kinetic Monte Carlo**
- **Cluster Dynamics**
- **Phase Field**
- **Finite Elements**

Material science needs diffusion/transport coefficients

How do we get diffusion coefficients?

Difficult to measure experimentally

- Long experiments
- Use of radioactive tracers

Diffusion coefficients are not enough
=> Onsager (or transport coefficients)

- Matrix of coefficients
- Only measured in a small number of systems (Anthony)

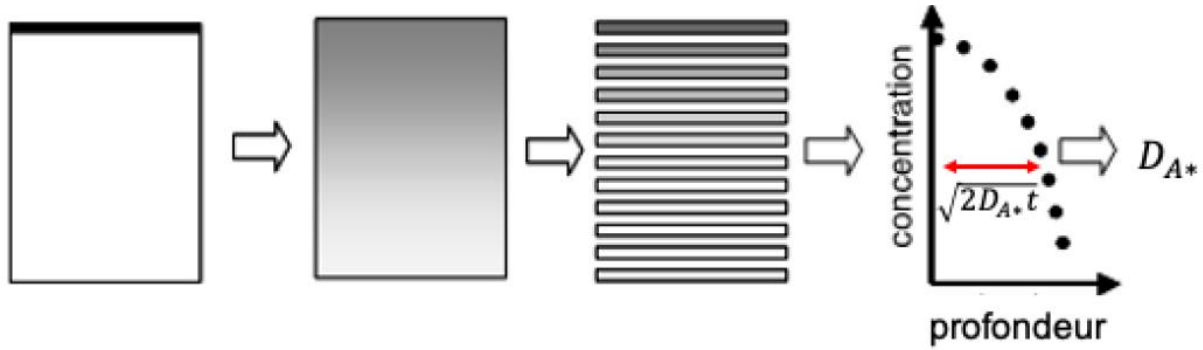
Onsager equation

$$\vec{J}_i = -\sum_j L_{ij} \vec{\nabla} \mu_j$$

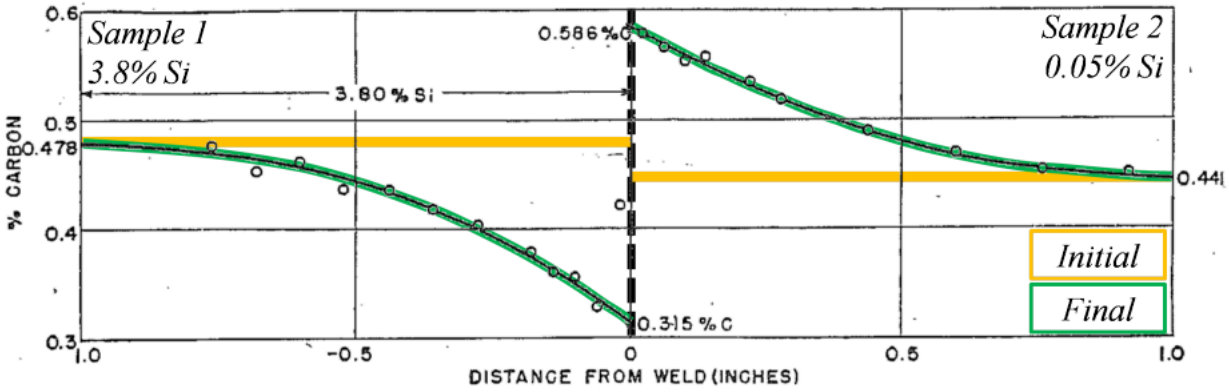
(matrix formulation)

$$\begin{pmatrix} \mathbf{J}_\mathrm{A} \\ \mathbf{J}_\mathrm{B} \\ \mathbf{J}_\mathrm{C} \end{pmatrix} = - \begin{pmatrix} L_{\mathrm{AA}} & L_{\mathrm{AB}} & L_{\mathrm{AC}} \\ L_{\mathrm{BA}} & L_{\mathrm{BB}} & L_{\mathrm{BC}} \\ L_{\mathrm{CA}} & L_{\mathrm{CB}} & L_{\mathrm{CC}} \end{pmatrix} \begin{pmatrix} \nabla \mu_\mathrm{A} \\ \nabla \mu_\mathrm{B} \\ \nabla \mu_\mathrm{C} \end{pmatrix}$$

Tracer diffusion experiment



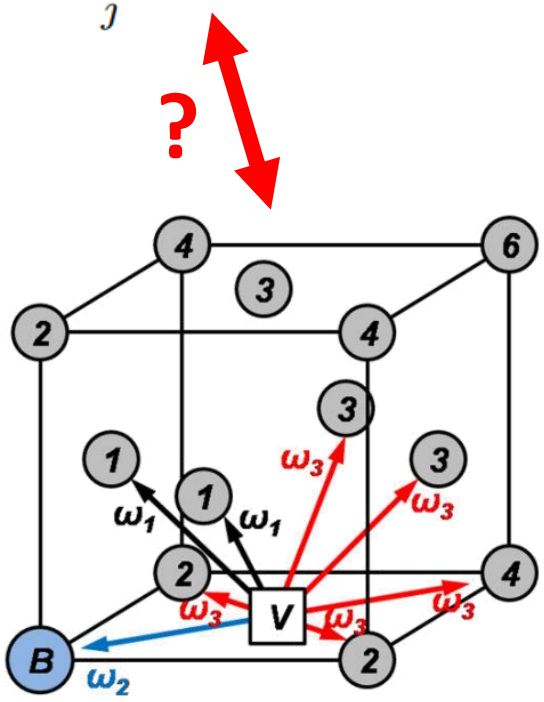
Darken's experiment



Outline

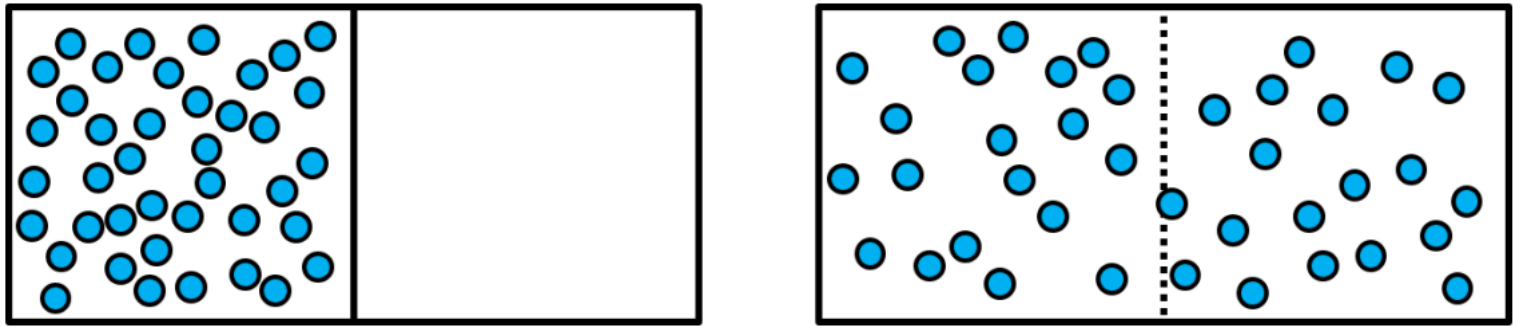
$$\vec{J}_i = -\sum_j L_{ij}\vec{\nabla}\mu_j$$

