MESOSCALE MODELLING TECHNIQUES (RPV)

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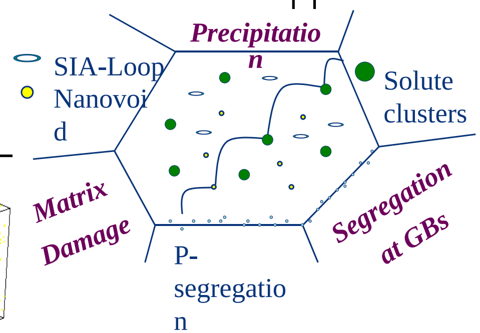
Radiation damage

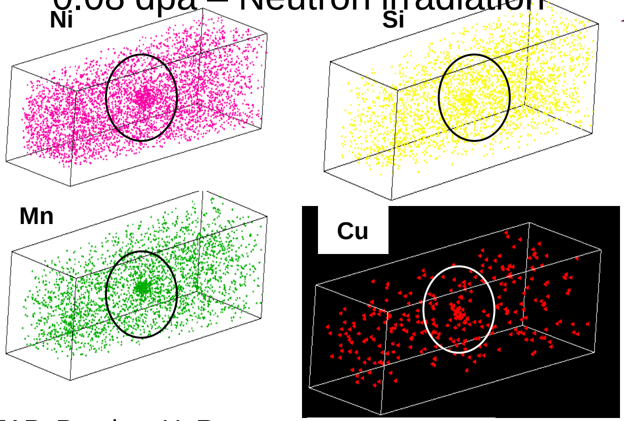
Material:
Fe
+ alloying elements: Cu, Ni, Mn, Si, …
+ carbon, nitrogen

+ dislocations

Irradiation:
Electron:
Frenkel pairs
Ion and neutron:
displacement cascades (10-100 keV)
vacancies and interstitials:
isolated and in clusters

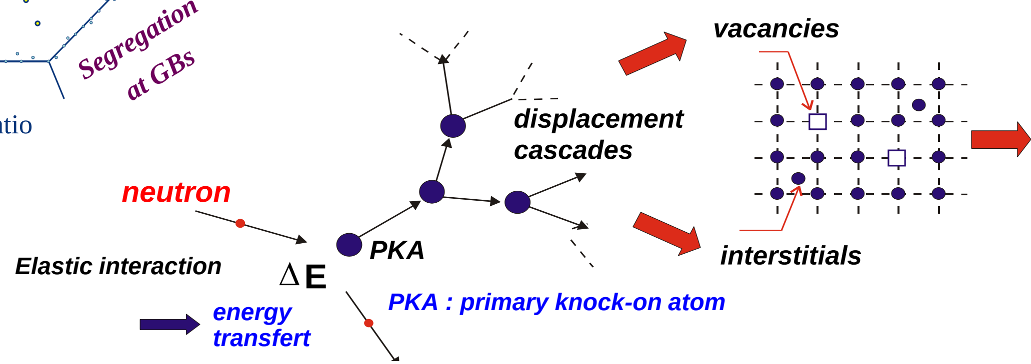


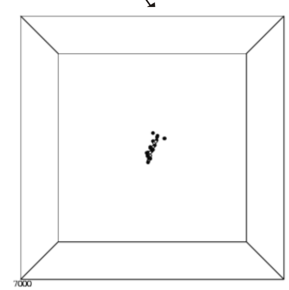
0.08 dpa – Neutron irradiation

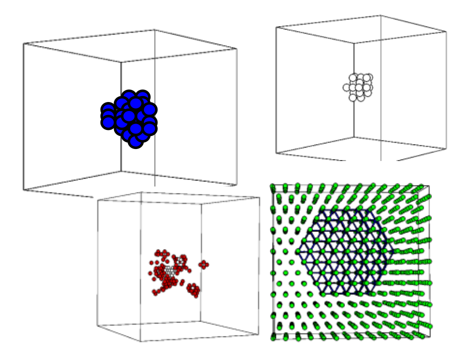


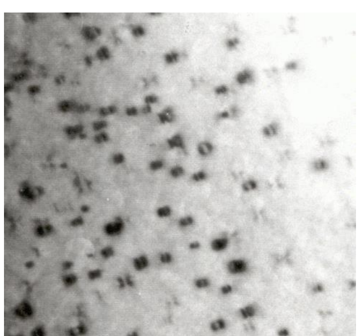
TAP, Pareige, U. Rouen

15x15x50 nm





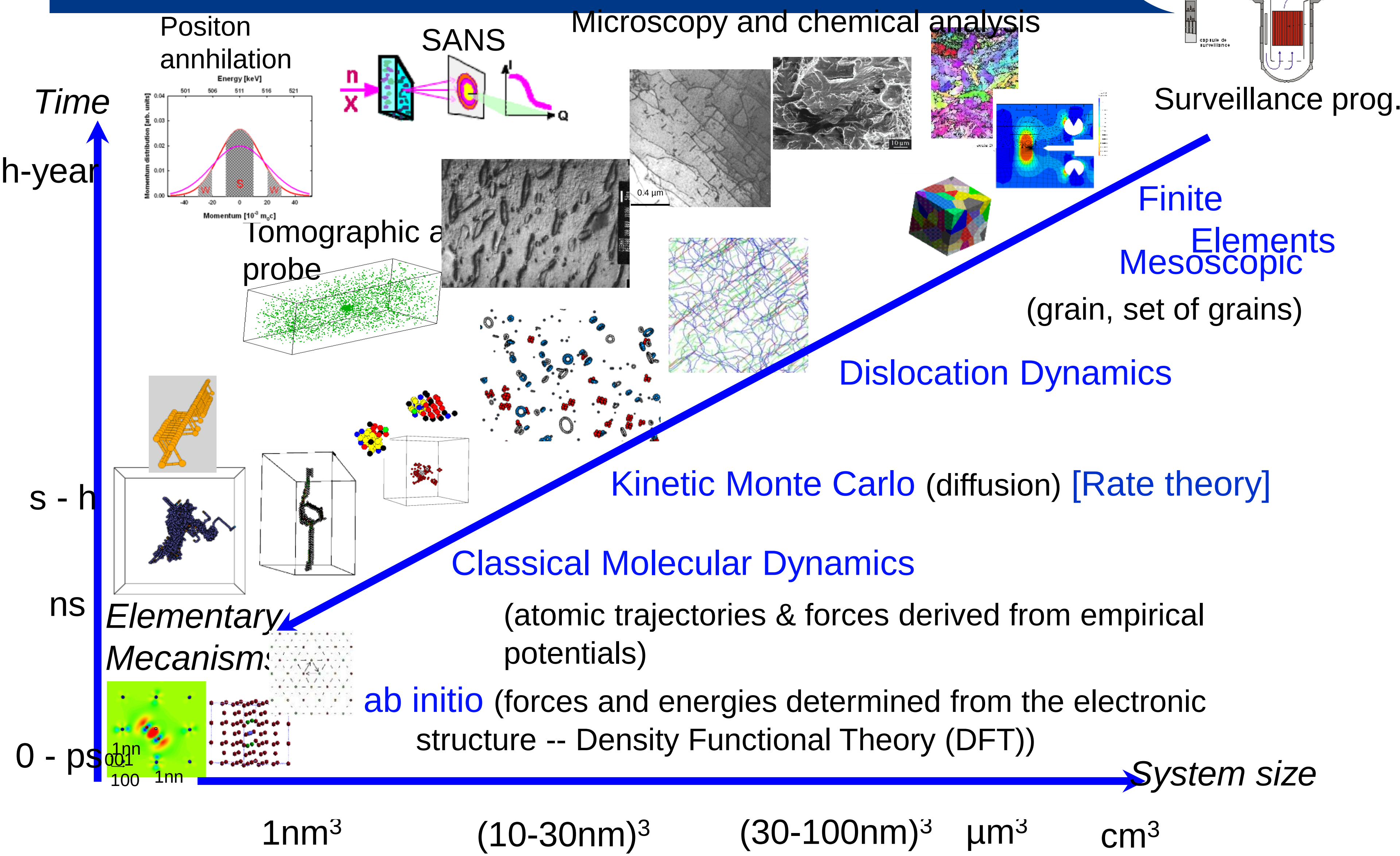




TEM, Barbu, CEA

Microstructure evolution:
point defect clusters: nanovoids, dislocation loops
solute clusters (# or \# point defects)

Simulation tools



Relevant phenomena and appropriate computational methods for microstructure evolution

SOTERIA

Phenomena

single displacement cascade

multiple cascades, cascade overlap

defect and solute migration and clustering

void swelling, hardening, embrittlement, creep, stress corrosion cracking, ...

collisional phase

quenching

annealing phase

defect/solute diffusion

microstructure evolution

mechanical property changes

10^{-14} s 10^{-11} s 10^{-8} s 10^{1} s 10^{4} s $> 10^{6}$ s

Methods

molecular dynamics

kinetic Monte Carlo

finite element

ab initio

MD dislocation dynamics

reaction rate theory, phase field 3D dislocation dynamics

10^{-9} m 10^{-7} m 10^{-6} m $> 10^{-3}$ m

Mesoscale modelling techniques

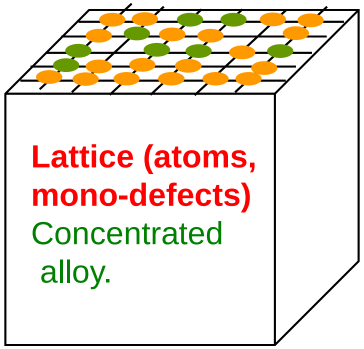
- Object / event kinetic Monte Carlo
- Cluster dynamics (rate theory)
- Phase field
- Coarse graining

Medium/long term evolution modelling methods

atoms ← → gaz of clusters

Atomic Kinetic Monte Carlo (AKMC)

Microchemical changes



V ≈ 10^{-4} μm^3
t ≈ 10^{11} jumps

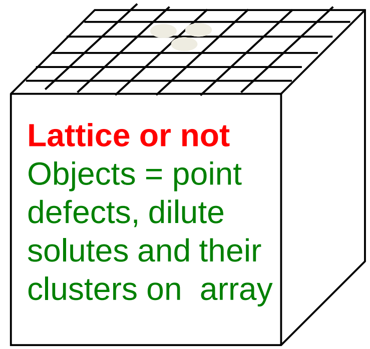
- Atom or defect on every lattice site
- **Jump probabilities of atoms**
- Interactions between atoms

Full thermodynamics

Solute cluster or RIS modelling

Object Kinetic Monte Carlo (OKMC)

Point defect clusters



V ≈ 10^{-4} μm^3;
t ≈ limited (T, G dependent)

- Gaz of cluster
- **Jump probabilities of objects**
- ω_α , $E^f_{cluster}$, r_c

Cluster Dynamics (CD) (Rate theory)

Point defect clusters

Rate equations (homogeneous in space and time)

Number density of objects / cm^3 (point defects, solutes and their clusters)

