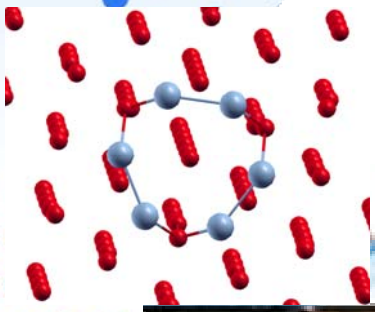
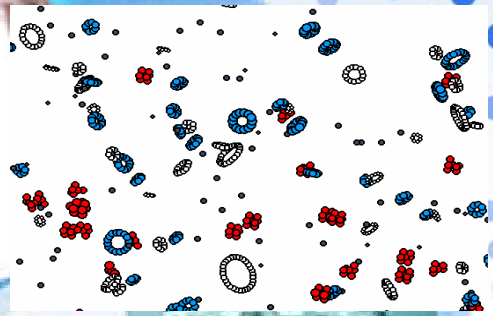
PERFORM 60

FP7 Project

GETMAT FP7 PROJECT

Time accelerated Atomic Kinetic Monte Carlo for radiation damage modelling





C. Domain, C.S. Becquart, R. Ngayam-Happy

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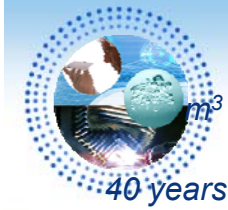
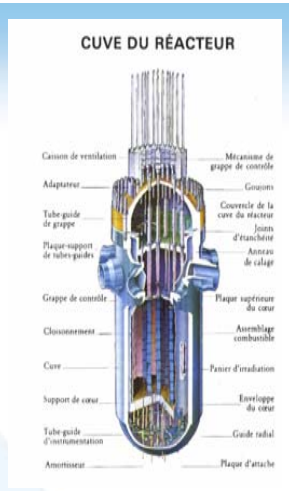
mai

EDF R&D



m³

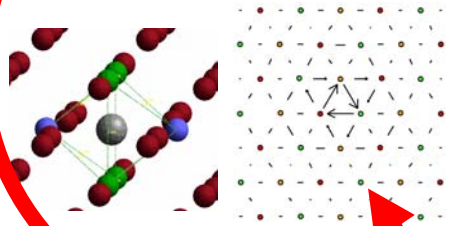
40 years



1nm³

0 - ps

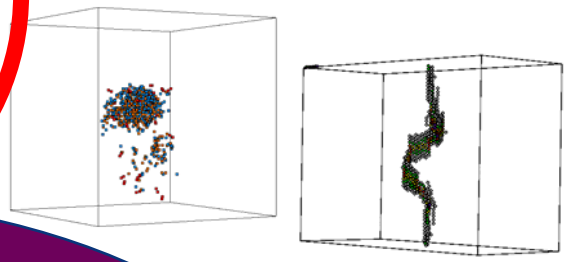
ab initio



(10-30nm)³

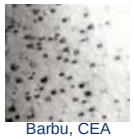
ns

Molecular dynamics

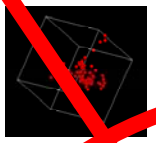


Finite elements

Multi-scale modelling



Barbu, CEA



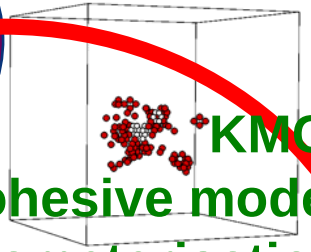
Pareige, U Rouen

+ experimental validation

PERFORM 60

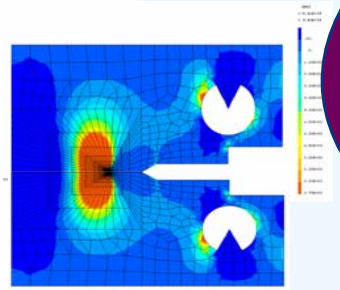
FP7 Project

s - h

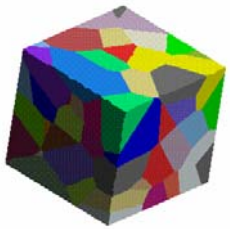


KMC cohesive model & parameterisation

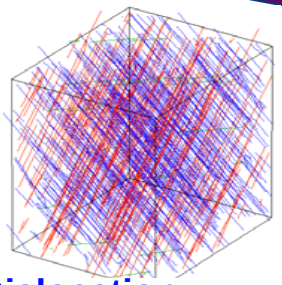
cm³



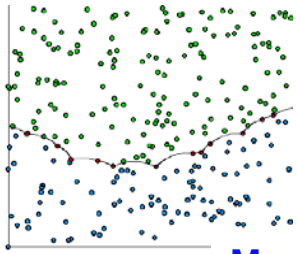
Micro-macro



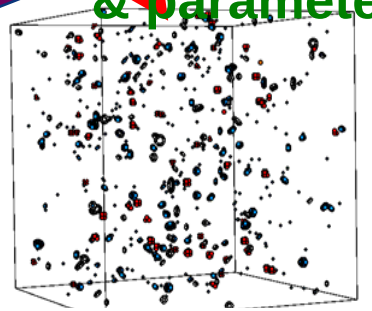
µm³



Dislocation dynamics



Mesoscopic



(30-100nm)³

h-year

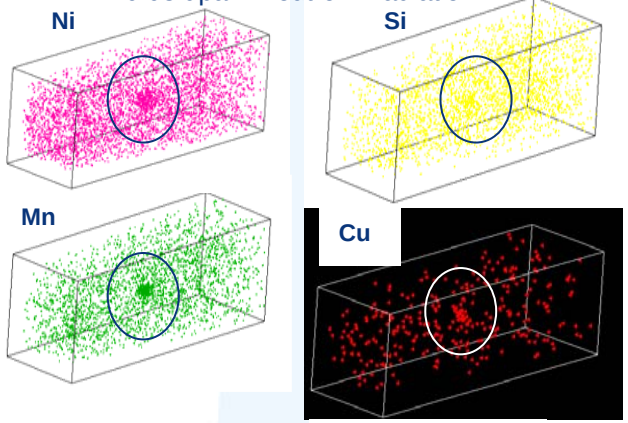
Radiation damage

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

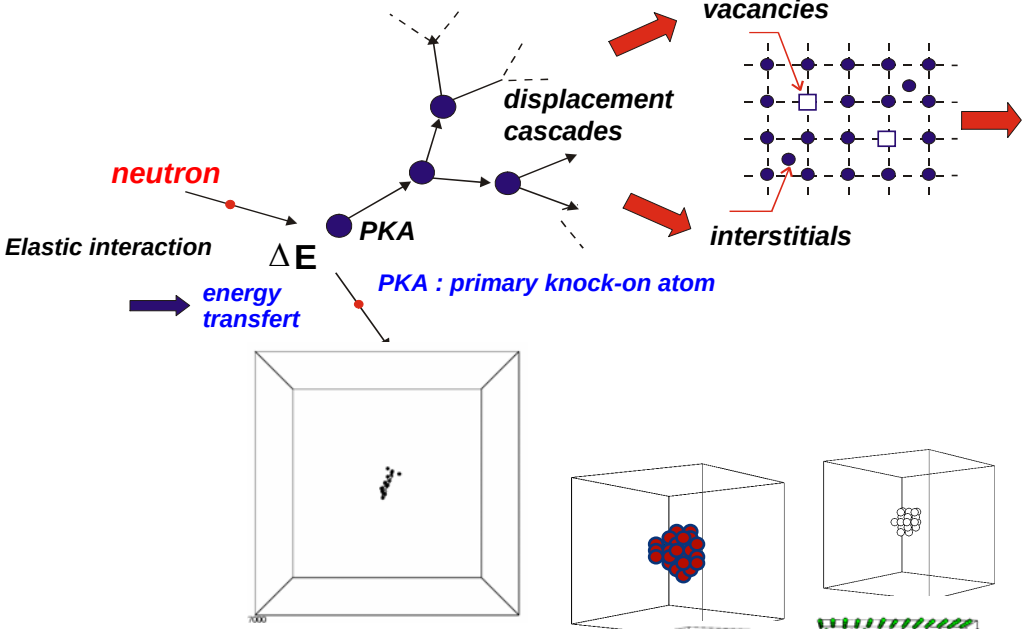
+ dislocations

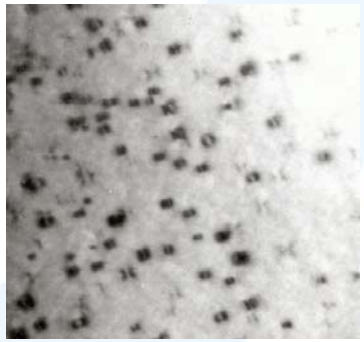
Irradiation:
Electron:
Frenkel pairs
Ion and neutron:
displacement cascades (10 - 100 keV)
vacancies and interstitials:
isolated and in clusters