Jump	$E_m(if)$	ν_{if}^d
ω_0^I	0.128	2.35
ω_0^V	0.717	3.47
ω_{ex}^V	0.473	7.26
ω_{11}^V	0.945	4.68
ω_{12}^V	0.830	5.10
ω_{13}^V	0.805	5.32
ω_{14}^V	0.747	5.22
ω_{23}^V	0.793	5.16
ω_{25}^V	0.673	5.03
ω_{33}^V	0.699	4.86
ω_{34}^V	0.776	4.83
ω_{35}^V	0.676	4.96
ω_{36}^V	0.737	5.01
ω_{37}^V	0.717	5.01
ω_{45}^V	0.665	4.88
ω_{47}^V	0.746	4.95
ω_{48}^V	0.709	4.94



- Phenomenological approach : Fick's law
- 1-D random walk model
- Diffusion coefficient
  vs. equilibrium fluctuations of atomic positions
- Kinetic correlation
- Self-Consistent Mean-Field (SCMF) theory

Fick's first law at the microscopic scale



Particles perform a random walk in the available volume

Fick's first law

$$\vec{J}_\alpha = -D_\alpha \vec{\nabla} C_\alpha$$

At the macroscopic scale, diffusion is an irreversible phenomenon.
At the microscopic scale, diffusion is reversible.

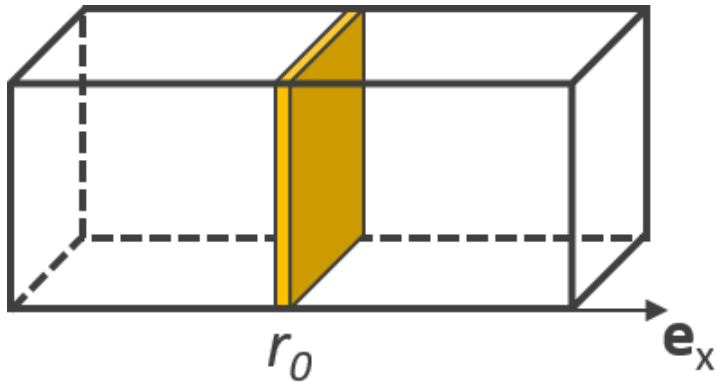
Phenomenological law: Fick and solution to the diffusion equation

Matter conservation law
(continuity equation)

$$\frac{\partial C_{\mathrm{A}}(\mathbf{r},t)}{\partial t} + \boldsymbol{\nabla}\cdot\mathbf{J}_{\mathrm{A}} = 0$$

Diffusion equation
(2nd Fick law)

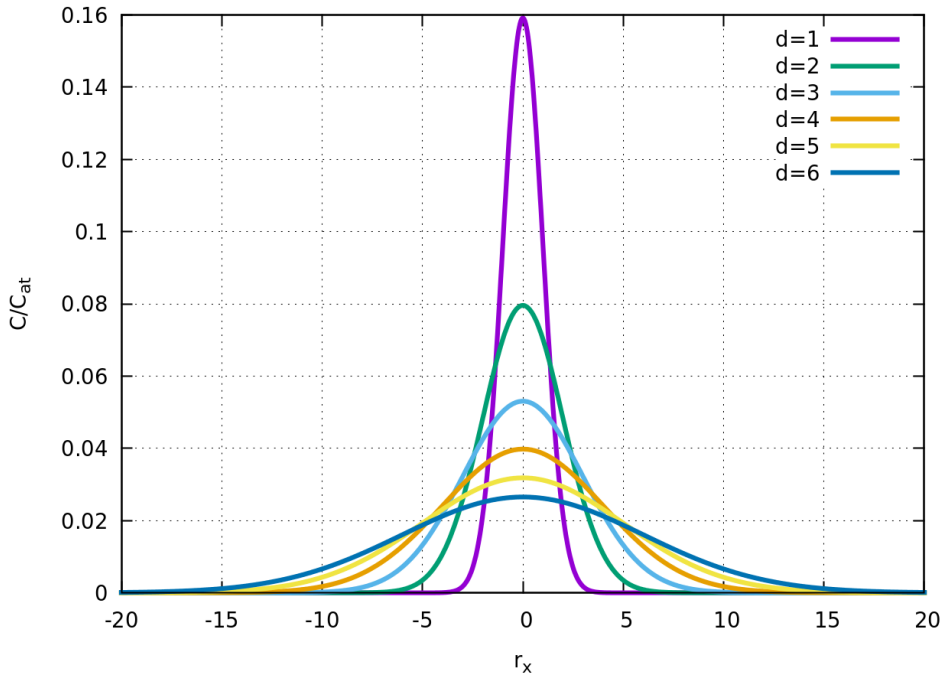
$$\frac{\partial C_{\mathrm{A}}(\mathbf{r},t)}{\partial t} = D_{\mathrm{A}} \triangle C_{\mathrm{A}}(r,t)$$



Solution of the diffusion equation:

$$C_{\mathrm{A}}(r_x,t) = \frac{C_{at}}{\sqrt{2\pi}\delta_x}\exp\left(\frac{-(r_x-r_0)^2}{2\delta_x^2}\right)$$