V unlimited
t unlimited

- Gaz of cluster
- **Set of DE**

$$\frac{\partial C_j}{\partial t} = F(C_j, C_k, \ldots)$$

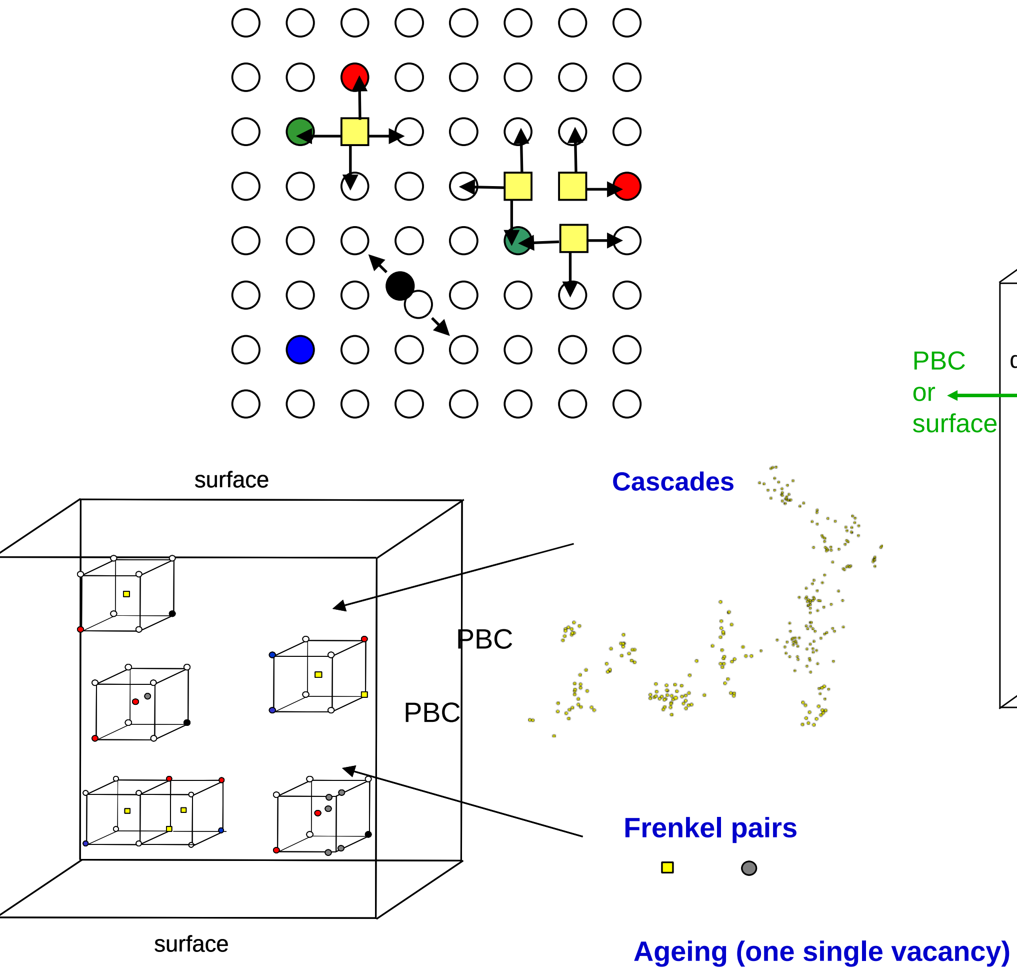
- D_α , $E^f_{cluster}$, r_c

Microstructure modelling

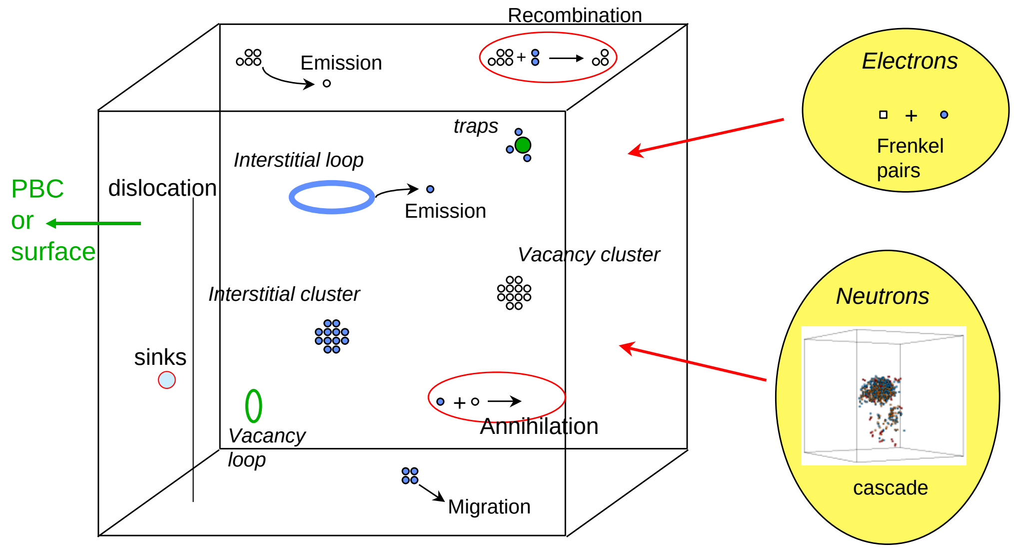
Courtesy A. Barbu

Kinetic Monte Carlo simulation of irradiation

Atomic KMC



Object KMC

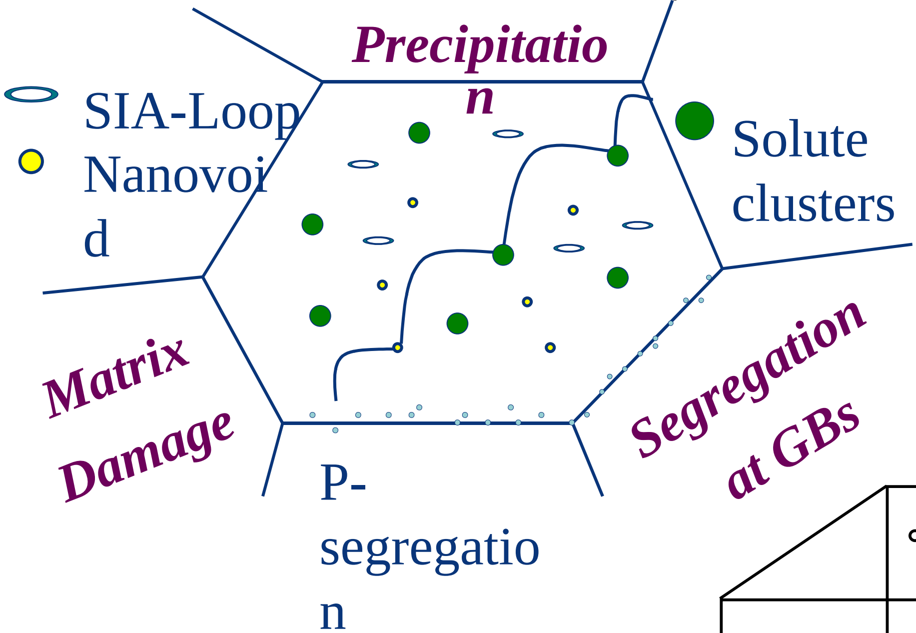


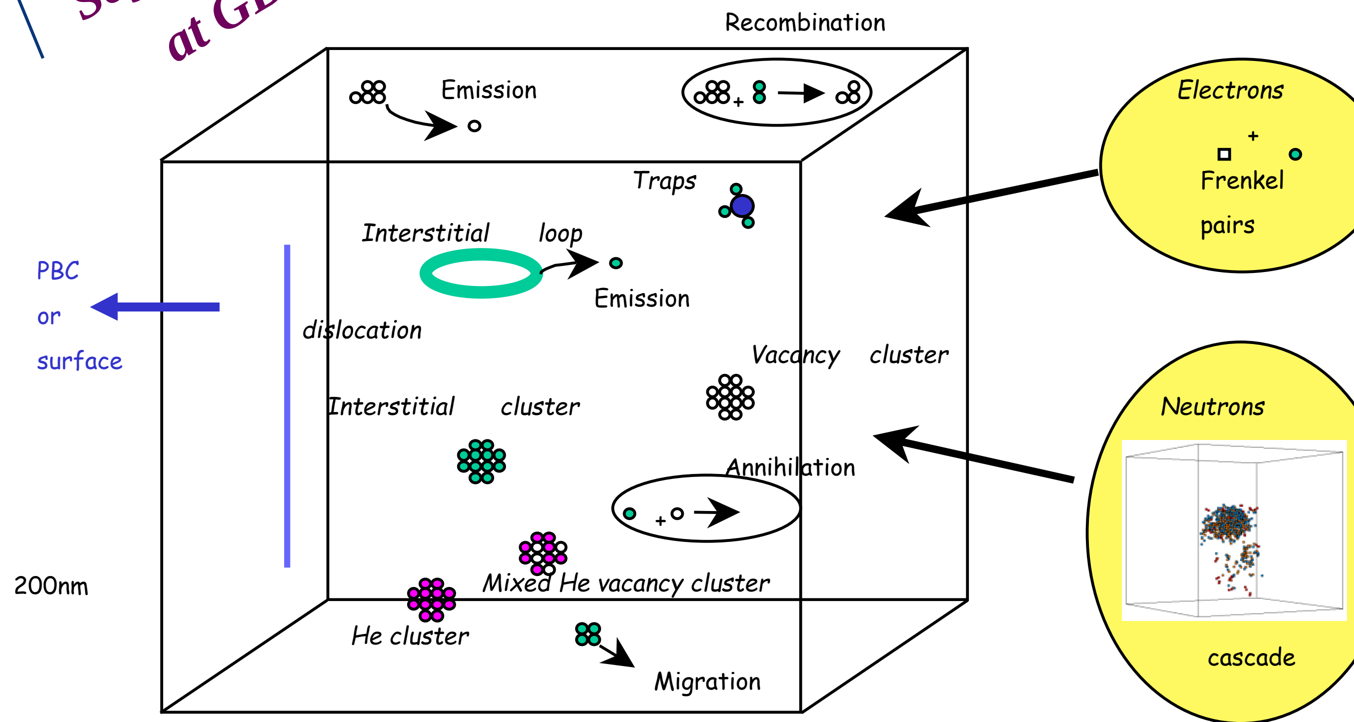
[JNM 335 (2004) 121–145]

Object Kinetic Monte Carlo

Objects:

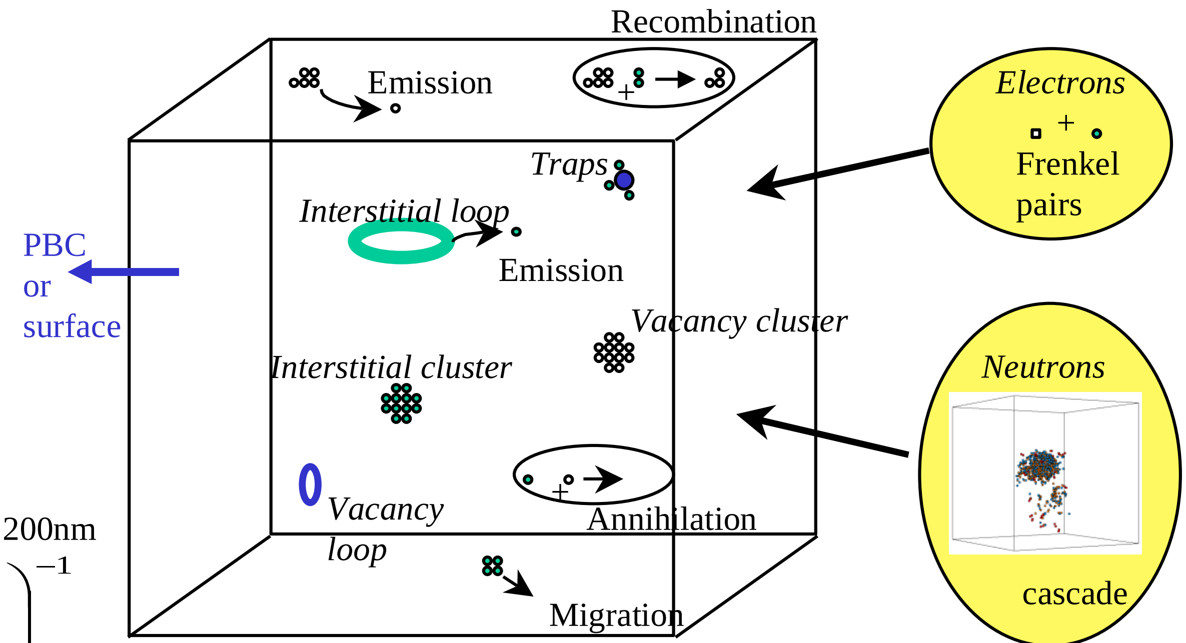
- vacancy
- self interstitial
- dilute solute (with vacancy interactions)
- sink (e.g. grain boundaries, …)
- trap (e.g. impurities, …)
- dislocation
- foreign interstitial atoms
  - He in austenitic alloys
  - C or N in ferritic or austenitic alloys





Object Kinetic Monte Carlo

- Each object defined by:
  - type
  - centre-of-mass position
  - reaction radius
  - possible reactions



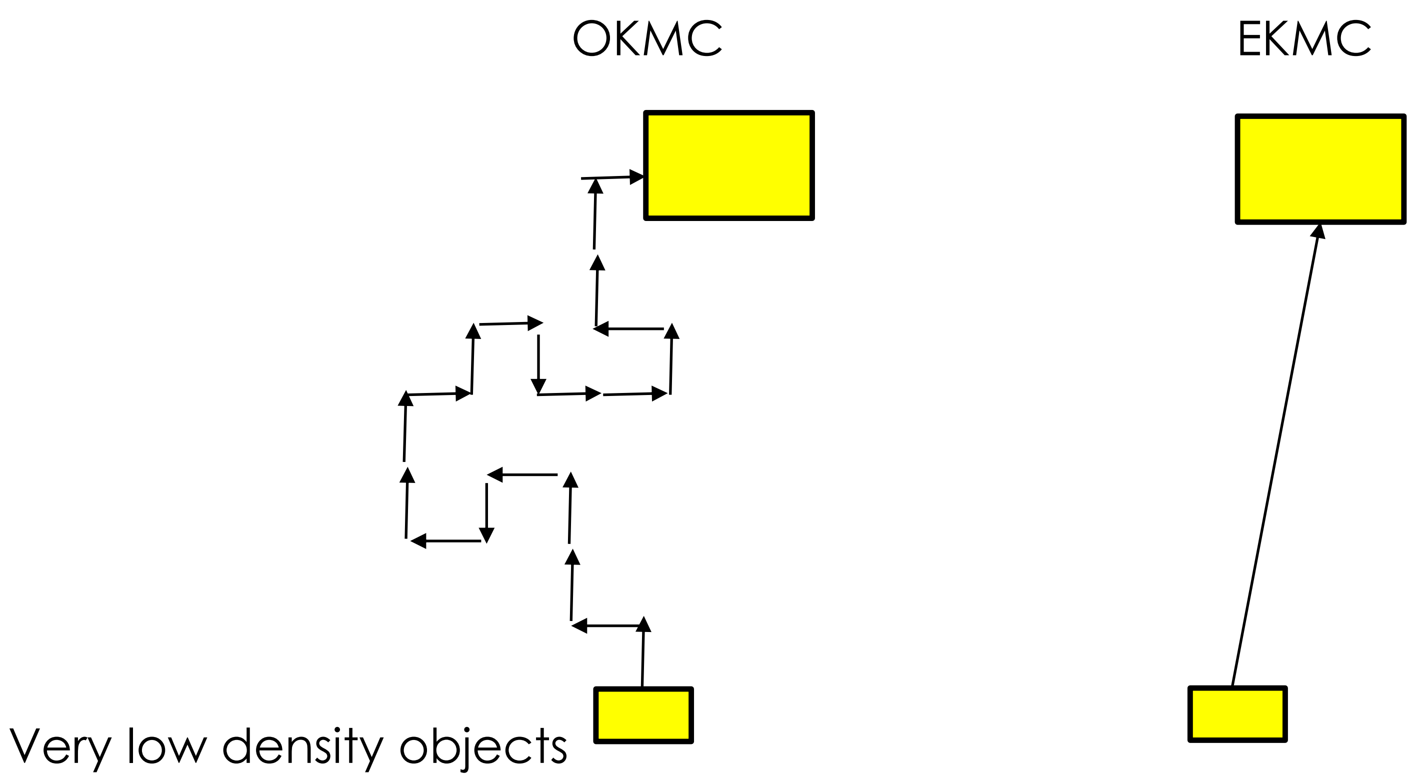
$$\Gamma_i = \Gamma_i^0 \exp(-E_a / kT)$$

$$\text{Time step} = \left(\sum_{\substack{\text{internal} \\ \text{events}}} \Gamma_i + \sum_{\substack{\text{external} \\ \text{events}}} \Gamma_i \right)^{-1}$$

- Advantages:
  - Flexibility
  - Computing efficiency
  - Spatial distribution

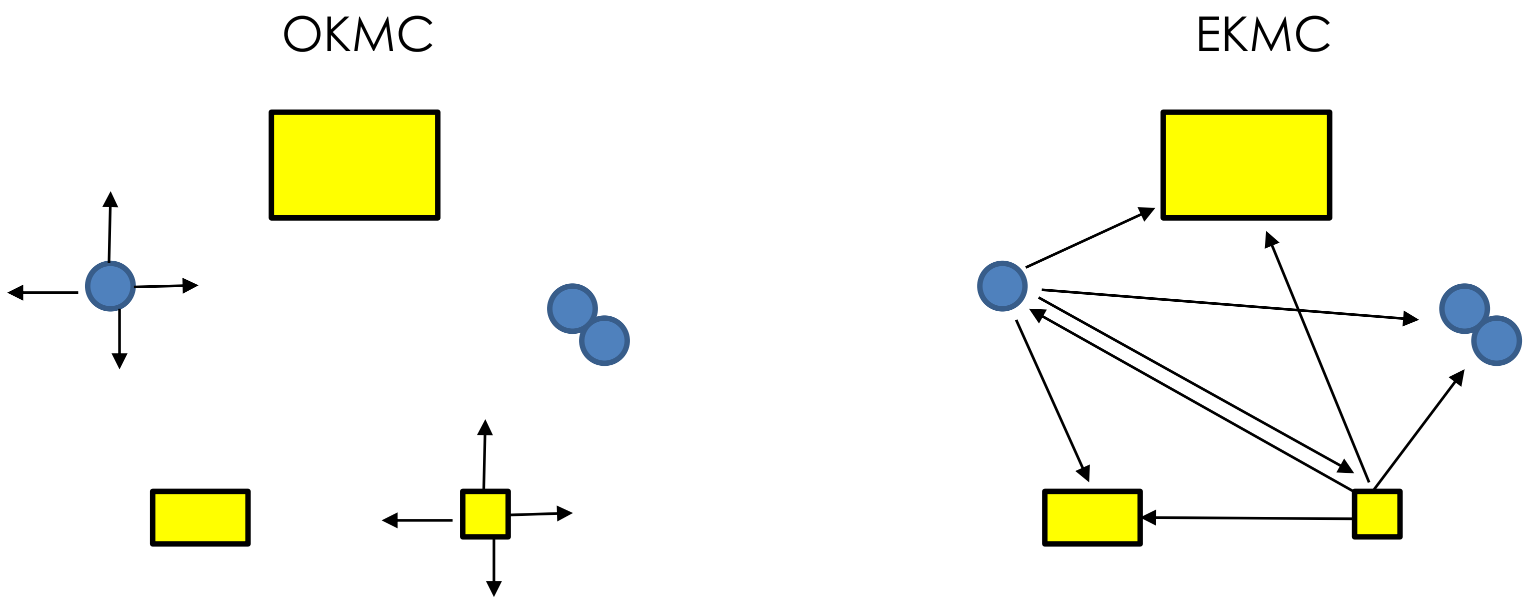
- Drawbacks:
  - Large number of physical parameters
  - No atomic configurations

Object Kinetic Monte Carlo: Object vs Event



- Advantages:
  - EKMC → fast
- Drawbacks:
  - OKMC → many steps before reaction

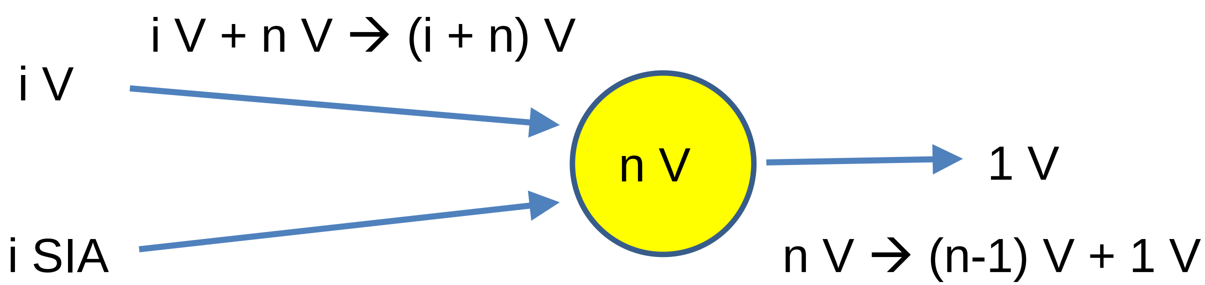
Object Kinetic Monte Carlo: Object vs Event



High density objects

- Advantages:
  - OKMC → local rules
- Drawbacks:
  - EKMC → many different reactions