0.08 dpa – Neutron irradiation



TAP, Pareige, U. Rouen



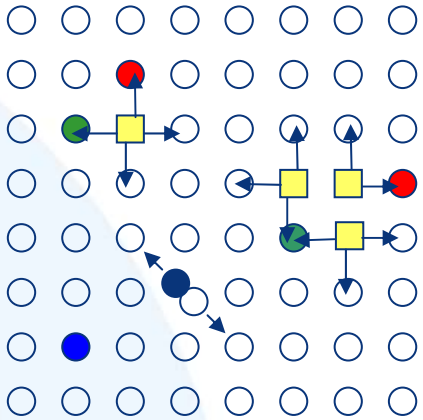


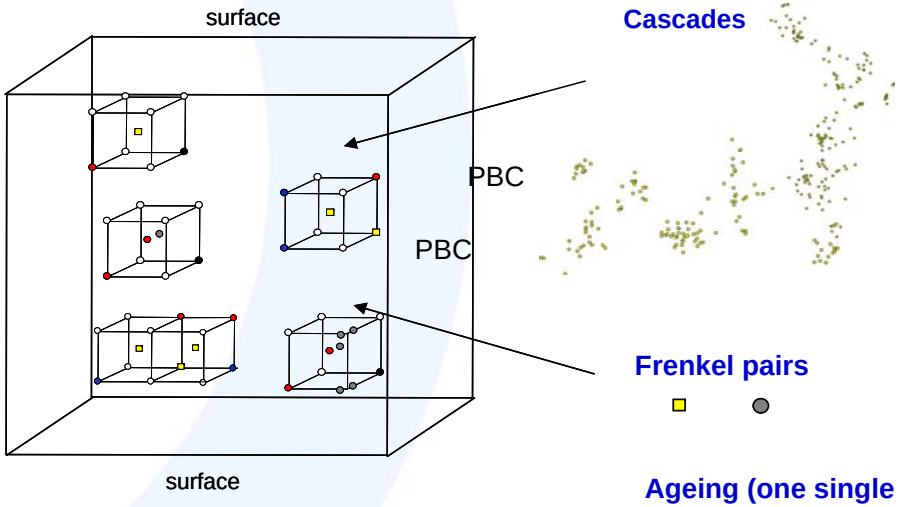
TEM, Barbu, CEA

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

Kinetic Monte Carlo simulation of irradiation

Atomic KMC



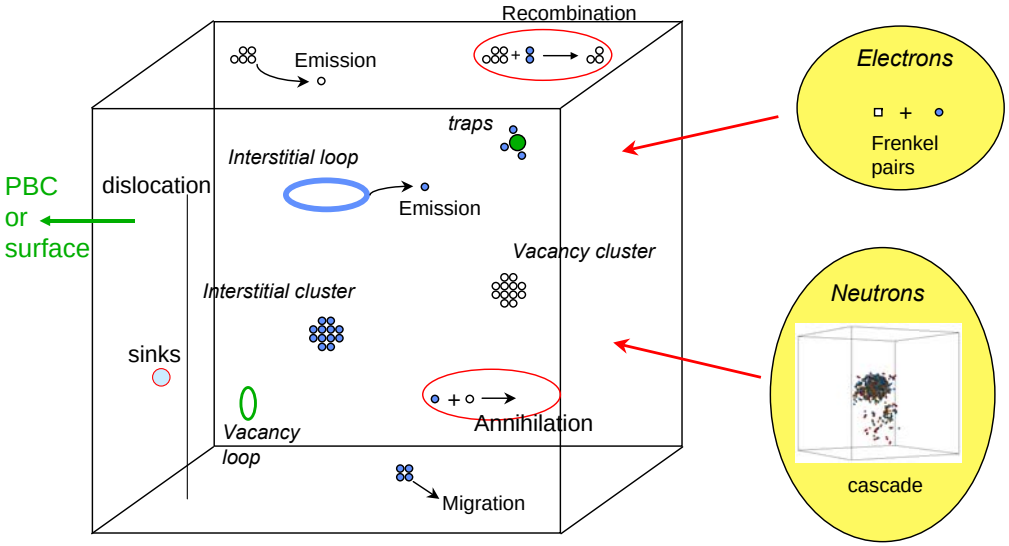


Cascades

Frenkel pairs

Ageing (one single vacancy)

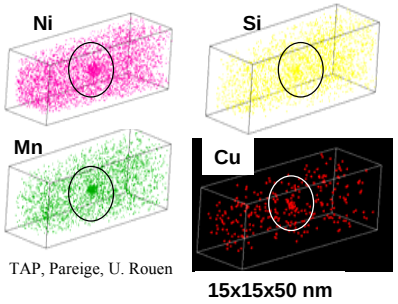
Object KMC

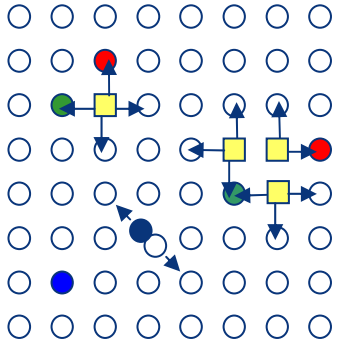


[JNM 335 (2004) 121–145]

Atomic Kinetic Monte Carlo of microstructure evolution

Objective:
Simulation formation of solute rich complexes (observed by TAP) under irradiation

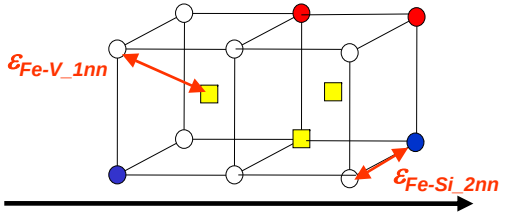




Ab initio

Solute interactions (Cu, Ni, Mn, Si)
(interface energies,
mixing energies …)

Experimental data and
Thermodynamical data



Parameterisation
cohesive model

AKMC

Solute diffusion by
- vacancy mechanisms
- interstitial mechanisms

$$E_{mixing} = -4\varepsilon^{(1)}_{(Fe-Fe)} - 3\varepsilon^{(2)}_{(Fe-Fe)} + 8\varepsilon^{(1)}_{(Fe-X)} + 6\varepsilon^{(2)}_{(Fe-X)} - 4\varepsilon^{(1)}_{(X-X)} - 3\varepsilon^{(2)}_{(X-X)}$$

$$E_{formation}(V^Z) = 8\varepsilon^{(1)}_{(V-Z)} + 6\varepsilon^{(2)}_{(V-Z)} - 4\varepsilon^{(1)}_{(Z-Z)} - 3\varepsilon^{(2)}_{(Z-Z)}$$

$$E^{(1)}_{binding(V-X)} = \varepsilon^{(1)}_{(Fe-V)} + \varepsilon^{(1)}_{(Fe-X)} - \varepsilon^{(1)}_{(Fe-Fe)} - \varepsilon^{(1)}_{(V-X)}$$

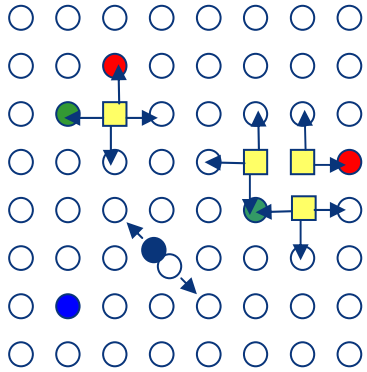
Experimental validation: TAP, SANS, SAXS, PA, TEP

Atomistic Kinetic Monte Carlo (AKMC)

- Treatment of multi-component systems on a rigid lattice
  - Substitutional elements
  - Interstitial elements