$$\delta_x = \sqrt{2D_{\mathrm{A}}^x t}$$

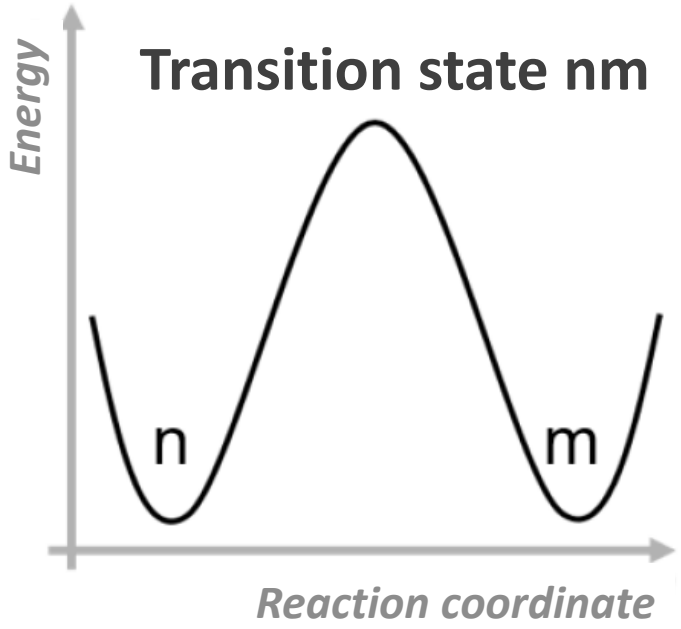


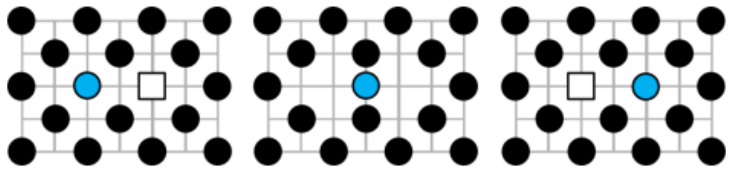
Various interpretations of C_A

- Time average
- Ensemble average
- Average over space

Going to the atomic scale : Transition state theory

$$\omega_{nm} = \nu_{nm} \exp\left(-\frac{G^{mig}(n \to m)}{k_B T}\right) = \nu_{nm} \exp\left(-\frac{G^{TS}_{nm} - G^{TS}_{n}}{k_B T}\right)$$

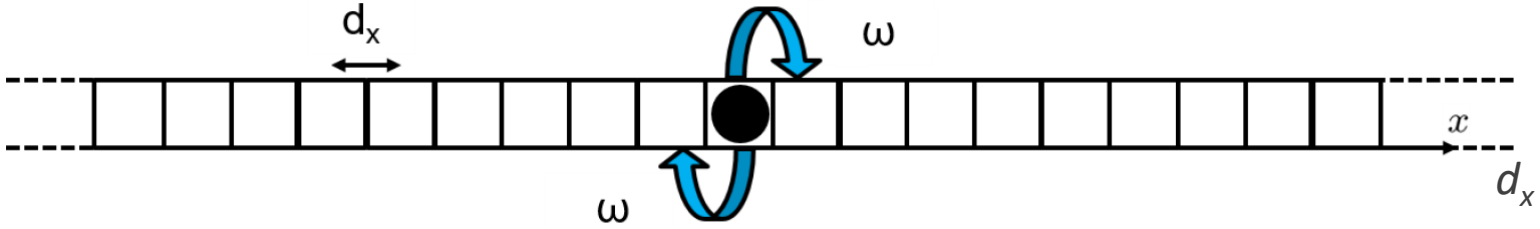




Additional assumption :

If migration energies are large enough compared with $k_B T$, the system has **no memory** in the sense that the probability to perform a given jump will not depend on the preceding jumps. Such process is called a **Markov process**.

First model : random walk on a 1D lattice



x : diffusion direction
d_x : distance between two sites
r_x : position of the particle
ω : jump frequency to a neighboring site
n : total number of jumps performed during time t
p : probability to jump to the right
$p_n(k)$: probability of performing k jumps to the right for a total of n jumps

Link between our problem and the classical binomial problem

$$\begin{cases} n = 2\omega t \\ r_x = d_x(2k-n) \\ p = 1/2 \end{cases}$$

$$\langle r_x \rangle = 0 \qquad \langle r_x^2 \rangle = 2d_x^2 \omega t$$

$$\delta_x = \sqrt{\langle r_x^2 \rangle - \langle r_x \rangle^2} = \sqrt{2d_x^2 \omega t}$$

Reminder: characteristic diffusion length $\delta_x = \sqrt{2D_\alpha^x t}$

$$D_\alpha^x = d_x^2 \omega$$

Results for the binomial law

$$p_n(k) = \binom{n}{k} p^k (1-p)^{n-k}$$

$$\langle k^m \rangle = \sum_{k=0}^{n} k^m p_n(k)$$

$$\langle k \rangle = np$$

$$\langle k^2 \rangle = n^2 p^2 + np(1-p)$$

The « equilibrium fluctuations » point of view

The Einstein-Smoluchowski formula for 3D systems

$$D_\alpha = \frac{\left\langle \vec{R}^2 \right\rangle}{6\tau}$$

For a random walk where all transitions have equivalent jump length
(*z* is the coordination number of the lattice)

$$\left\langle \vec{R}^2 \right\rangle = n_\tau \times \vec{d}^{\,2} = z\omega\tau\vec{d}^{\,2}$$

For a cubic lattice (SC, BCC, FCC) where atoms jump by first nearest neighbor jumps, we always have the following relation (*a* is the lattice parameter) :

$$\frac{z\vec{d}^{\,2}}{6} = a^2 \quad \Rightarrow \quad D_\alpha = a^2\omega$$

Diffusion coefficient vs. transport coefficient

Tracer diffusion coefficient

Einstein-Smoluchowski formula

$$D_\alpha = \frac{\langle \vec{R}^2 \rangle}{6\tau} = \frac{\left\langle \left(\sum_{i=0}^{\tau/\delta t} \vec{R}_i \right)^2 \right\rangle}{6\tau}$$

We can average the result obtained for a tracer atom on a population of N_α traced atoms

$$D_\alpha = \frac{1}{N_\alpha} \sum_{k=1}^{N_\alpha} \frac{\langle \vec{R}(k)^2 \rangle}{6\tau} = \frac{\left\langle \sum_{k=1}^{N_\alpha} \left(\sum_{i=0}^{\tau/\delta t} \vec{R}_i(k) \right)^2 \right\rangle}{6\tau N_\alpha}$$

A tracer diffusion coefficient characterizes the mobility of a **single particle.**

Transport coefficient

Allnatt formula

$$L_{\alpha\beta} = \frac{\left\langle \vec{R}(\alpha)\vec{R}(\beta) \right\rangle}{6\tau V k_B T}$$

Displacement of the group of atoms belonging to species α

$$\vec{R}(\alpha) = \sum_{k=1}^{N_\alpha} \vec{R}(k)$$

$$L_{\alpha\alpha} = \frac{C_\alpha}{k_B T} \frac{\left\langle \left(\sum_{k=1}^{N_\alpha} \sum_{i=0}^{\tau/\delta t} \vec{R}_i(k) \right)^2 \right\rangle}{6\tau N_\alpha}$$

A transport coefficient characterizes the mobility of a **group of particles** (mobility of the center of gravity of atoms belonging to a given species).

In the dilute limit :

$$D_\alpha = k_B T L_{\alpha\alpha} / C_\alpha$$

Deviation from random walk : kinetic correlation

The correlation coefficient ($0 \leq f_\alpha \leq 1$) quantifies the deviation from random walk.

A coefficient close to 0 relates to strongly correlated diffusion.

A coefficient equal to 1 relates to uncorrelated or random diffusion.

Correlations effects **always slow down** diffusion.