OKMC reactions



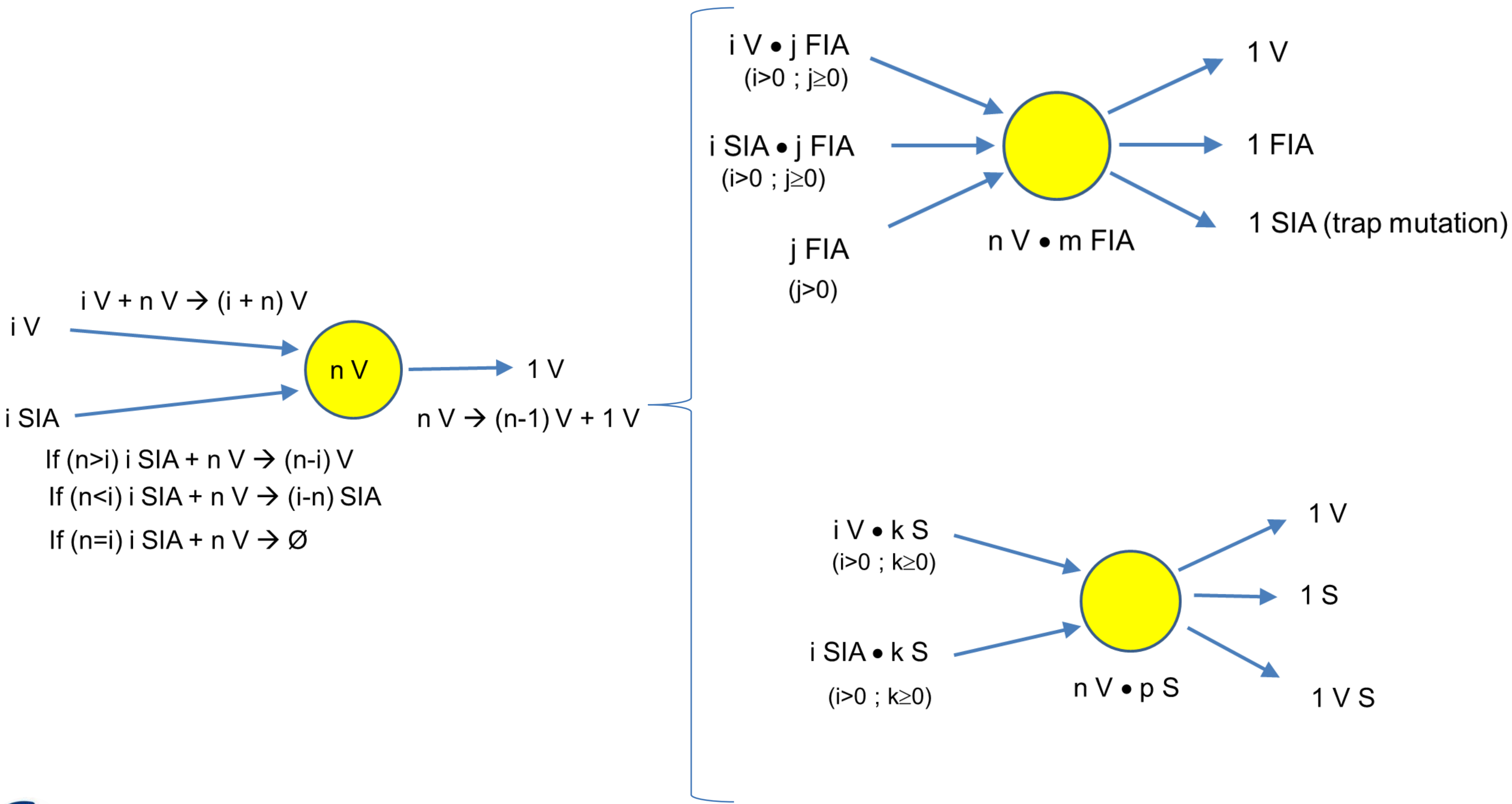
If (n>i) i SIA + n V → (n-i) V

If (n<i) i SIA + n V → (i-n) SIA

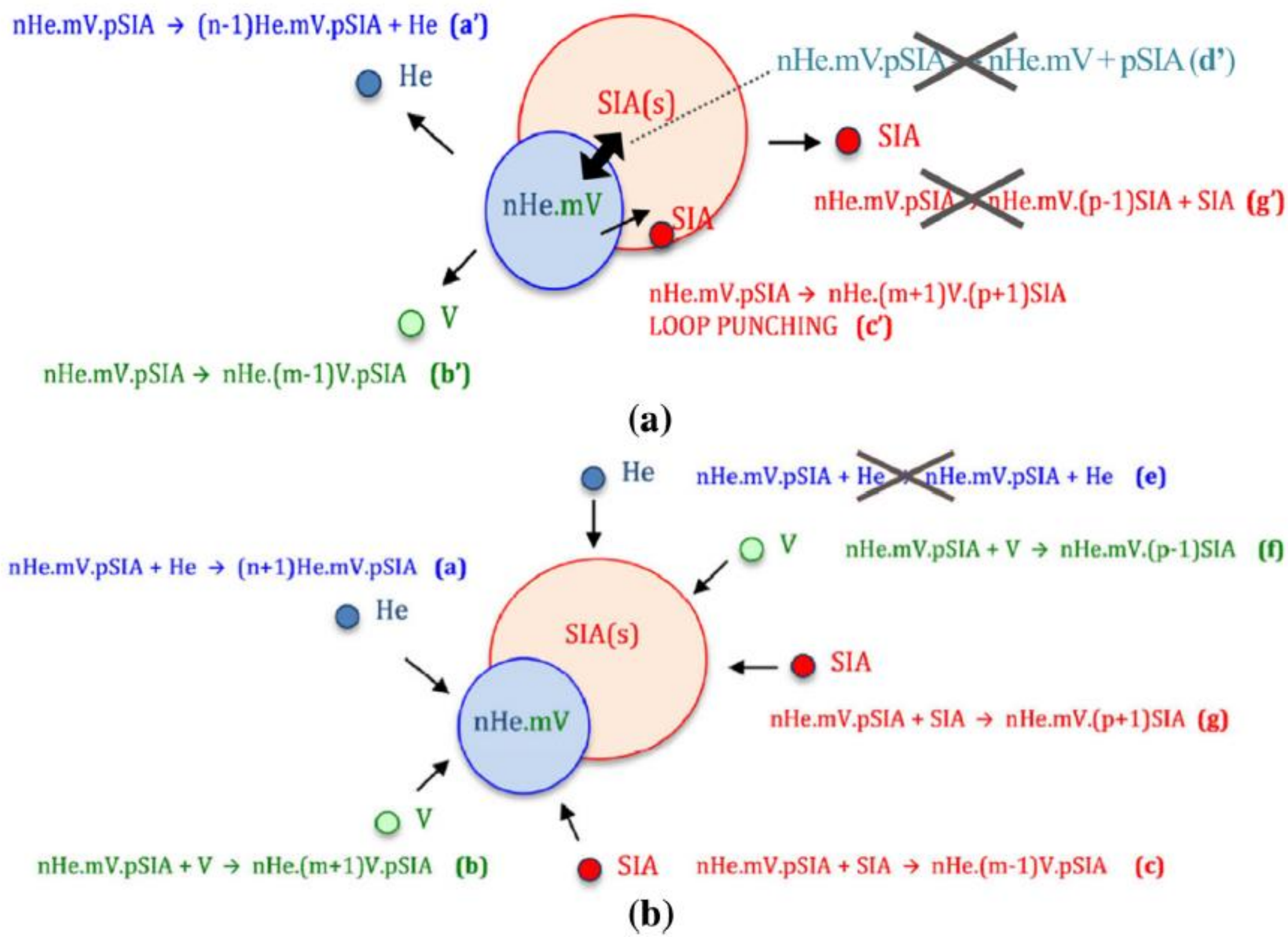
If (n=i) i SIA + n V → Ø

Input: binding energies (from MD / DFT)