Vincent et al. NIMB 255 (2007) 78
Vincent et al. JNM 382 (2008) 154

Code: LAKIMOCA

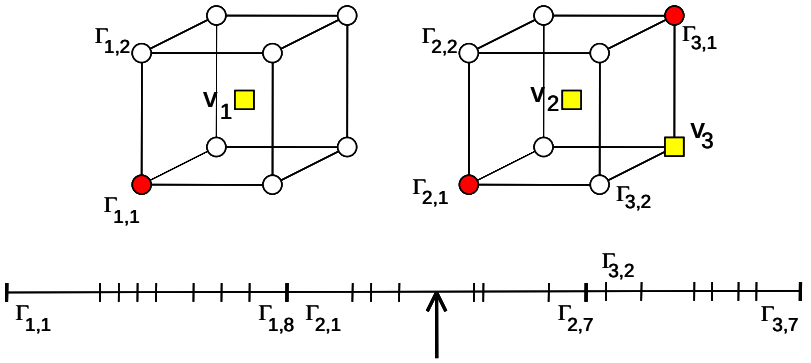


- Diffusion by 1nn jumps
  - Via vacancies
  - Via interstitials

Jump Probability: $\Gamma_X = \nu_X \exp\left(-\frac{Ea}{kT}\right)$ ν_X = attempt frequency

- Residence Time Algorithm applied to all events
  - Vacancy and Interstitial jumps
  - Frenkel Pairs and Cascade flux for irradiation

Average time step: $\Delta t = \frac{1}{\sum_{j,k} \Gamma_{jk}}$



→ Environment dependant form of activation energy Ea

$$Ea = Ea(X_i) + \frac{Ef - Ei}{2}$$

AKMC irradiation simulation conditions

For electron irradiation: Frenkel Pair (FP) flux

For neutron irradiation: flux of

- **20 keV and 100 keV cascades debris obtained by Molecular Dynamics**

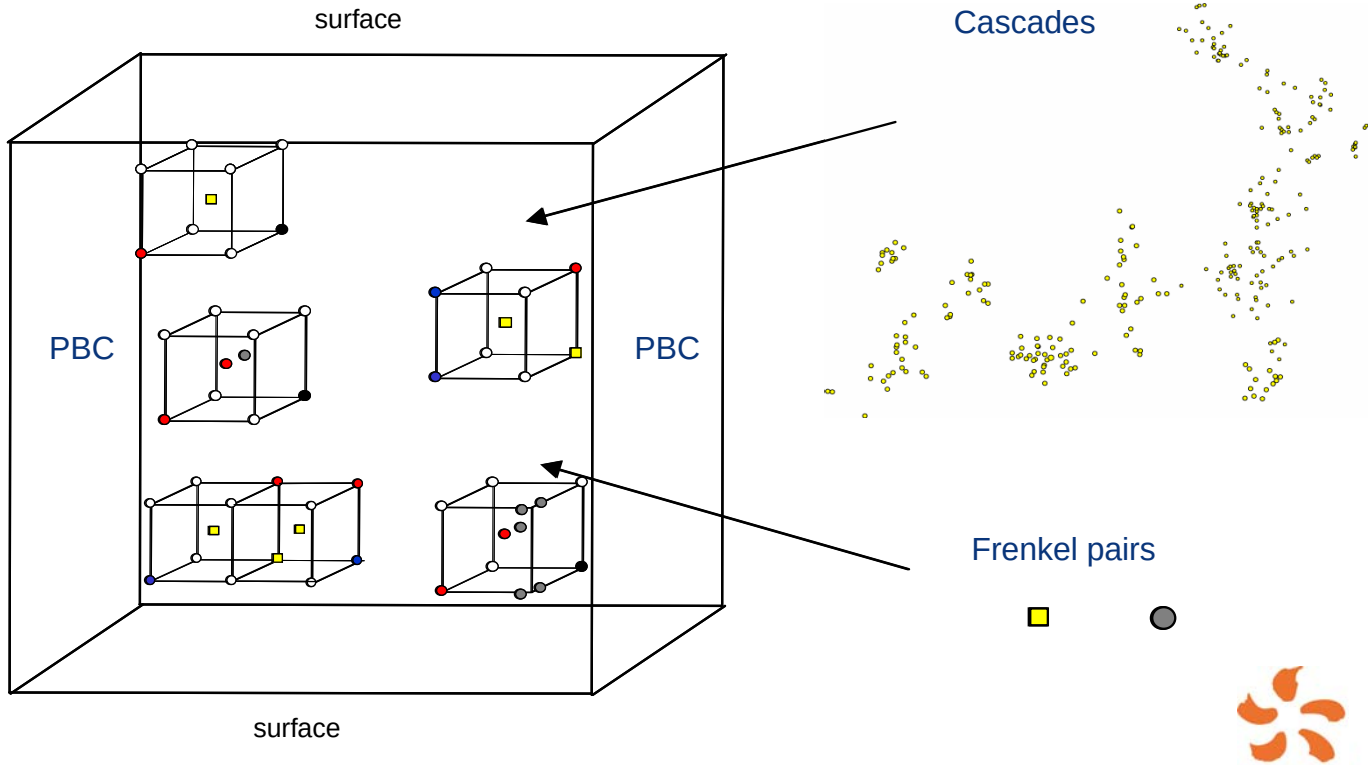
  (R. Stoller, J. Nucl. Mater. 307-311 (2002) 935)

- **Frenkel Pairs**

Typical simulation box:

1.01×10^{-17} cm^3 boxes

$8.65\ 10^6$ atoms



AKMC simulation of radiation damage accumulation

Target dose: 0.1 dpa

Irradiation duration: 2 days (10^5 s) up to 40 years (10^9 s)

Irradiation temperature: 573 K

Defect accumulation: > 100 point defects in the simulation box

Events:

Self interstitial migration (0.3 eV) : time step : 10^{-10} s

Vacancy migration (0.65 eV) : time step : 10^{-7} s

Rapidly: annihilation or formation point defect clusters

Point defect migration within point defect - solute clusters or trapping with solutes

Very large number of jumps required to have “significant event”
(ie emission or diffusion)

Other jumps with high migration energies (1 eV) : time step : 10^{-4} s

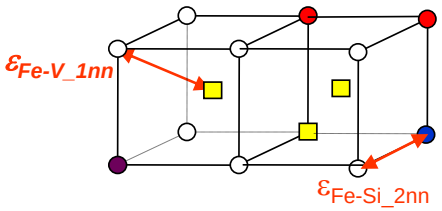
Computational limitation: ~10^{10} steps / month

Very complex situation: many events with different time scale & long simulation required

Cohesive energy model

$$Ea = Ea(X_i) + \frac{Ef - Ei}{2}$$

Vacancy:

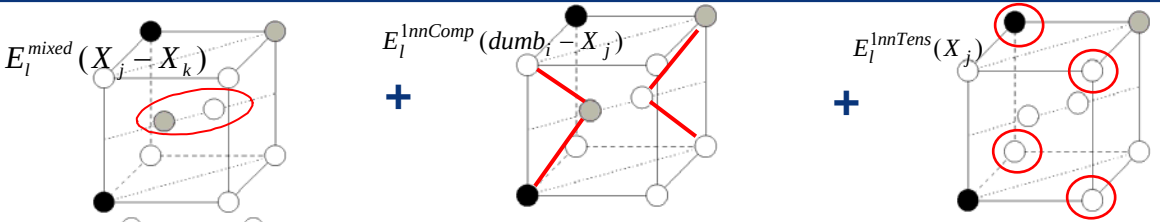


$$E = \sum_j \varepsilon^{(i)}_{(Fe-Fe)} + \sum_k \varepsilon^{(i)}_{(V-V)} + \sum_l \varepsilon^{(i)}_{(Fe-V)} + \sum_m \varepsilon^{(i)}_{(Fe-X)} + \sum_n \varepsilon^{(i)}_{(V-X)} + \sum_p \varepsilon^{(i)}_{(X-Y)}$$

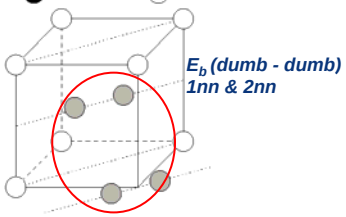
- RPV: 1nn and 2nn pair interactions
- FeCr: 2BM potential

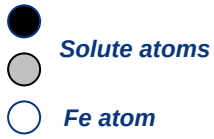
SIA:

- **solute - dumbbell**



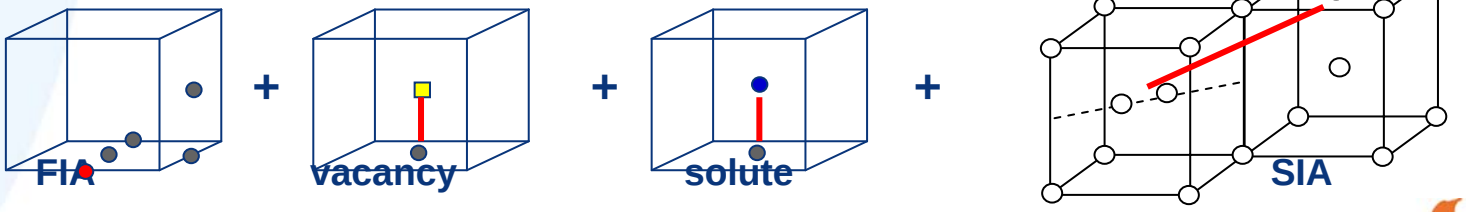
- **dumbbell - dumbbell**





$$E_{dumb} = \sum_i \left(E_f + \sum_j E_l^{1nnComp}(dumb_i - X_j) + \sum_j E_l^{1nnTens}(X_j) + \sum_{i,j} E_l^{mixte}(X_j - X_k) + \sum E_l(dumb - dumb) \right)$$

FIA (C):



~ 100 ab initio data considered in the model

Cohesive model: ε_{X-Y} and ε_{V-X} determination

Binary alloys

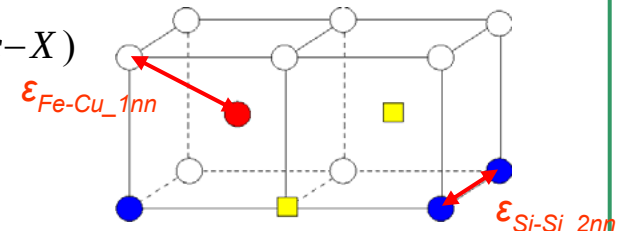
- $E_{mélange} = -4\varepsilon^{(1)}_{(Fe-Fe)} - 3\varepsilon^{(2)}_{(Fe-Fe)} + 8\varepsilon^{(1)}_{(Fe-X)} + 6\varepsilon^{(2)}_{(Fe-X)} - 4\varepsilon^{(1)}_{(X-X)} - 3\varepsilon^{(2)}_{(X-X)}$
- $E_{interface(100)} = -2\varepsilon^{(1)}_{(Fe-Fe)} - \varepsilon^{(2)}_{(Fe-Fe)} + 4\varepsilon^{(1)}_{(Fe-X)} + 2\varepsilon^{(2)}_{(Fe-X)} - 2\varepsilon^{(1)}_{(X-X)} - \varepsilon^{(2)}_{(X-X)}$
- $E_{cohésion}(Z) = 4\varepsilon^{(1)}_{(Z-Z)} + 3\varepsilon^{(2)}_{(Z-Z)}$
- $E_{formation}(lac^{Z}) = 8\varepsilon^{(1)}_{(lac-Z)} + 6\varepsilon^{(2)}_{(lac-Z)} - 4\varepsilon^{(1)}_{(Z-Z)} - 3\varepsilon^{(2)}_{(Z-Z)}$
- $E^{(i)}_{liaison}(lac-lac) = 2\varepsilon^{(i)}_{(Fe-lac)} - \varepsilon^{(i)}_{(Fe-Fe)} - \varepsilon^{(i)}_{(lac-lac)}$

$E^{(1)}_{liaison}(lac-X) = \varepsilon^{(1)}_{(Fe-lac)} + \varepsilon^{(1)}_{(Fe-X)} - \varepsilon^{(1)}_{(Fe-Fe)} - \varepsilon^{(1)}_{(lac-X)}$

i = 1 or 2

X, Y = solute atoms

Z = Fe or solute atom



Ternary alloys…

$E^{(i)}_{liaison}(X-Y) = \varepsilon^{(i)}_{(Fe-X)} + \varepsilon^{(i)}_{(Fe-Y)} - \varepsilon^{(i)}_{(Fe-Fe)} - \varepsilon^{(i)}_{(X-Y)}$

Ab initio data

Parameters

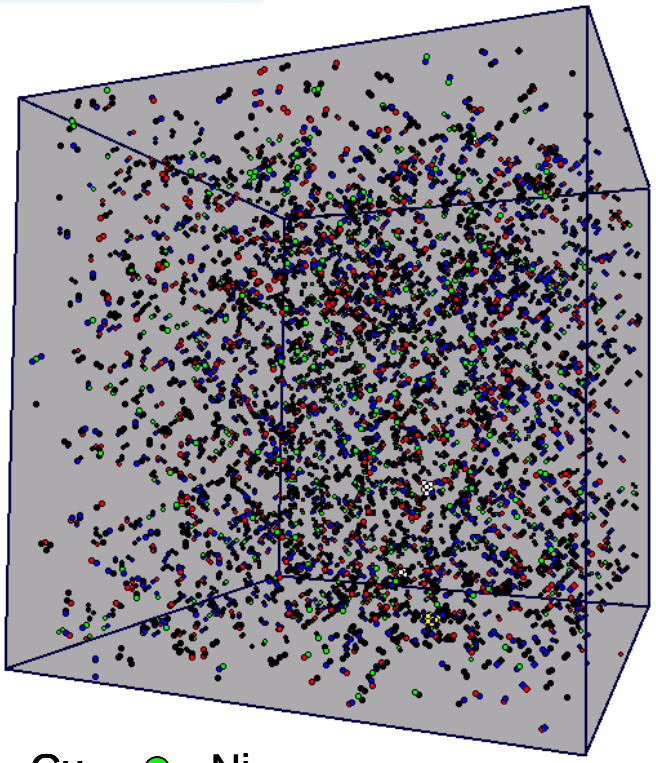
Adjustment on thermal annealing experiment

Neutron irradiation of FeCuNiMnSi alloys
Medium term evolution by atomic Kinetic Monte Carlo

Fe-0.2Cu-0.53Ni-1.26Mn-0.63Si (at.%) at 300°C

Flux: 6.5 10^{-5} dpa.s^{-1}

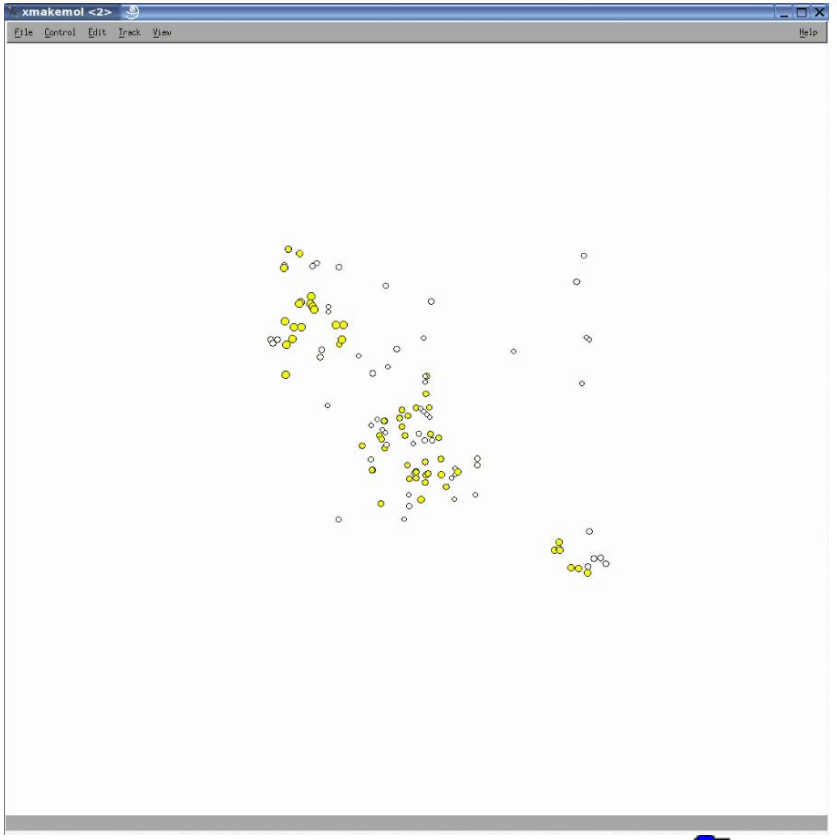
Dose: 1.3 10^{-3} dpa



Cu Ni

Si V

Mn SIA



V-solute complex

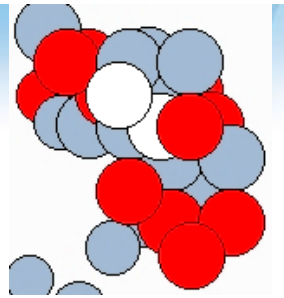
SIA-solute complexes

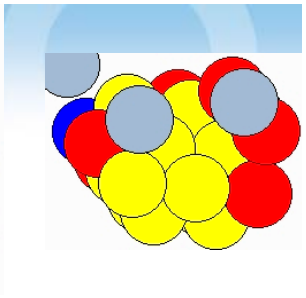
Small solute clusters

Point defect clusters = germs for precipitation

[> 1 month on 1 CPU]