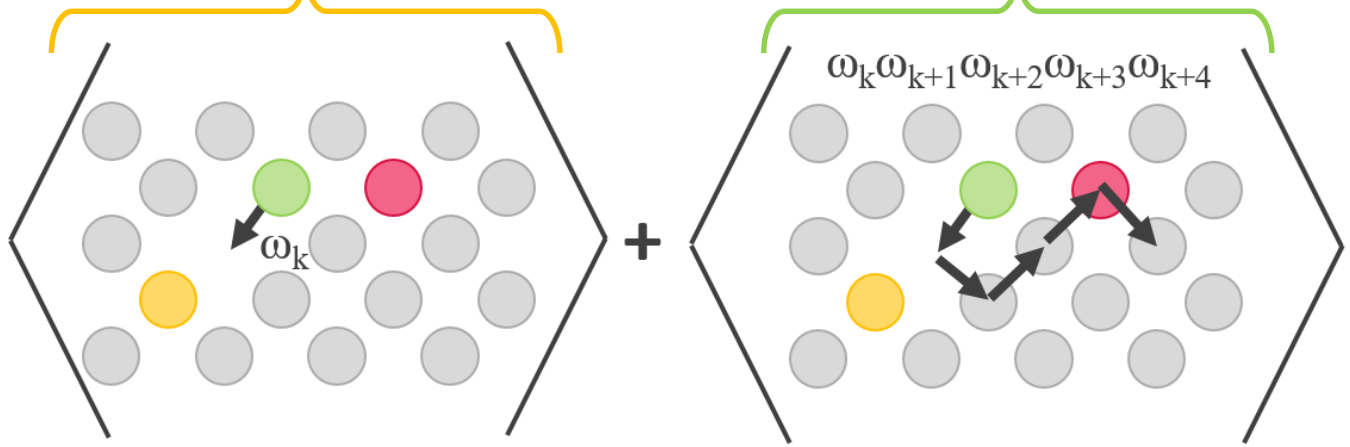
It can be seen as a loss of efficiency in the motion of atoms.

$$f_\alpha = \frac{D_\alpha}{D_\alpha^0}$$

$$D_\alpha = \frac{\langle \vec{R}^2 \rangle}{6\tau} = \frac{\left\langle \left(\sum_i \vec{R}_i \right)^2 \right\rangle}{6\tau} = \frac{\left\langle \sum_i \vec{R}_i^2 + \sum_i \sum_{j \neq i} \vec{R}_i \vec{R}_j \right\rangle}{6\tau} = f_\alpha D_\alpha^0$$

Random walk, ***Average of individual contributions*** *from each jump*

$$D_\alpha^0 = \frac{\sum_i \left\langle \vec{R}_i^2 \right\rangle}{6\tau}$$



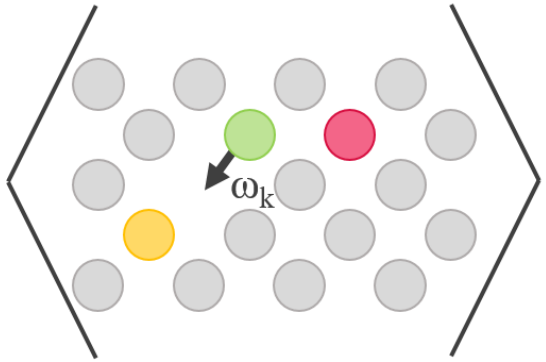
Kinetic correlations accounting for the ***probability of each trajectory, a multi-body contribution which is hard to compute***

$$f_\alpha = 1 + 2\frac{\sum_i \sum_{j>i} \left\langle \vec{R}_i \vec{R}_j \right\rangle}{\sum_i \left\langle \vec{R}_i^2 \right\rangle}$$

Computing the random walk contribution

Random walk, ***Average of individual contributions*** *from each jump*

$$D^0_\alpha = \frac{\sum_i \left\langle \vec{R}_i^2 \right\rangle}{6\tau}$$



$$\frac{\sum_i \left\langle \vec{R}_i^2 \right\rangle}{6\tau} = \frac{1}{6\tau} \sum_i P_i \vec{R}_i^2$$

i : trajectory step
n_i : configuration of the system before step *i*
m_i : configuration of the system after step *i*
$P_{n_i \to m_i}$: probability of jumping from *n* to *m* (at step *i*)
$W_{n_i m_i}$: jump rate [s^{-1}] between configurations *n* and *m* (independent of *i*, Markov process)
θ_n : available jumps from configuration *n*
τ_{n_i} : average residence time on configuation *n*
P_n^{eq} : equilibrium configuration probability (Boltzmann statistics)
G_n : Gibbs free energy associated with configuration *n*
G_{nm}^{TS} : Gibbs free energy at the saddle point between *n* and *m*
z : number of jumps available (coordination number)
a : lattice parameter
$\mathcal{Z}$: partition function
ν_0 : attempt frequency [s^{-1}]

$$\mathcal{Z} = \sum_n \exp\left(-\frac{G_n}{k_B T}\right)$$

Computing the random walk contribution

Random walk,
***Average of individual contributions** from each jump*

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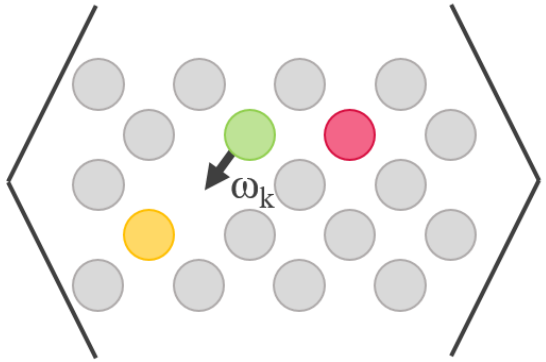

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$$\mathcal{Z} = \sum_n \exp\left(-\frac{G_n}{k_B T}\right)$$

$$\begin{aligned}
\frac{\sum_i \left\langle \vec{R}_i^2 \right\rangle}{6\tau} &= \frac{1}{6\tau}\sum_i P_i \vec{R}_i^2 \\
&= \frac{1}{6\tau}\sum_i P_{n_i \to m_i} \vec{R}^2_{n_i \to m_i} \\
&= \frac{1}{6\tau}\sum_i \frac{W_{n_i m_i}}{\sum_{k \in \theta_{n_i}} W_{n_i k}} \vec{R}^2_{n_i \to m_i} \\
&= \frac{1}{6}\sum_i \frac{\tau_{n_i}}{\tau} W_{n_i m_i} \vec{R}^2_{n_i \to m_i} \\
&\xrightarrow[\tau \to \infty]{} \frac{1}{6}\sum_n P_n^{eq} \sum_{m \in \theta_n} W_{nm} \vec{R}^2_{n \to m} \qquad \textbf{Equilibrium (ergodicity principle)} \\
&= \frac{1}{6\mathcal{Z}}\sum_n \exp\left(-\frac{G_n}{k_B T}\right) \sum_{m \in \theta_n} W_{nm} \vec{R}^2_{n \to m} \\
&= \frac{1}{6\mathcal{Z}}\sum_n \exp\left(-\frac{G_n}{k_B T}\right) \sum_{m \in \theta_n} \nu_0 \exp\left(-\frac{G_{nm}^{TS} - G_n}{k_B T}\right) \vec{R}^2_{n \to m} \\
&= \frac{\nu_0}{6\mathcal{Z}}\sum_n \sum_{m \in \theta_n} \exp\left(-\frac{G_{nm}^{TS}}{k_B T}\right) \vec{R}^2_{n \to m} \\
&= \frac{a^2 \nu_0}{\mathcal{Z}}\sum_n \frac{1}{z}\sum_{m \in \theta_n} \exp\left(-\frac{G_{nm}^{TS}}{k_B T}\right). \qquad \textbf{Cubic system + 1NN jumps}
\end{aligned}$$