OKMC reactions



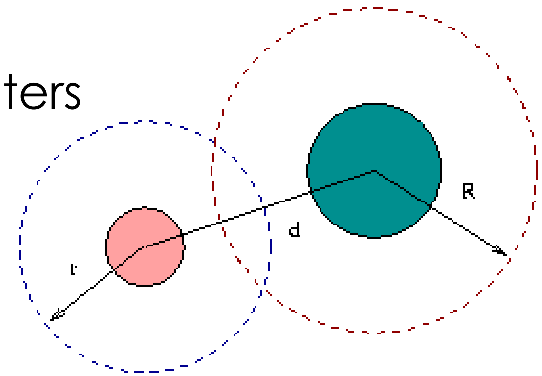
OKMC reactions

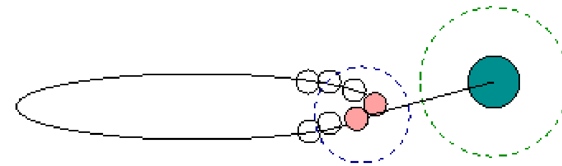


OKMC reactions
Recombination distances / sink strength

Recombinaison criteria between 2 defects: $d<R1+R2$

Clusters





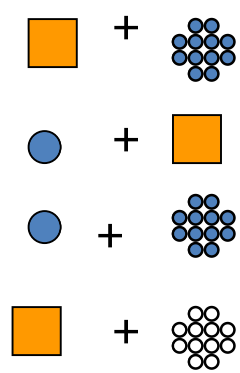
Loops

$v+i_n \leftrightarrow i_{n-1}$ — Recombinaison

$v+i \rightarrow 0$ — Annihilation

$i+i_n \rightarrow i_{n+1}$ — Cluster growth

$v+v_n \leftrightarrow v_{n+1}$

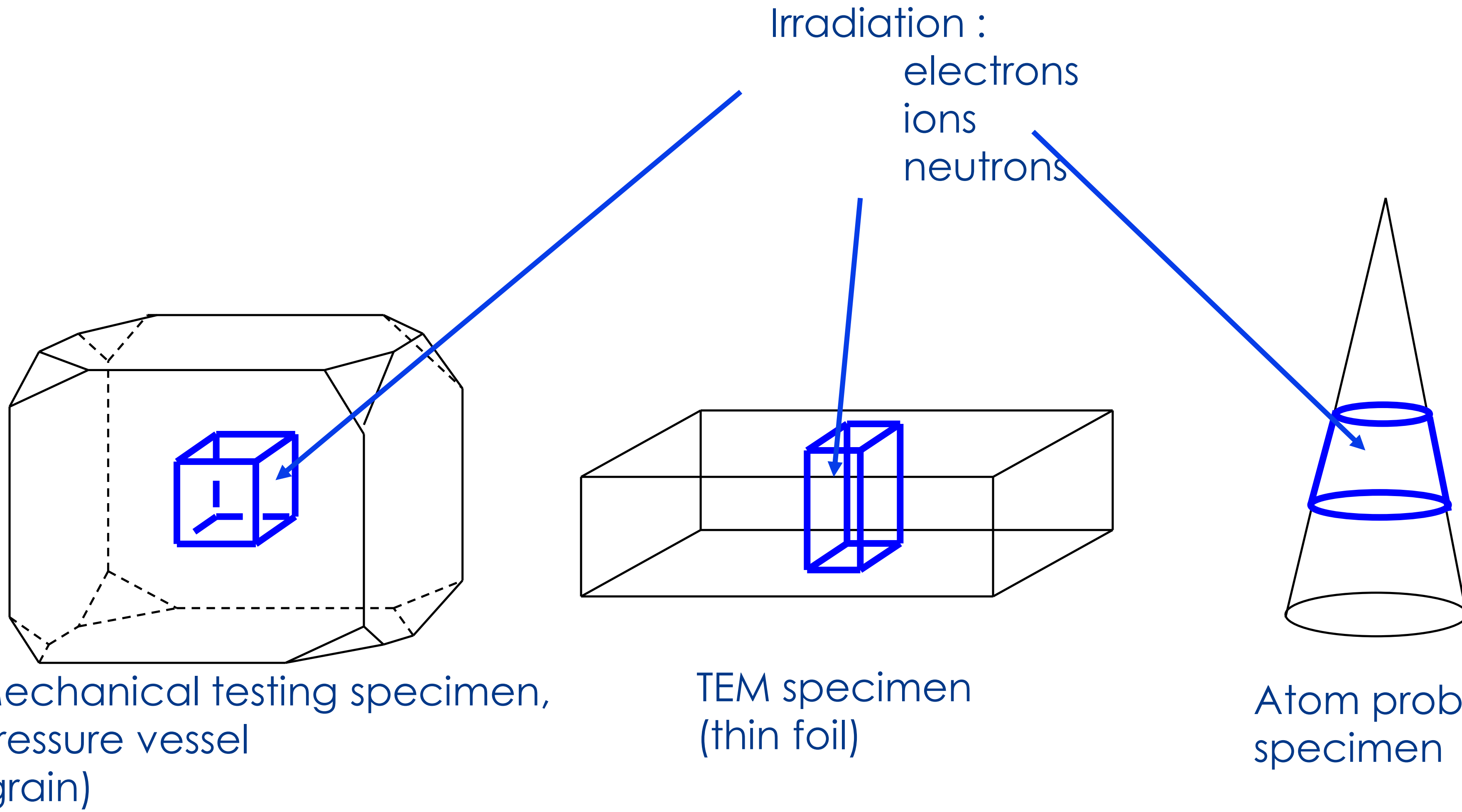


+ reactions with very dilute elements (e.g. Cu in Fe)
+ reactions with foreign interstitial atoms (e.g. C or He)

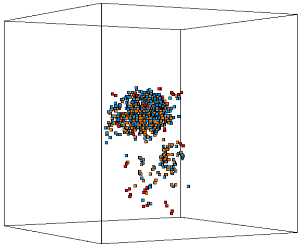
OKMC parameter determination / adjustement

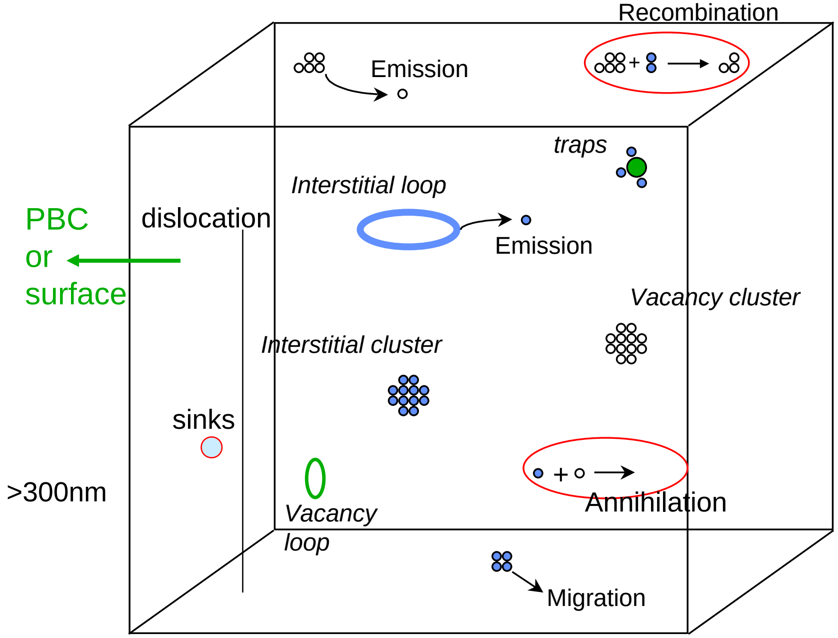
- Parameters ?
  - Interstitial & vacancy clusters mobility
    - diffusion coefficient (migration energy and jump frequency)
  - Recombination radius
  - Emission : binding energies
  - …
- How to get these parameters ?
  - experimental data
  - atomic simulations
    - ✓ molecular dynamics
    - ✓ ab initio calculations
  - Fitting on “dedicated” lab. experiments (electrons, ions irradiation)

OKMC: SIMULATIONS ADAPTED TO DIFFERENT EXPERIMENTAL SPECIMENS



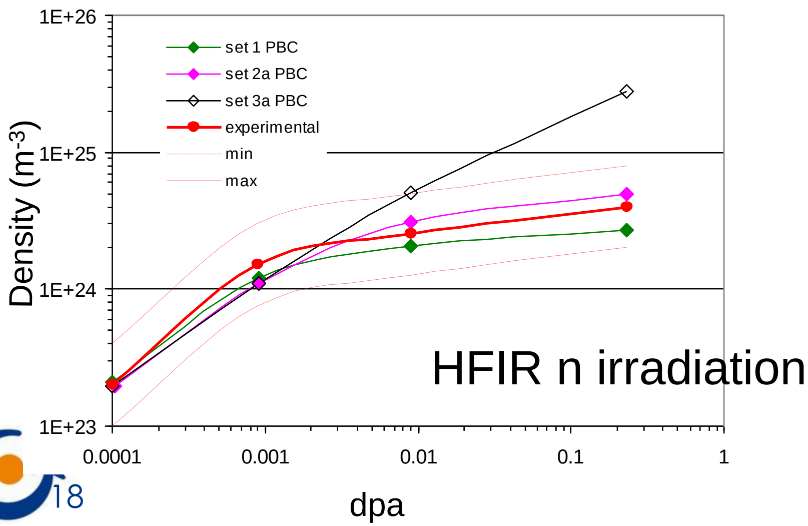
Long term simulation of the microstructure under irradiation by object kinetic Monte Carlo