Fe – CuMnNiSiP (at.%) alloys

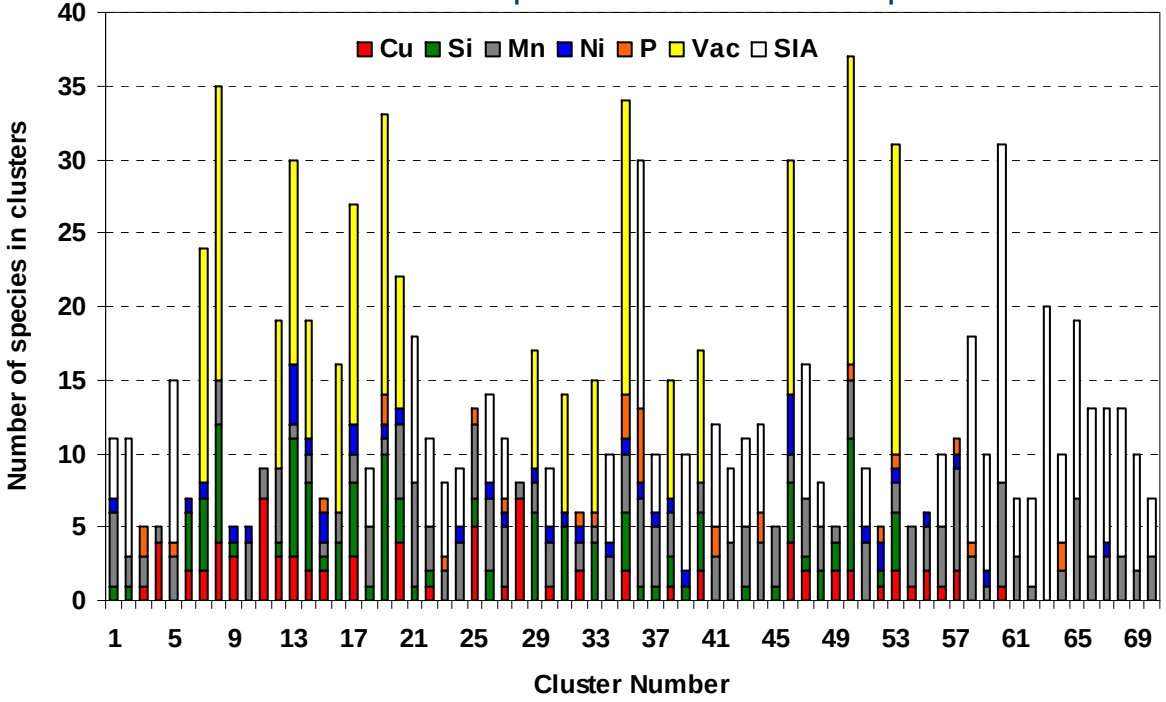


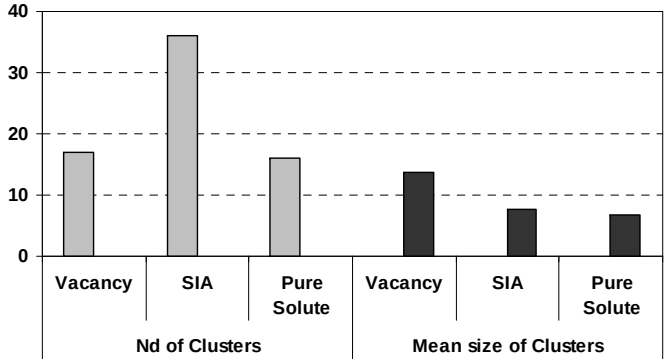


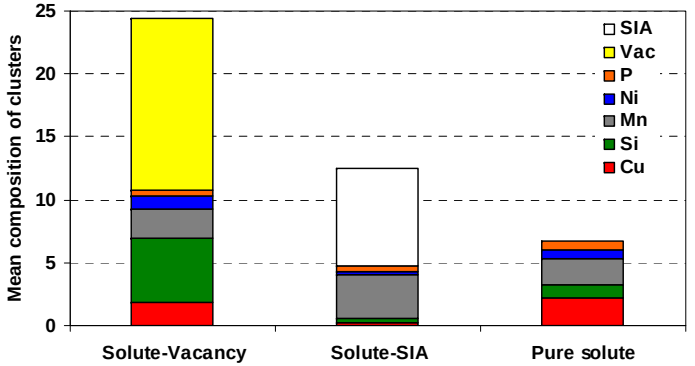
- Distribution and composition of clusters:

0.18Cu 1.38Mn 0.69Ni 0.43Si 0.01P (A533B plate)

5.79x10^{-4} dpa/s - 300°C - 9.03 mdpa

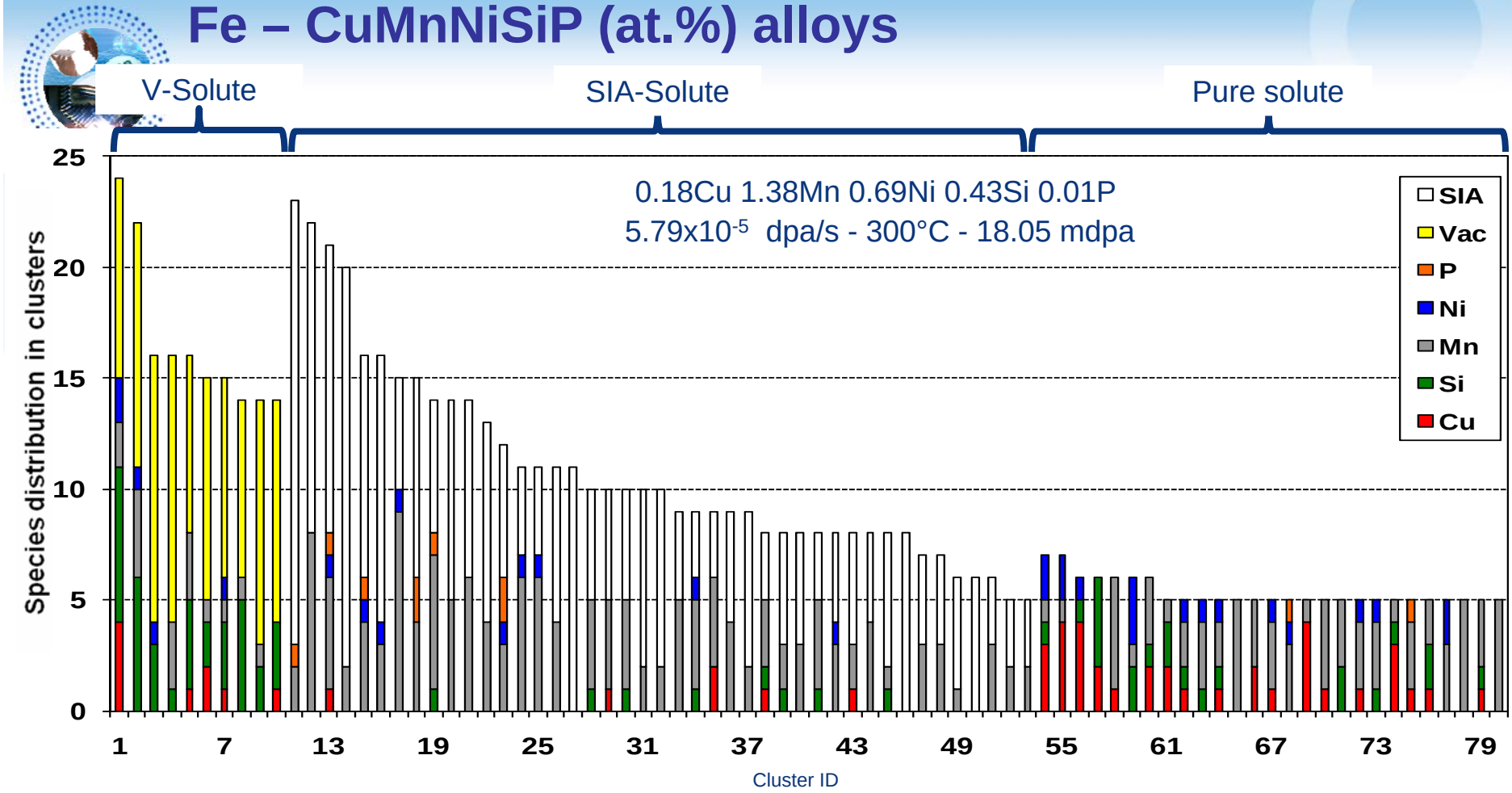






- High Nd of PD clusters
  Vacancy clusters are bigger and less numerous than SIA clusters
- Solute clusters form on PD clusters (induced segregation)
  Clusters associated with SIA clusters are enriched in Mn
  Clusters associated with vacancy clusters are enriched in Si/Cu/Mn and Ni/P
- Cu enriched clusters observed (enhanced precipitation)