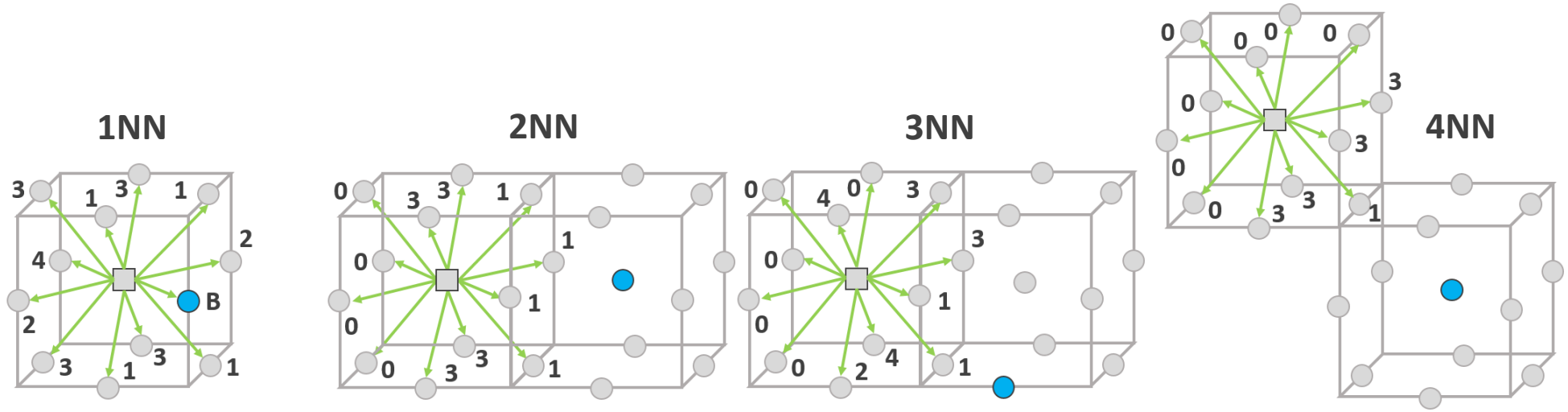
Computing the random walk contribution in a system with interactions
Example : substitutional solute-vacancy pair in a FCC crystal

$$D_\alpha^0 = \frac{a^2\nu_0}{z}\frac{\sum_n\sum_{m\in\theta_n}\exp\left(-\frac{G_{nm}^{TS}}{k_BT}\right)}{\sum_n\exp\left(-\frac{G_n}{k_BT}\right)} = \frac{a^2\nu_0}{z}\frac{\sum_n\sum_{m\in\theta_n}Y_{nm}}{\sum_n Y_n}$$

Monovacancy :

$$D_V^0 = \frac{a^2\nu_0}{z}\frac{z\exp\left(-\frac{G^{for}(V)+G^{mig}(V)}{k_BT}\right)}{\exp\left(-\frac{G^{for}(V)}{k_BT}\right)} = a^2\omega_V$$

Solute vacancy pair (up to 4nn):



Denominator	12 x Y_1	6 x Y_2	24 x Y_3	12 x Y_4
Numerator	12 x ($4Y_{11}+Y_{11B}+2Y_{12}+4Y_{13}+Y_{14}$)	6 x ($4Y_{21}+4Y_{23}+4Y_{20}$)	24 x ($2Y_{31}+2Y_{33}+2Y_{34}+Y_{32}+5Y_{30}$)	12 x ($Y_{41}+4Y_{43}+7Y_{40}$)

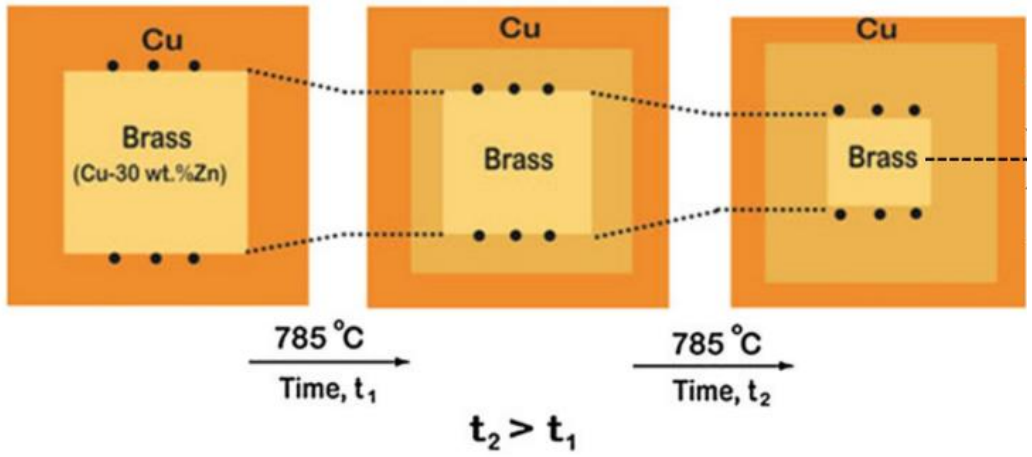
**col=Saddle-Point*

Why vacancies ?

$$X_V^{eq} = \exp\left(-\frac{G^{for}(V)}{k_B T}\right)$$

From a thermodynamic point of view, equilibrium vacancies result from a competition between the energetic cost of a vacancy (all neighboring atoms lose one of the chemical bonds which ensure the stability of the structure) and the disorder created by vacancies, as one vacancy can be located on any site of the cristal, and this possibility generates configurational entropy. At equilibrium, the site concentraiton of vacancies is a function of its formation free energy.

Kirkendall's exeperiment



Point defect concentrations are monitored at every instant at extended crystal defects (dislocations, joints de grains, surfaces, interfaces).

Point defect concentrations can be increased by placing the system in out-of-equilibrium conditions, for instance under irradiation, after quenching or during severe plastic deformation. Diffusion properties are automatically modified under such conditions.

Deviation from random walk : kinetic correlation

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A coefficient close to 0 relates to strongly correlated diffusion.