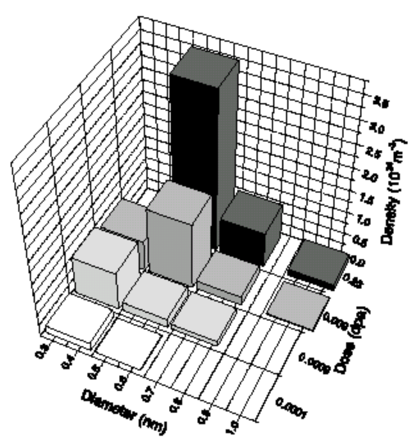


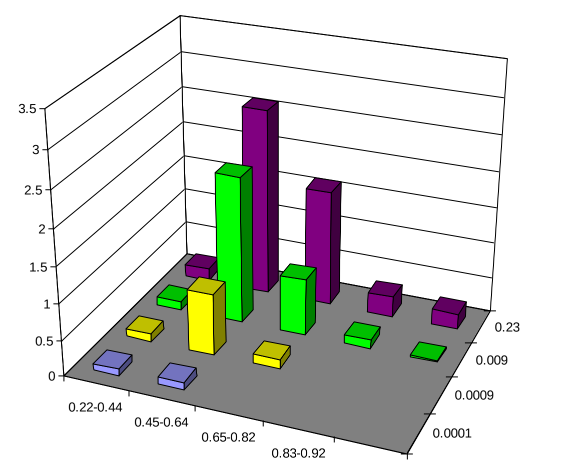


Input required: Mobility: diffusion coefficient

Local interaction rules: Interaction and binding energies



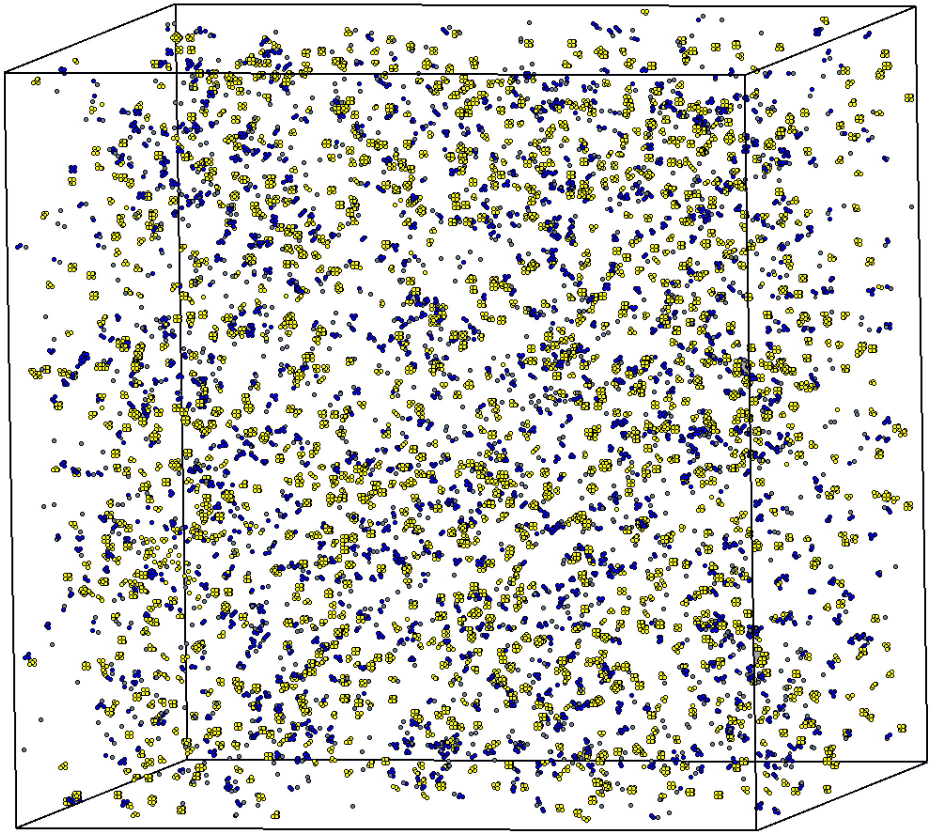




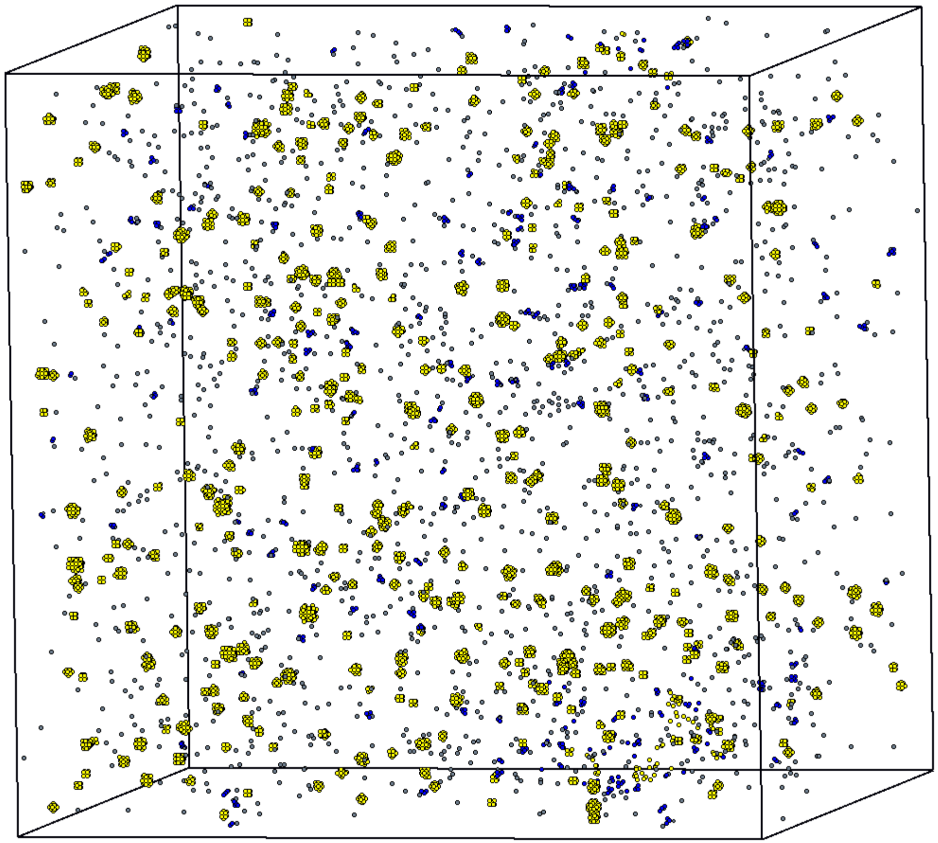
Long term simulation of the microstructure: Application example: flux effect study

DEFECT POPULATION at 0.1 dpa

343K



$7\ 10^{-5}$ dpa/s



$7\ 10^{-11}$ dpa/s

(param Set II)

Object KMC - applications

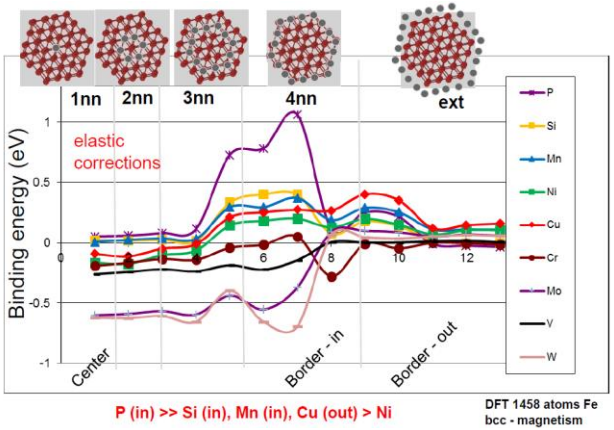
- Objectives: 3D simulation of time evolution microstructure
  - cascade annealing (generation term for rate theory)
  - sink strength calculation (input data for rate theory modelling)

- Irradiation experiment simulations
  - isochronal annealing (after electron or neutron irradiation)
  - electron irradiation under flux
  - neutron irradiation under flux
  - proton irradiation under flux

- Different conditions (bulk, surface, …)

Object KMC – Irradiation Fe(C)MnNi alloys

DFT



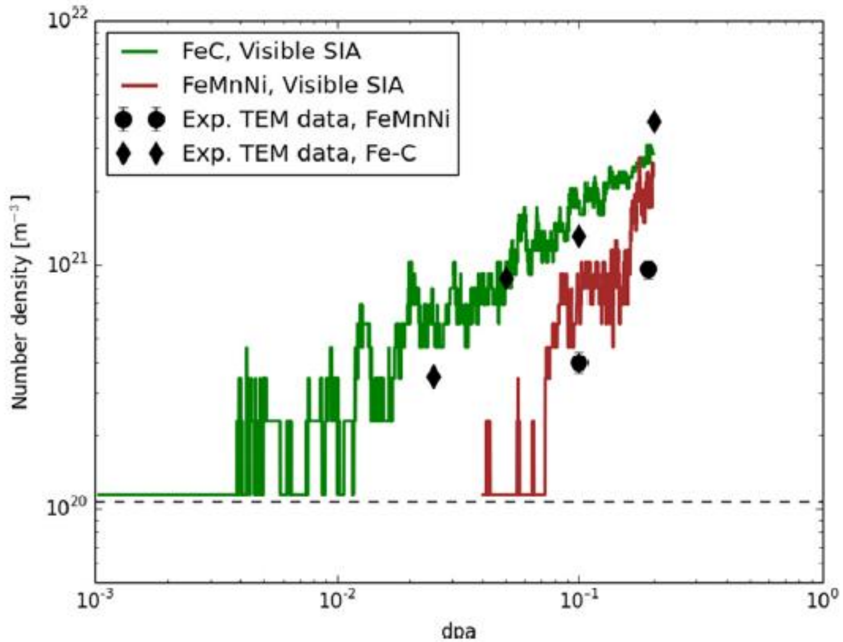
Loop mobility model

$$D_n^{FeMn} = D_n^{Fe} e^{\beta \Delta F_n}$$

$$\Delta F_n \approx -K_n E_{b1}$$

$$K_n = n n_I x_{Mn}$$

OKMC microstructure



[Chiapetto PhD]
[Chiapetto, Malerba, Becquart et al]

Mesoscale methods: MFRT

Cluster Dynamics (CD) or Mean Field Rate Theory (MFRT)

- Analytical method
- Set of N coupled ordinary differential equations (ODEs) of balance
- Mean-field approximation: only defect concentration

Example for single vacancy concentration:

$$\frac{dc_V}{dt} = K_V - k_V^2 D_V c_V - \alpha c_I c_V$$

Coupling with SIA concentration equation

Vacancy production rate

Disappearance of vacancies at sinks

Vacancy-SIA recombination rate

Need to provide k^2_V, D_V and α

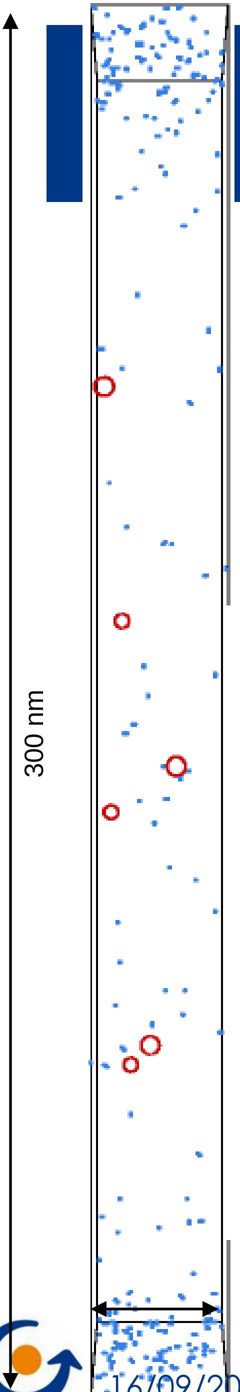
Advantages: no volume and time limits, short computing time

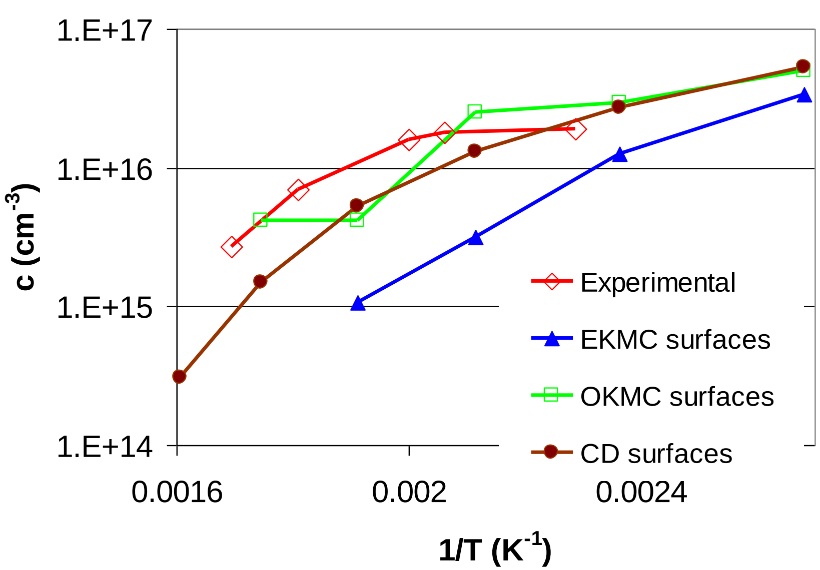
Drawbacks: spatial inhomogeneities not treated

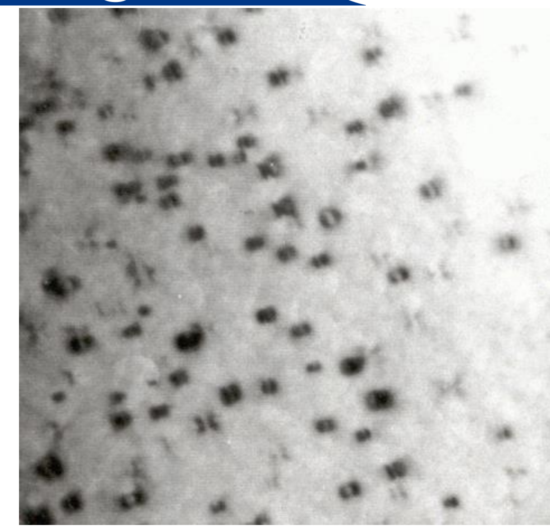
OKMC & MFRT electron irradiation modelling

Electron Irradiation

150°C, 0.1dpa, 1000 s







[Phil Mag 2005]