Fe – CuMnNiSiP (at.%) alloys



- **The biggest solute clusters are associated with PD clusters**
  - **In agreement with induced segregation mechanism to account for solute clusters formation**
- **Clusters associated with interstitial clusters are enriched in Mn, and P/Ni**
- **Clusters associated with vacancy clusters are enriched in Si/Cu/Mn (mostly) and Ni**
- **I-Solute complexes > V-Solute complexes**

Isochronal annealing: pure Fe

Isochronal annealing in pure Fe

DT/Dt = 2K/300s (T<30K)

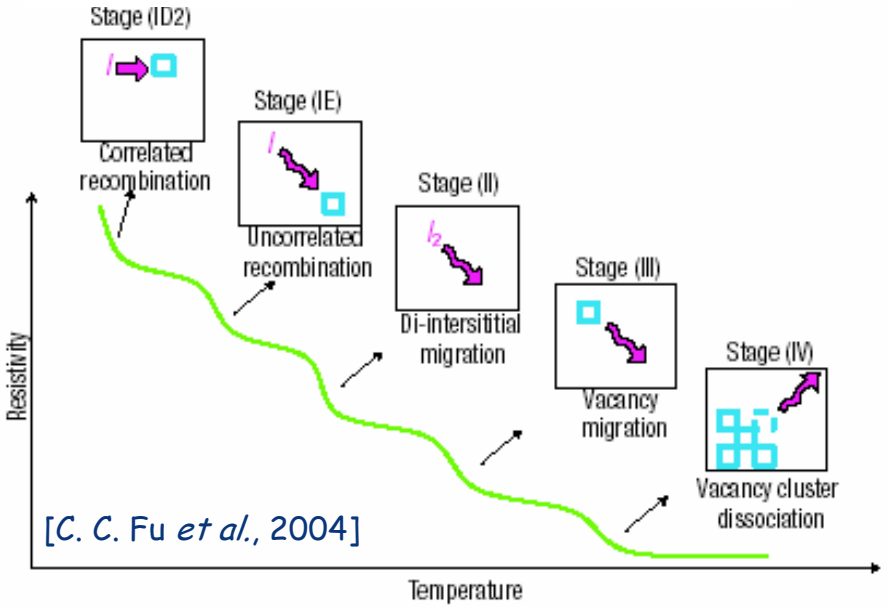
DT/TDt = 0.03K/300s (T>30K)

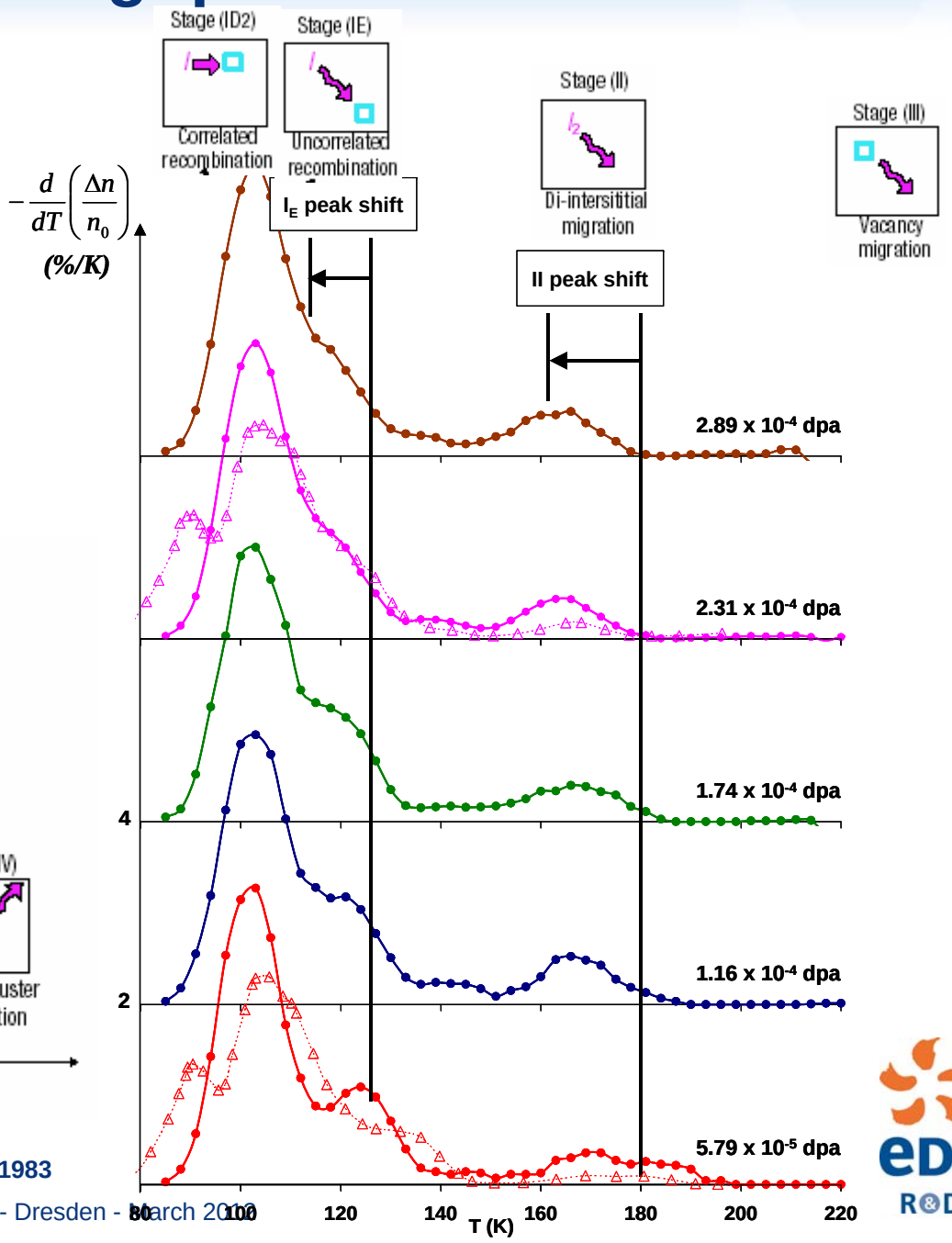
Tirrad = 4.5 K

ρ (Resistivity)➔ n (number of defects)