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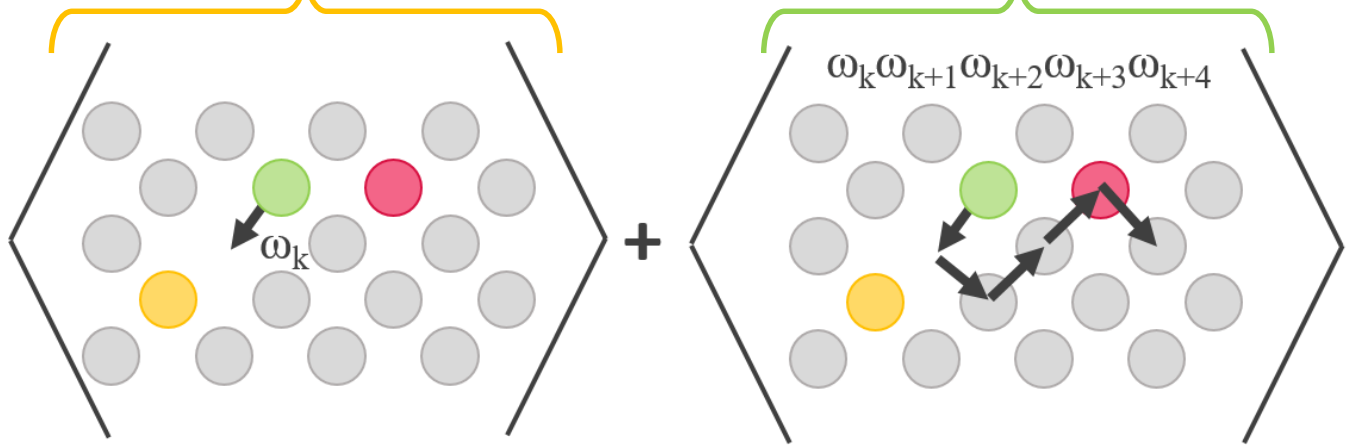
$$D_\alpha^0 = \frac{\sum_i \left\langle \vec{R}_i^2 \right\rangle}{6\tau}$$



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Kinetic correlation effects

The diffusion of an isolated vacancy in a pure metal is non-correlated.

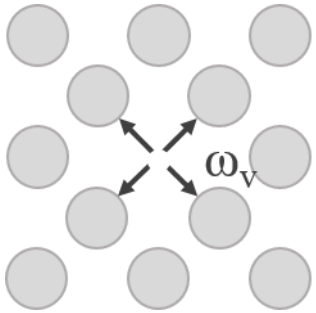
The diffusion of an interstitial atom in a dilute alloy is non-correlated.

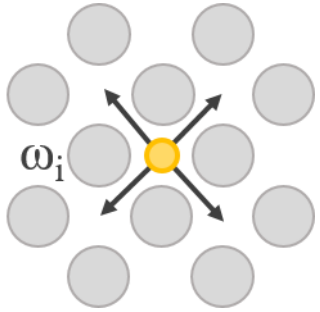
The diffusion of a substitutional solute with vacancy-mediated diffusion is correlated.

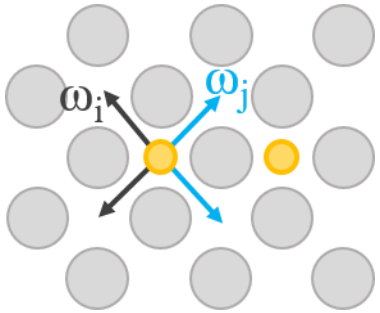
As soon as there are interactions between atoms and/or defects that are different from the interactions with the matrix atoms, diffusion is generally correlated.

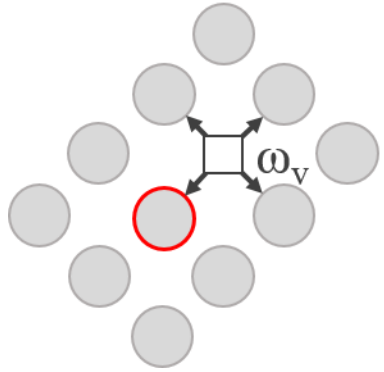
$$f_\alpha = 1 + 2\frac{\sum_i \sum_{j>i} \left\langle \vec{R}_i \vec{R}_j \right\rangle}{\sum_i \left\langle \vec{R}_i^2 \right\rangle}$$

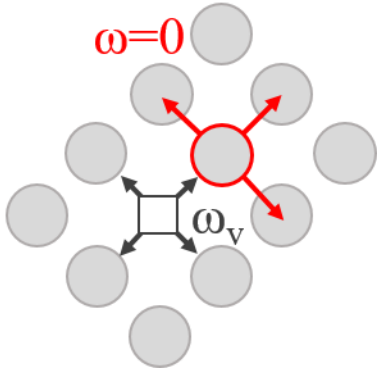
Let's see if we can understand why…







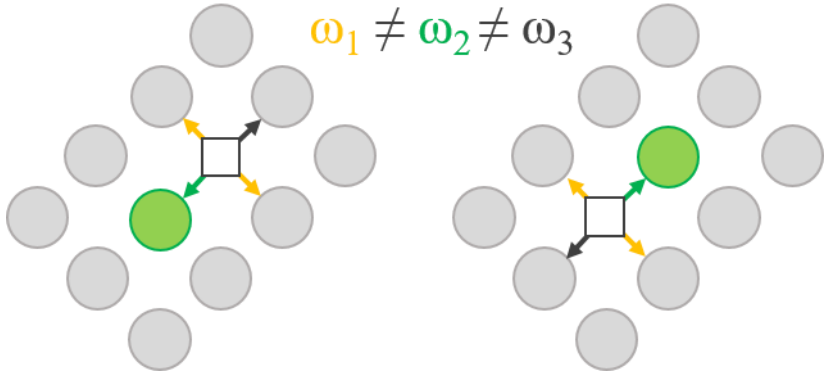




For a tracer atom, the correlation coefficient is purely geometric and it can be estimated to first order as :

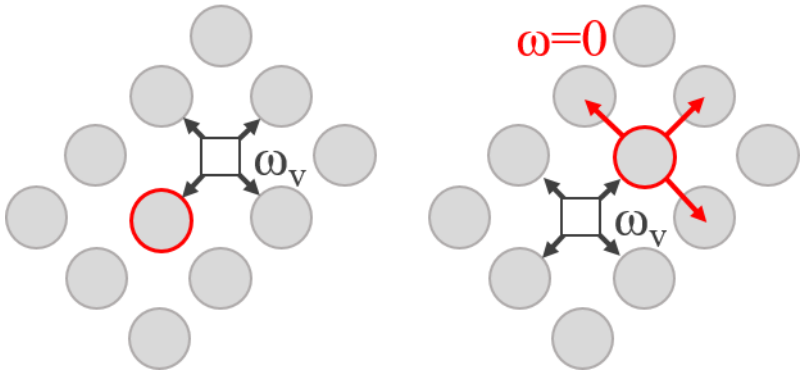
$$f \simeq \frac{z-1}{z+1}$$

Lattice	f_0
Square	0.46705
Hexagonal	0.56006
Honeycomb	0.33333
Diamond	0.50000
Simple cubic	0.65310
Body-centered cubic	0.72719
Face-centered cubic	0.78145
Hexagonal compact (basal)	0.78121
Hexagonal compact (non basal)	0.78145