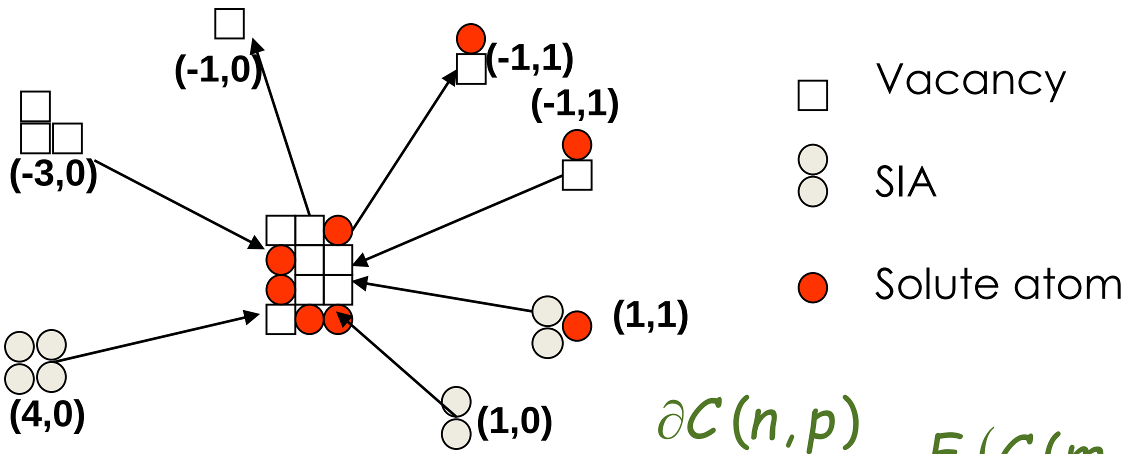
Mesoscale methods: MFRT

$$\frac{dC_n}{dt} = G_n + \sum_m w_{m\to n} C_m - \sum_q w_{n\to q} C_n - K_n C_n$$

All the physics is contains in the coefficients $G(j)$, $w(k,j)$, K_j

Rate theory calculation

- to treat austenic alloy as "grey" alloy + He treatment
- to treat ferritic alloy as "grey" alloy + one solute (Cu)



C(n,p)

nb de défauts ponctuels

nb de d'atomes de solutés

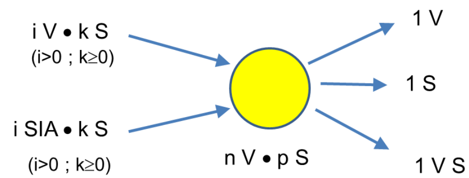
$$\frac{\partial C(n,p)}{\partial t} = F\left(C(m,q), C(k,l), \ldots.\right)$$

Many equations & system hard to integrate!

Alternative approach: Guillepsie method (stochastic treatment of the reactions/equations)

Mesoscale methods: MFRT

Reactions:



$$(n,p) + (m,q) \overset{B((n,p),(m,q))}{\longrightarrow} (n+m, p+q).$$

$$(n,p) \overset{A((n,p),(1,0))}{\longrightarrow} (n-1,p) + (1,0), \quad \text{for } n \geqslant 2$$
$$(n,p) \overset{A((n,p),(-1,0))}{\longrightarrow} (n+1,p) + (-1,0),$$
$$(n,p) \overset{A((n,p),(1,1))}{\longrightarrow} (n-1,p-1) + (1,1), \quad \text{for } n \geqslant 2$$
$$(n,p) \overset{A((n,p),(-1,1))}{\longrightarrow} (n+1,p-1) + (-1,1)$$

$$B((n,p),(m,q)) = 4\pi r^*((n,p),(m,q))[D(n,p) + D(m,q)],$$

Sink strength

$$A((n,p),(m,q)) = B((n-m,p-q),(m,q))\frac{1}{V_{at}} \times \exp\left(\frac{-E_b((n,p),(m,q))}{k_B T}\right),$$

Binding energies

$$\begin{aligned}\frac{\partial C(n,p)}{\partial t} = {} & G_{MD}(n) - A((n,p),(1,0|1))C(n,p) \\ & - A((n,p),(\bar{1},0|1))C(n,p) + A((n+1,p),(1,0|1)) \\ & \times C(n+1,p) + A((n-1,p),(\bar{1},0|1))C(n-1,p) \\ & + \sum_{m=1}^{\min(n-Nov,m_v)} \sum_{q=0}^{1} B((n-m,p-q),(m,q))C(n-m,p-q) \\ & \times C(m,q) + \sum_{m=1}^{\min(Noi-n,m_i)} \sum_{q=0}^{1} B((n+m,p-q),(m,q)) \\ & \times C(n+m,p-q)C(m,q) - \sum_{m=-m_v, m\neq 0}^{m_i} \sum_{q=0}^{\min(1,p)} B((n,p),(m,q)) \\ & \times C(n,p)C(m,q) - \mathbb{1}_{-m_v \leqslant n \leqslant m_i \text{ and } p \leqslant 1} B(n,p,n,p)[C(n,p)]^2 \\ & - L_{gb}(n,p)C(n,p) - L_d(n,p)C(n,p), \end{aligned} \quad (16)$$

Set of ODEs

(mobile defect clusters & solutes considered)

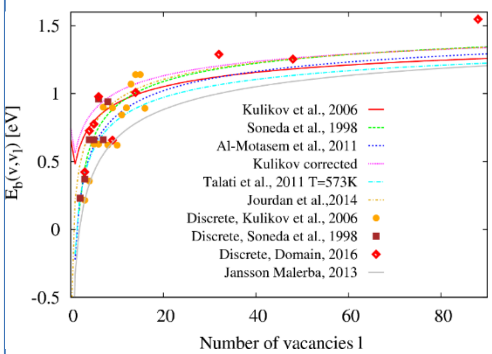
Numerical integration

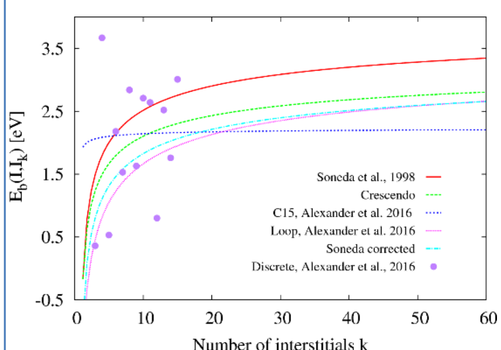
[Adjanor, JNM 2010]

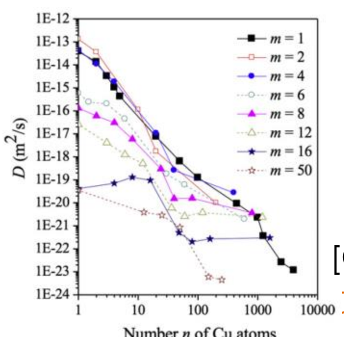
[Jourdan, JNM2014]

Cluster dynamics – irradiation Fe-0.1%Cu 0.1 dpa

DFT, MD, AKMC results

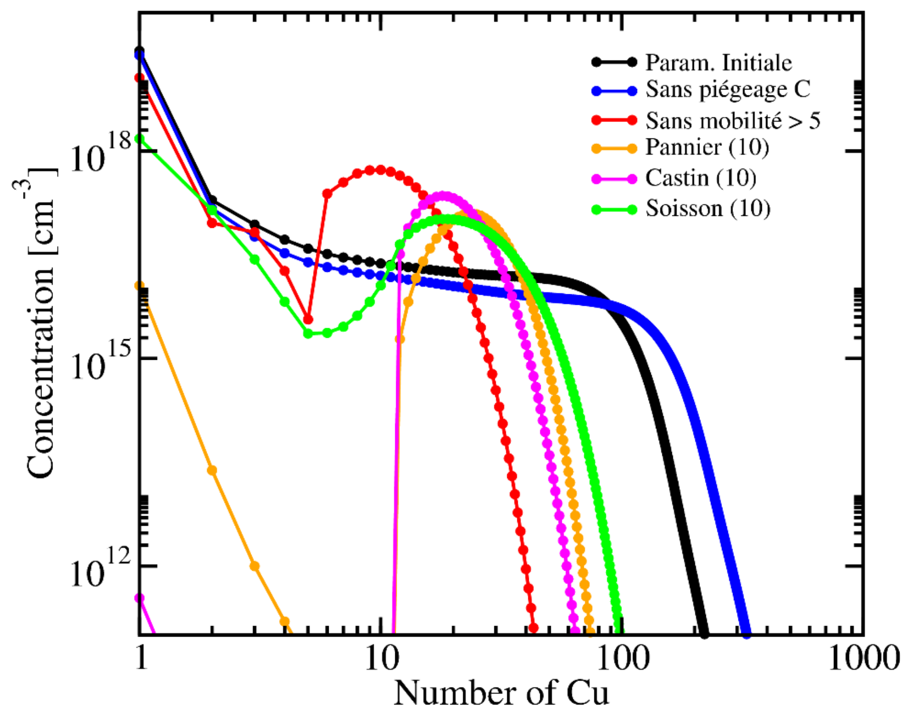






[Castin 2012]

CRESCENDO (co-dev CEA-EDF)



In progress:

Treat multi-component alloys
1D/3D + trapping

Mesoscale methods

MFRT and OKMC models are similar kinetic models

- can be used to simulate the same phenomena
- most details are handled quite differently in the 2 approaches

MFRT-OKMC: inherent differences

parameter or mechanism	MFRT	OKMC
solution method	deterministic	stochastic
time	explicit variable	inferred from processes and reaction rates
space	smeared, effective medium, possible multi-region RT	full spatial dependence
defect production	time and space-averaged, but …	discrete in time and space
sink strength, e.g. dislocations	explicit expression or input parameter	inferred from fate of point defects
defect or sink density	essentially unlimited	limited (computationally) by simulation cell size, i.e. $N = 1/(x \cdot y \cdot z)$

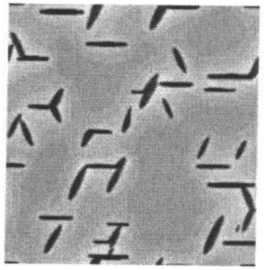
Phase field – Mesoscale 2D/3D

- Elements of the microstructure: "Order parameters"
  - Conserved order parameters: solute concentration
  - Non conserved order parameters: phase

$\eta_1(\mathbf{r},t)$, $\eta_2(\mathbf{r},t)$, $\eta_3(\mathbf{r},t)$, …

$\eta_i(\mathbf{r},t) = 0$ if there is matrix in $(\mathbf{r},t)$

$\eta_i(\mathbf{r},t) = 1$ if there is phase i in $(\mathbf{r},t)$



- Prediction of order parameters describe the microstructure evolution

Phase field – Thermodynamics & kinetic

- Free energy F
- $F = F_c + E_{el}$
- Chemical and structural contribution (short range)

$$F_c = \int_V \left[f\left(c(r,t), \eta_i(r,t)\right) + \sum_{i=1}^{3} \frac{\alpha_i}{2} \left(\nabla \eta_i(r,t)\right)^2 + \frac{\beta}{2} \left(\nabla c(r,t)\right)^2 \right] d^3 r$$

- Elastic contribution (long range)

$$E_{el} = E_0 + E_{relax}^{hom} + E_{relax}^{het} - \sigma_{ij}^{appl} \sum_{p=1}^{Np} \int_V \varepsilon_{ij}^{00}(p)\, \eta_{i(p)}^2 (r,t)\, d^3 r$$