Differential Fractional Recovery

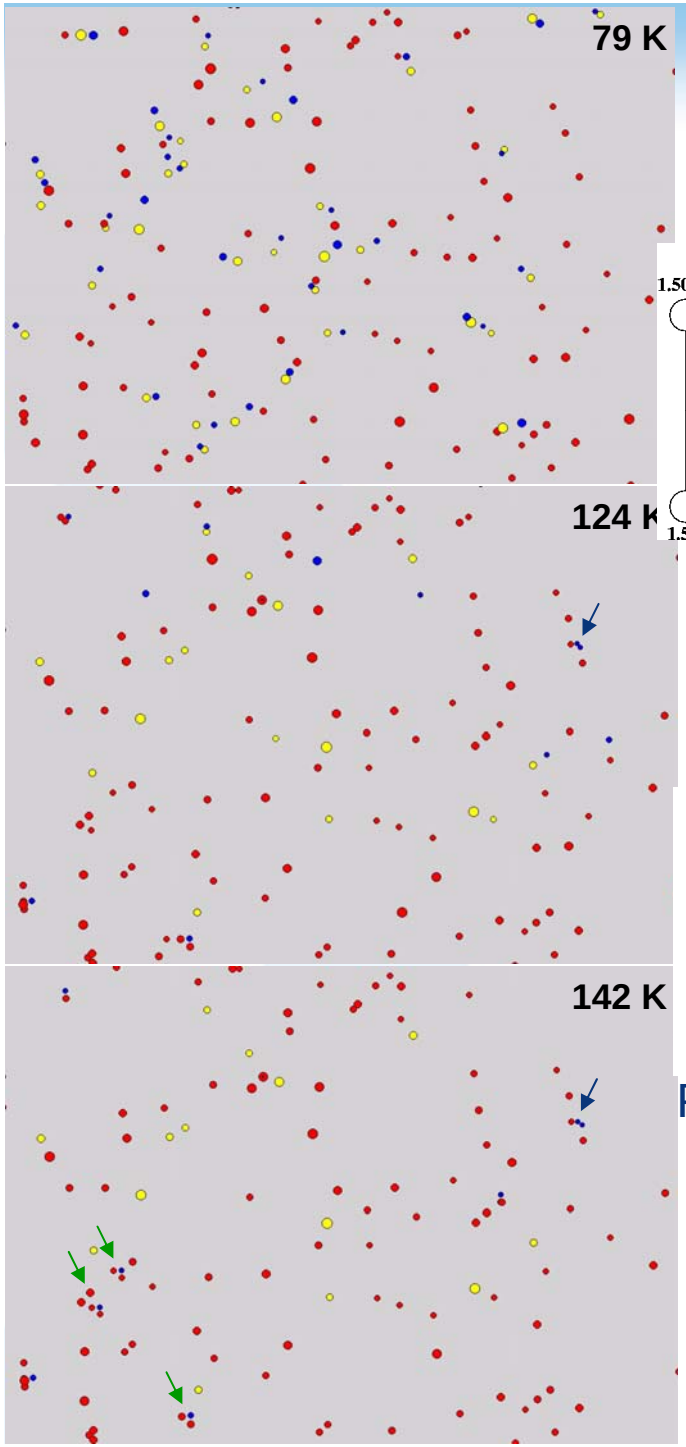
d/dT (Dρ /Dρ$_0$) ➔ d/dT (n/n$_i$)