Convergence of the tracer correlation coefficient with trajectory length

$$f_\alpha = 1 + 2\frac{\sum_i \sum_{j>i} \left\langle \vec{R}_i \vec{R}_j \right\rangle}{\sum_i \left\langle \vec{R}_i^2 \right\rangle}$$



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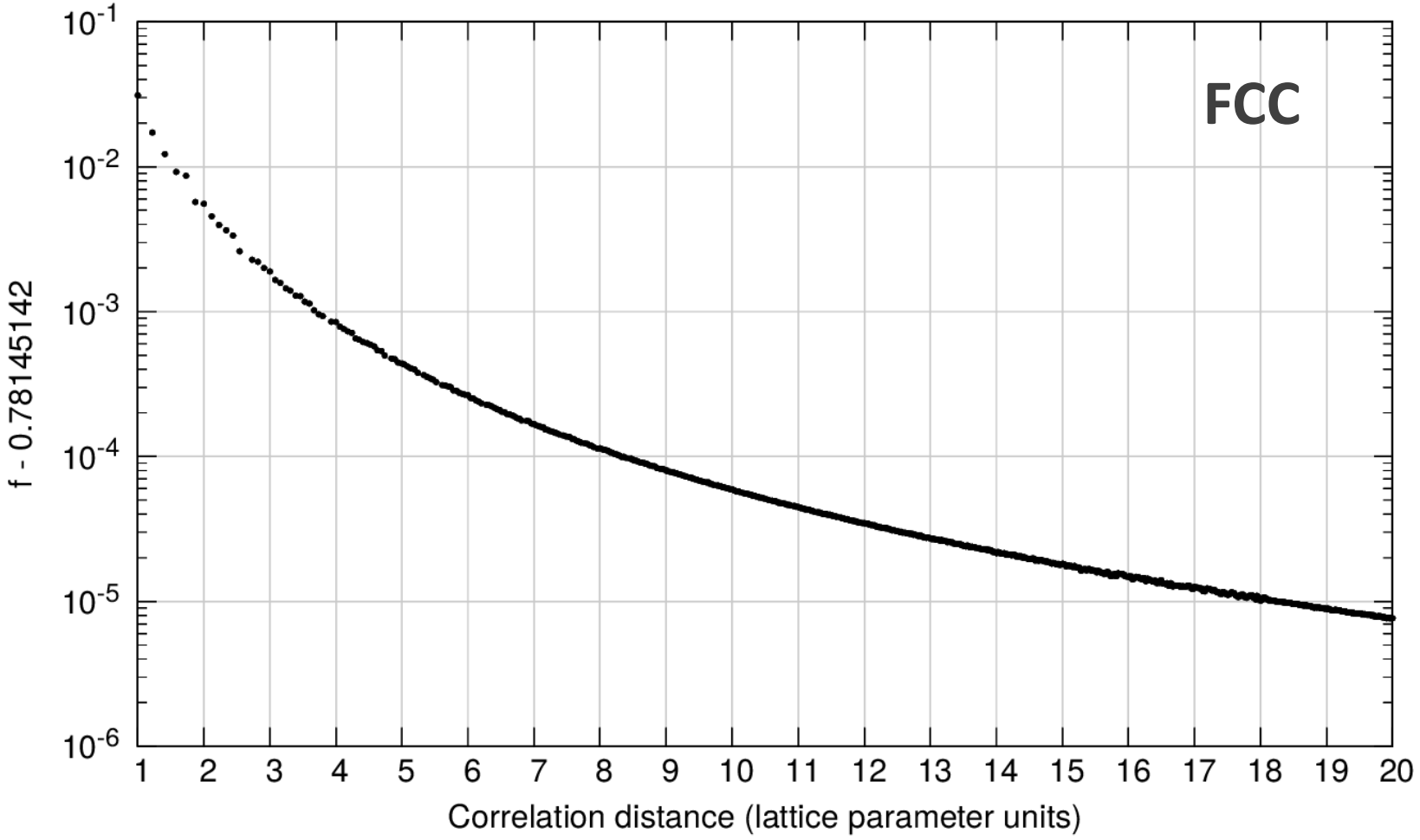


Kinetic correlation : 5-frequency model in FCC

Expression for the tracer diffusion coefficient. In this case, we explicitly find a Arrhenius relation

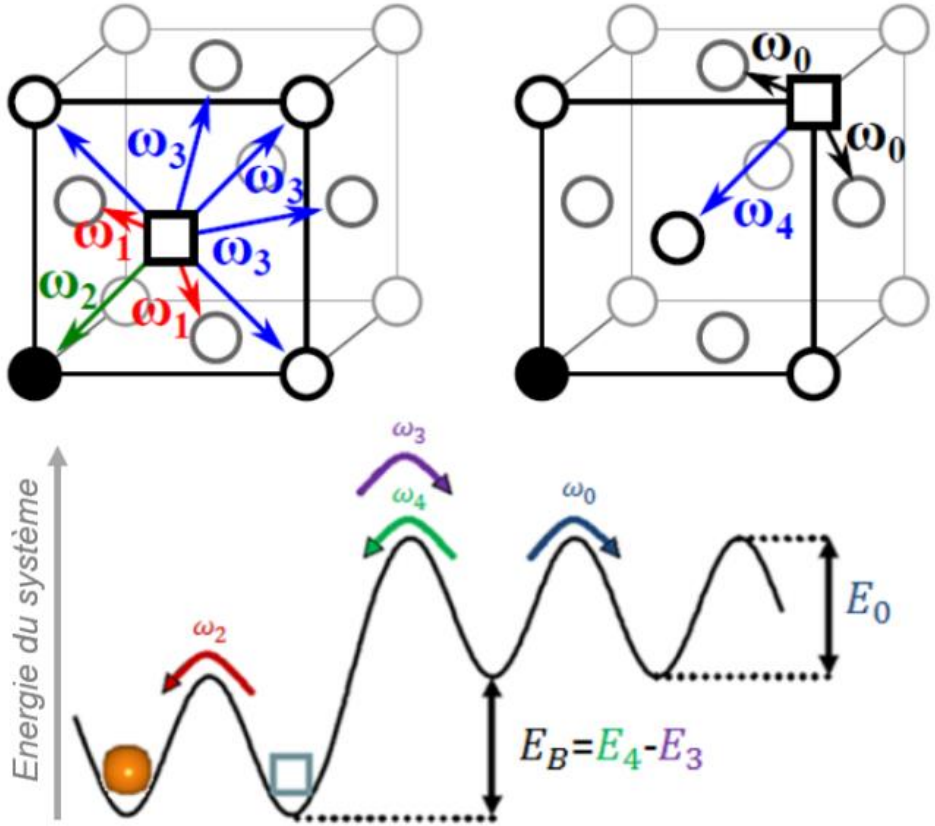
$$D_{\alpha^*} = X_V^{eq} f_0 \frac{zd^2}{6}\omega_0 = \frac{zd^2}{6} f_0 \nu_V \exp\left(-\frac{G^{for}(V) + G^{mig}(V)}{k_B T}\right)$$