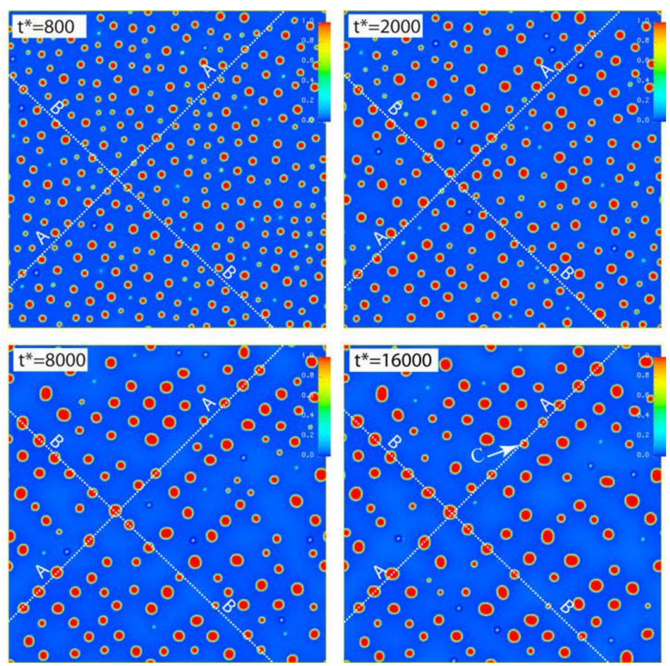
- Kinetic

$$\frac{\partial c(r,t)}{\partial t} = M \nabla^2 \frac{\delta F}{\delta c(\mathbf{r},t)}$$

Phase field - Applications

- Microstructure evolution under irradiation / thermal ageing

$$\frac{\partial c_v(r,t)}{\partial t} = M\nabla^2 \frac{\delta F}{\delta c_v} + \underbrace{\dot{g}(c_v(r,t))}_{\text{Production term}} - \underbrace{\dot{\gamma}(c_v(r,t), c_{SIA}(r,t))}_{\text{Recombination term}}$$

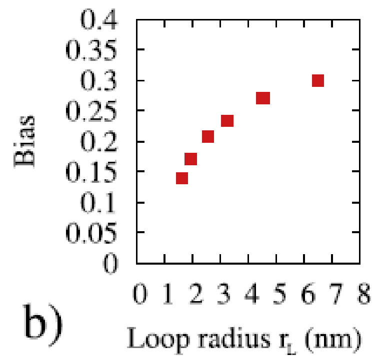


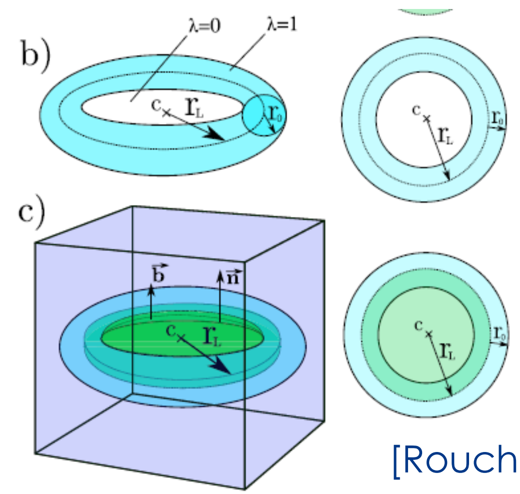
Void formation

Phase field - Applications

Sink strength calculations

$$B = \frac{Z_i - Z_v}{Z_i}$$



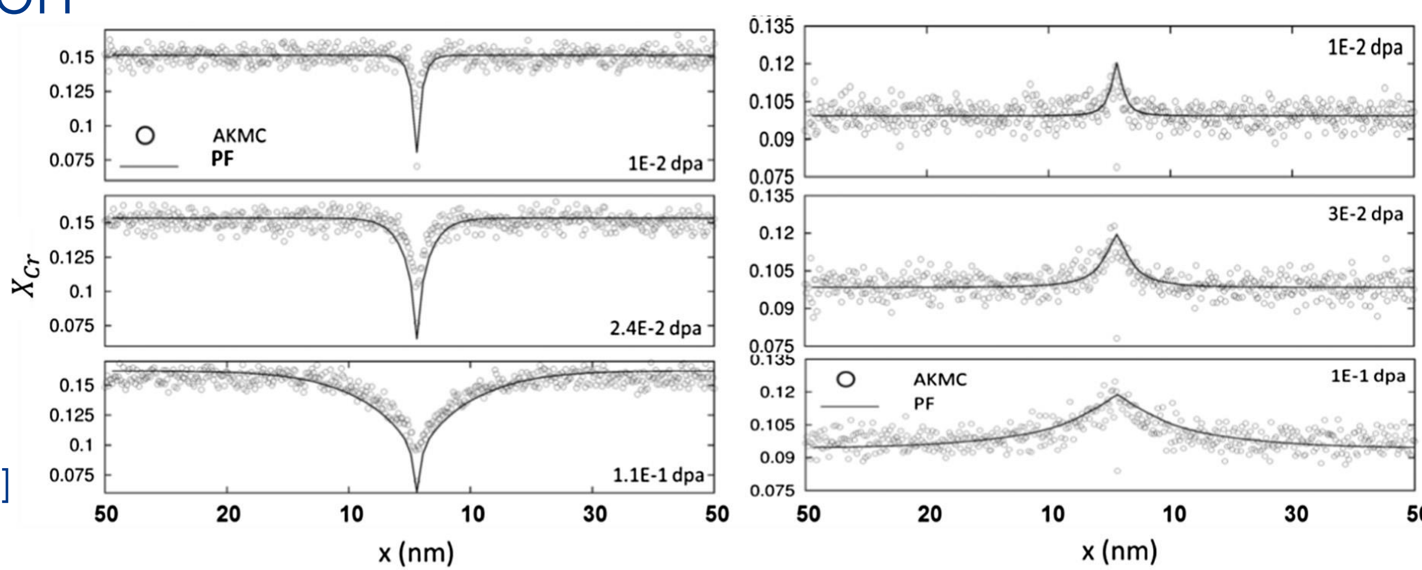


[Rouchette et al.]

Segregation

Fe-15%Cr @900K
Fe-10%Cr @700K

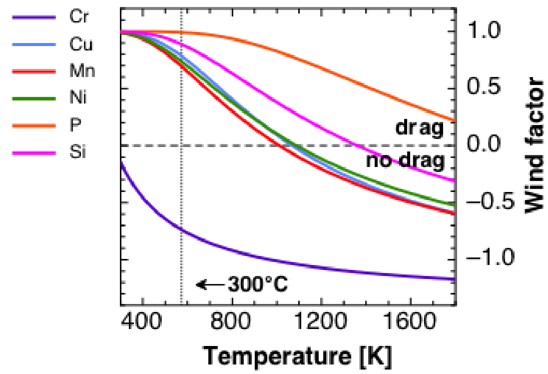
[Piochaud, CMS 2016]

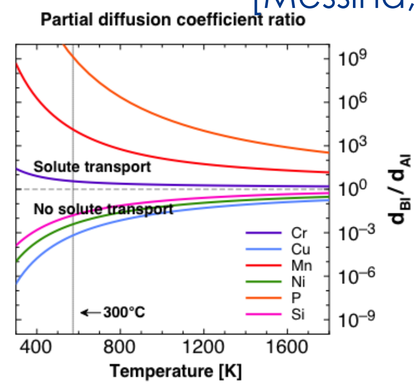


Segregation applications

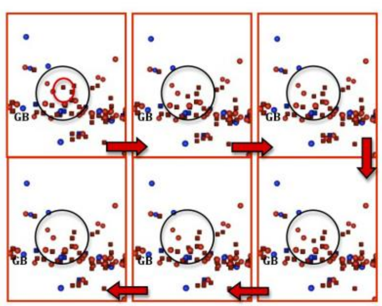
[Messina, Olsson et al.]
[Messina PhD]

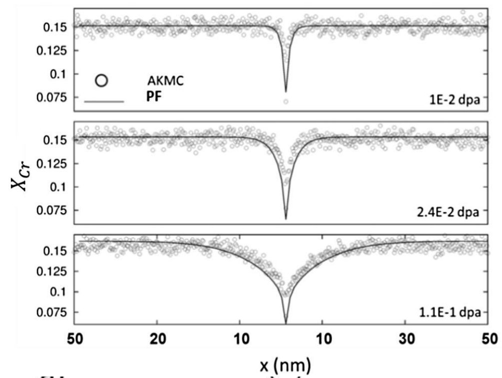
- Atomic data (DFT)
  - Diffusion coefficients, transport coefficients (Onsager coefficients)
  - Input for AKMC cohesive models

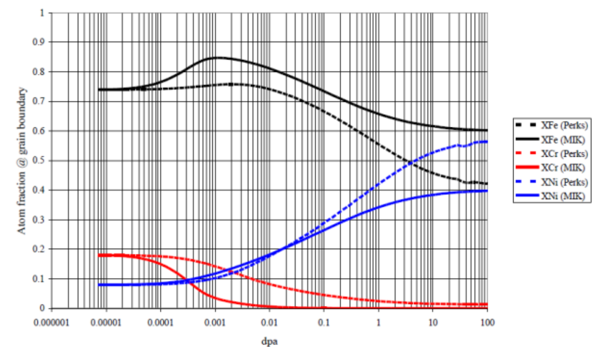




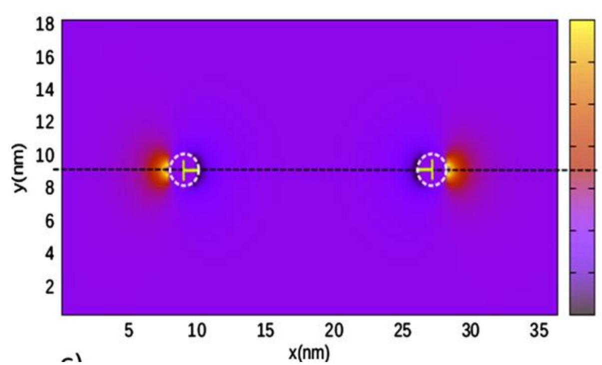
- Mechanisms (MD, of-lattice AKMC)

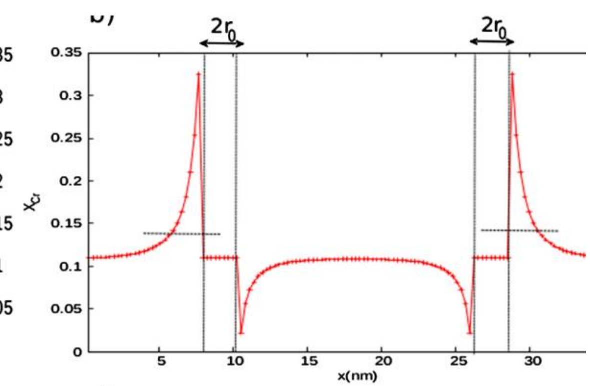






- Segregation simulation
  - AKMC
  - Phase field (+elasticity)
  - Finite elements





Material Multiscale Modeling Challenge

Complexity
(chemistry, clusters, interfaces)

Length-scale
(Angstrom, meter)

Integration
(codes, database, methods, …)

HPC
(High Performance Computing)
Exp validation

Time-scale
(fs, ps, years)

Accuracy
(ab initio, semi-empirical potentials, cohesive models)

Uncertainties
Statistics (sensitivity analysis)