Expression for the solute diffusion coefficient

$$D_B = X_V^{eq} f_B \frac{zd^2}{6}\omega_2$$

General expression for the solute correlation factor in whcich appears the competition between the vacancy-solute exchange (ω_2) and the effective vacancy escape frequency *H*.

$$f_B = \frac{H}{2\omega_2 + H}$$



In the 5-frequency model for vacancy-solute diffusion in FCC, The escape frequency reads :

$$H = 2\omega_1 + 7F_3\left(\omega_4/\omega_0\right)$$

$$7F_3\left(\frac{\omega_4}{\omega_0}\right) = 7 - \frac{10\left(\frac{\omega_4}{\omega_0}\right)^4 + 180.5\left(\frac{\omega_4}{\omega_0}\right)^3 + 927\left(\frac{\omega_4}{\omega_0}\right)^2 + 1341\left(\frac{\omega_4}{\omega_0}\right)}{2\left(\frac{\omega_4}{\omega_0}\right)^4 + 40.2\left(\frac{\omega_4}{\omega_0}\right)^3 + 254\left(\frac{\omega_4}{\omega_0}\right)^2 + 597\left(\frac{\omega_4}{\omega_0}\right) + 436}$$

The SCMF method(Self-Consistent Mean-Field theory)

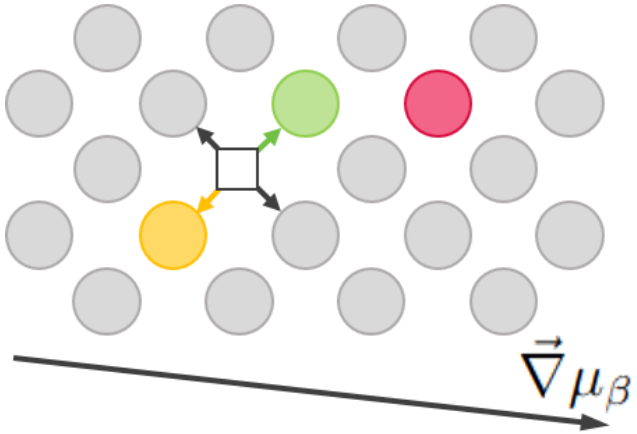
Out-of-equilibrium probability (weak driving force, hence the first order expansion)

$$P_n = P_n^0 \delta P_n = P_n^0 \exp\left(\frac{\delta\Omega - \nu_n + \sum_\beta \delta\mu_n^\beta}{k_B T}\right) \simeq P_n^0 \left(1 + \delta\Omega - \frac{\nu_n}{k_B T} + \sum_\beta \frac{\delta\mu_n^\beta}{k_B T}\right)$$

Expression for the out-of-equilibrium flux

$$\vec{J}_\alpha = \frac{1}{V}\sum_{n\in V} P_n \sum_m W_{nm}\vec{d}_{nm}^{\alpha} = \frac{1}{V}\sum_{n\in V} P_n^0 \delta P_n \sum_m W_{nm}\vec{d}_{nm}^{\alpha}$$

?



Master equation

$$\forall n,\quad \frac{dP_n}{dt} = \sum_m P_m W_{mn} - P_n W_{nm} = \sum_m P_m \delta P_m W_{mn} - P_n \delta P_n W_{nm}$$

$$= \sum_m P_m^0 W_{mn}\left(\delta P_m - \delta P_n\right) = \sum_m P_m^0 W_{mn}\left(\frac{\nu_n - \nu_m + \sum_\beta \vec{d}_{nm}\cdot\vec{\nabla}\mu_\beta}{k_B T}\right)$$

$$= 0$$

As a consequence of the stationnary condition, effective interactions are proportional to driving forces. Therefore the flux is proportional to driving forces which allow us to identify transport coefficients.

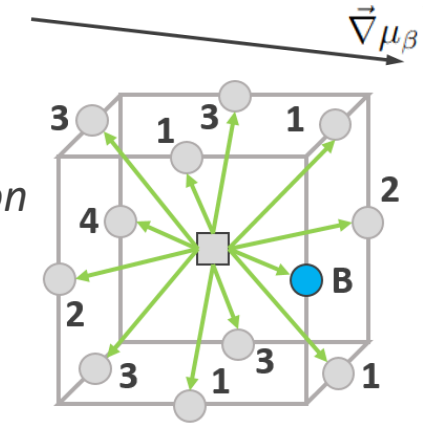
The SCMF method (Self-Consistent Mean-Field theory)
Finding the values of the effective interactions

$$\forall n,\ \forall \beta,\quad \sum_{m\in\theta_n} P_m^0 W_{mn}\left(\nu_n-\nu_m\right) = -\left(\sum_{m\in\theta_n} P_m^0 W_{mn}\vec{d}_{nm}\right)\cdot\vec{\nabla}\mu_\beta$$

The size of this system of equation we need to solve is a priori gigantic but it can be reduced by using :

- **Dilute system**, i.e. a small group of traced atoms and/or defects in a homogeneous material
- **Translation invariance** of the system (homogeneous crystal)
- **Crystal symmetries** for the out-of-equilibrium system (the chemical potential gradient breaks part of the crystal symmetries)
- An interaction **cut-off radius** (kinetic radius) which defines how far atoms interact (thermodynamic and « kinetic » interactions)

Vacancy solute 1NN configuration in a FCC crystal; CPG along the [100] direction



$$2Y_{11}(\nu_1-0)+Y_{11B}(\nu_1+\nu_1)+Y_{12}(\nu_1-0)+2Y_{11}(\nu_1-\nu_1)+2Y_{13}(\nu_1-\nu_3)$$
$$+2Y_{13}(\nu_1-\nu_{3'})+Y_{14}(\nu_1-\nu 4)+Y_{12}(\nu_1-\nu_2)=-\frac{a}{2}\left(2Y_{11}+Y_{11B}+Y_{12}-Y_{12}-2Y_{13}-Y_{14}\right)\nabla\mu_\beta$$

Then we do the same for all configurations below the cut-off radius, we solve this linear system by matrix inversion and we get the effective interactions which are proportionnal to chemical potential gradients

Don’t want to do this all by hand ?

Use KineCluE !

(It’s free)

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Editor’s Choice

KineCluE: A kinetic cluster expansion code to compute transport coefficients beyond the dilute limit

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Thank you for your attention

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