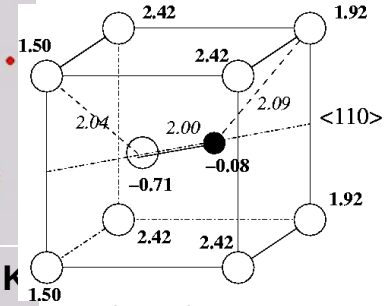


Triangle: Exp. Results: S. Takaki, et al., Radiat. Eff. 79, 87-122, 1983

Isochronal annealing FeP

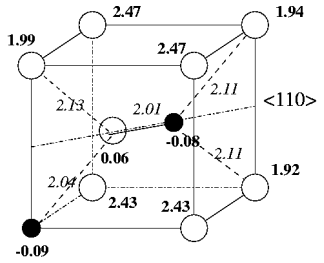


$$-\frac{d}{dT}\left(\frac{\Delta n}{n_0}\right) \quad (\%/K)$$



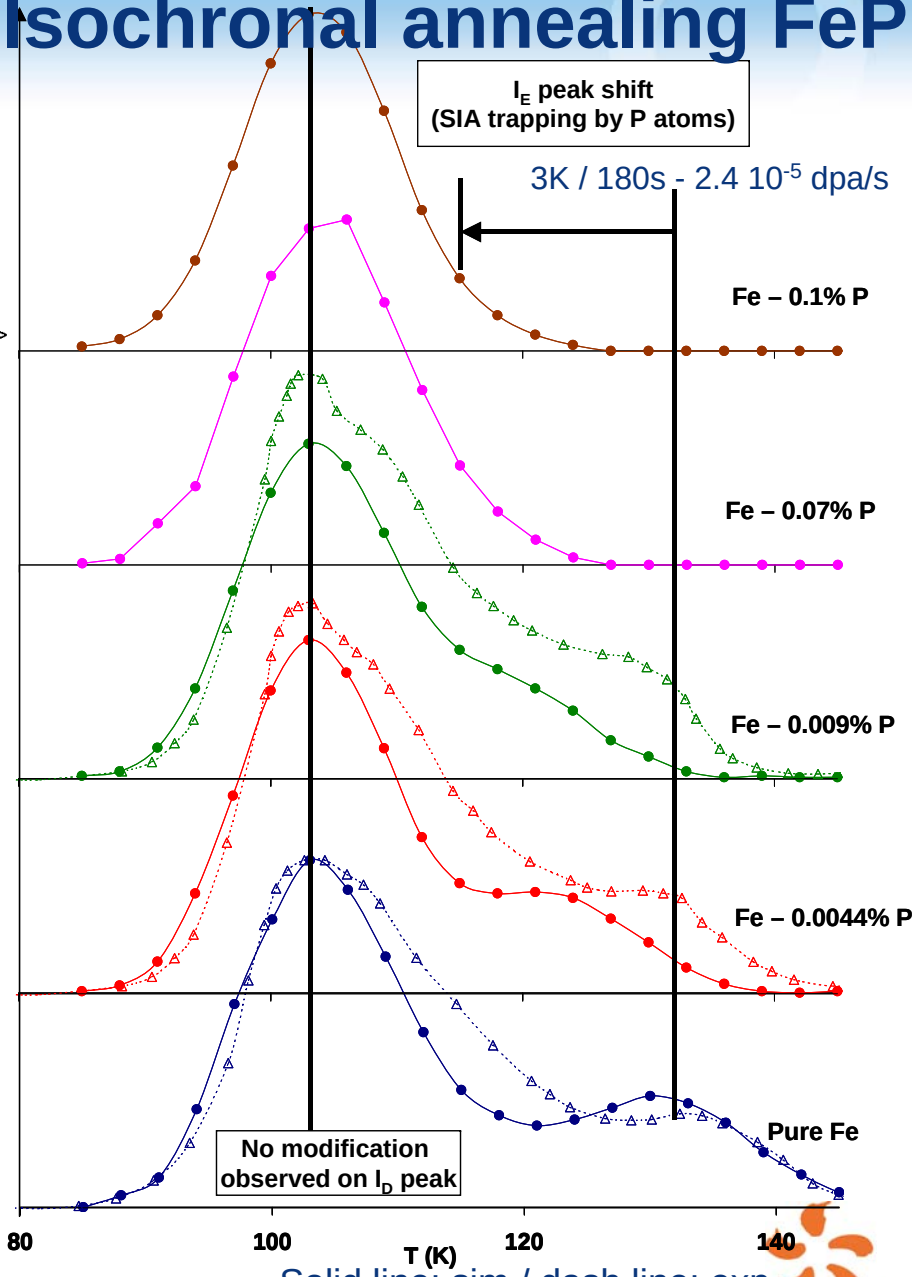
$\langle 110 \rangle_{Fe\text{-}P}$

Eb = 1.02 eV



$P_{subs} - \langle 110 \rangle_{Fe\text{-}P}$

Eb = 2.0 eV

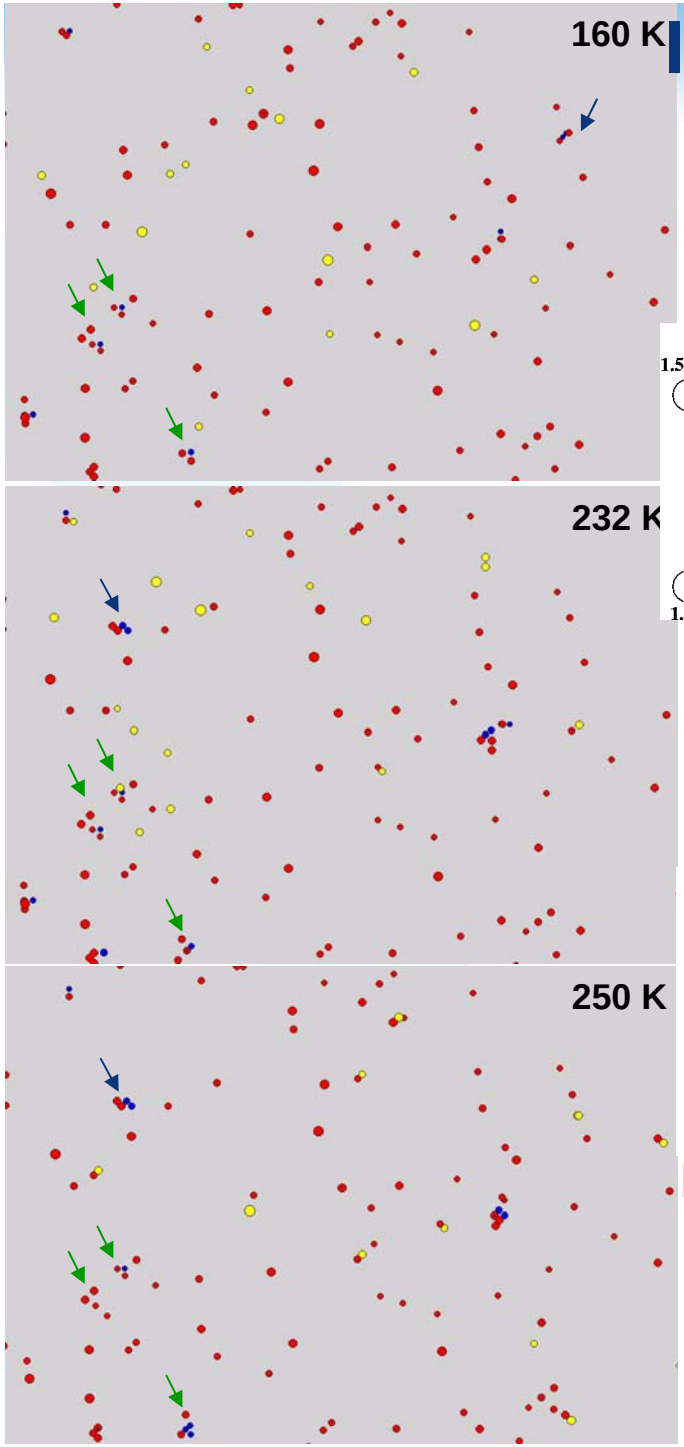


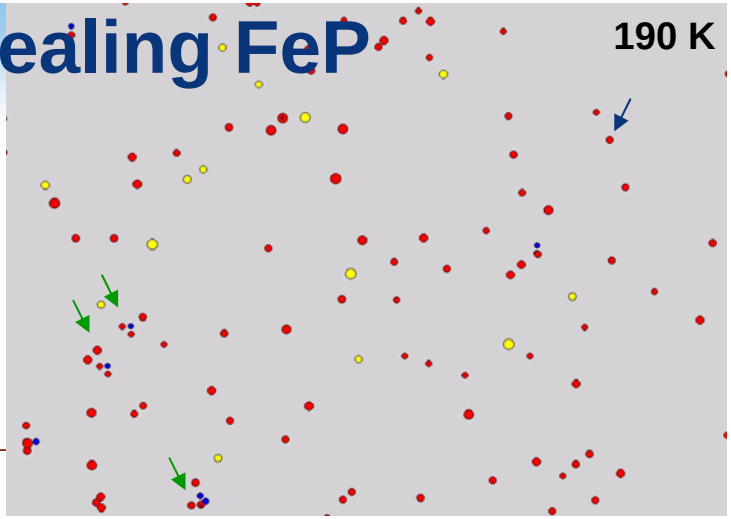
Solid line: sim / dash line: exp

Experimental results:

H. Abe, F. Kuramoto, J. Nucl. Mater. **271 & 272** (1999) 209.

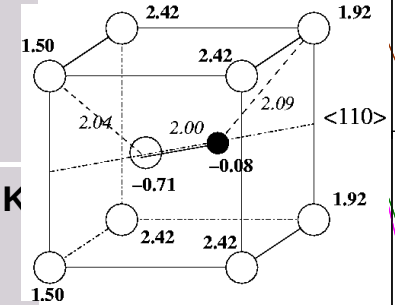
Isochronal annealing FeP





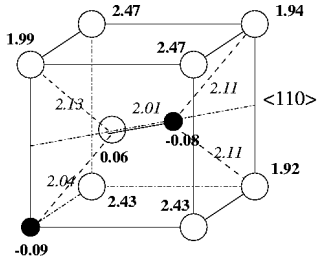
$$-\frac{d}{dT}\left(\frac{\Delta n}{n_{II}}\right)$$

(%/K)



$\langle 110 \rangle_{Fe\text{-}P}$

Eb = 1.02 eV



$P_{subs} - \langle 110 \rangle_{Fe\text{-}P}$

Eb = 2.0 eV

Solid line: sim / dash line: exp

Time Accelerated Dynamics in our AKMC

- With solutes, vacancy clusters & interstitial clusters (SIA and carbon), many “trapping” situations.
  - Associated time steps 10^{-10} s (other ones 10^{-5} s - 1 s)
  - Large number of SIAs and vacancies in the simulation box (>100)
  - Do not know a priori which object (point defect solute cluster) will be the usual suspect
  - During irradiation simulation, several different kind objects can be “trapping” situations

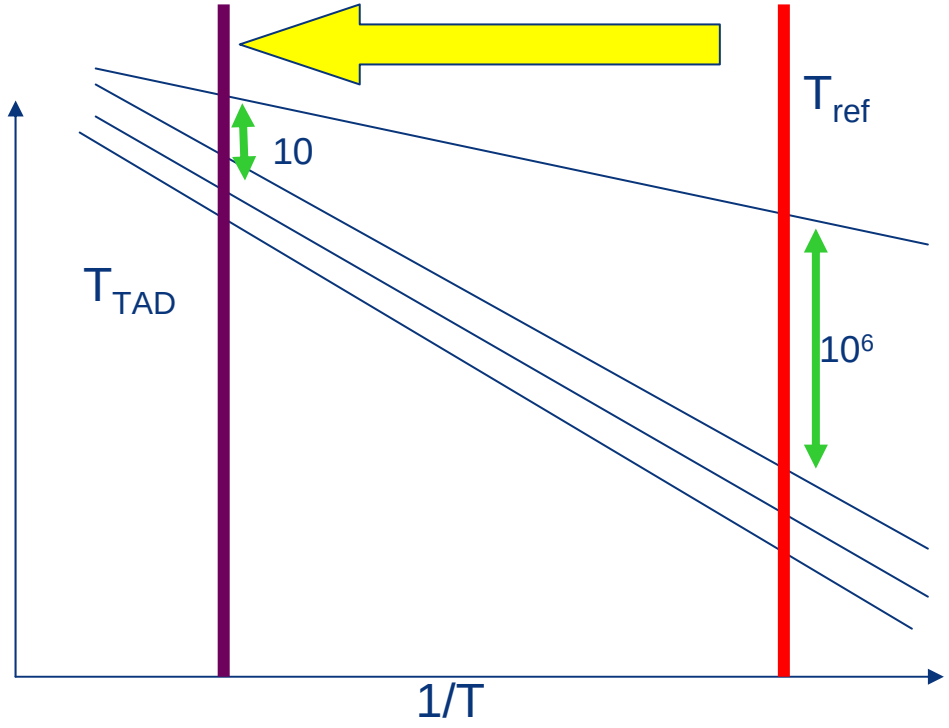
- Adapted version of the TAD algorithm of Voter et al. In our AKMC.
- Different from “pulsing algorithm” of Wirth & Odette (1998 & 2007).

- Based on temperature increase.

Time Accelerated Dynamics in our AKMC

Jump "probability" (s^{-1})

Attempt frequency are all similar



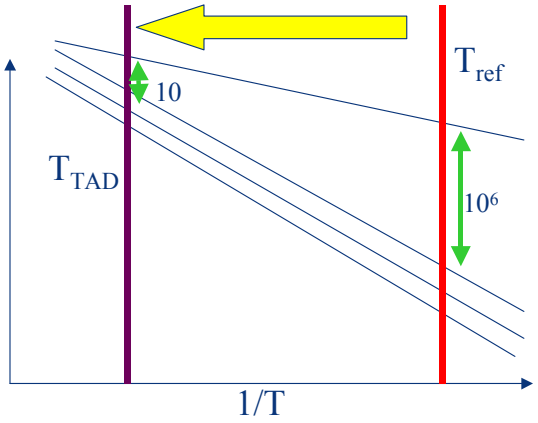
$$\delta t_{ref} = \delta t_{TAD} \exp[E_m / (1 / kT_{ref} - 1 / kT_{TAD})]$$

Time Accelerated Dynamics algorithm in our AKMC

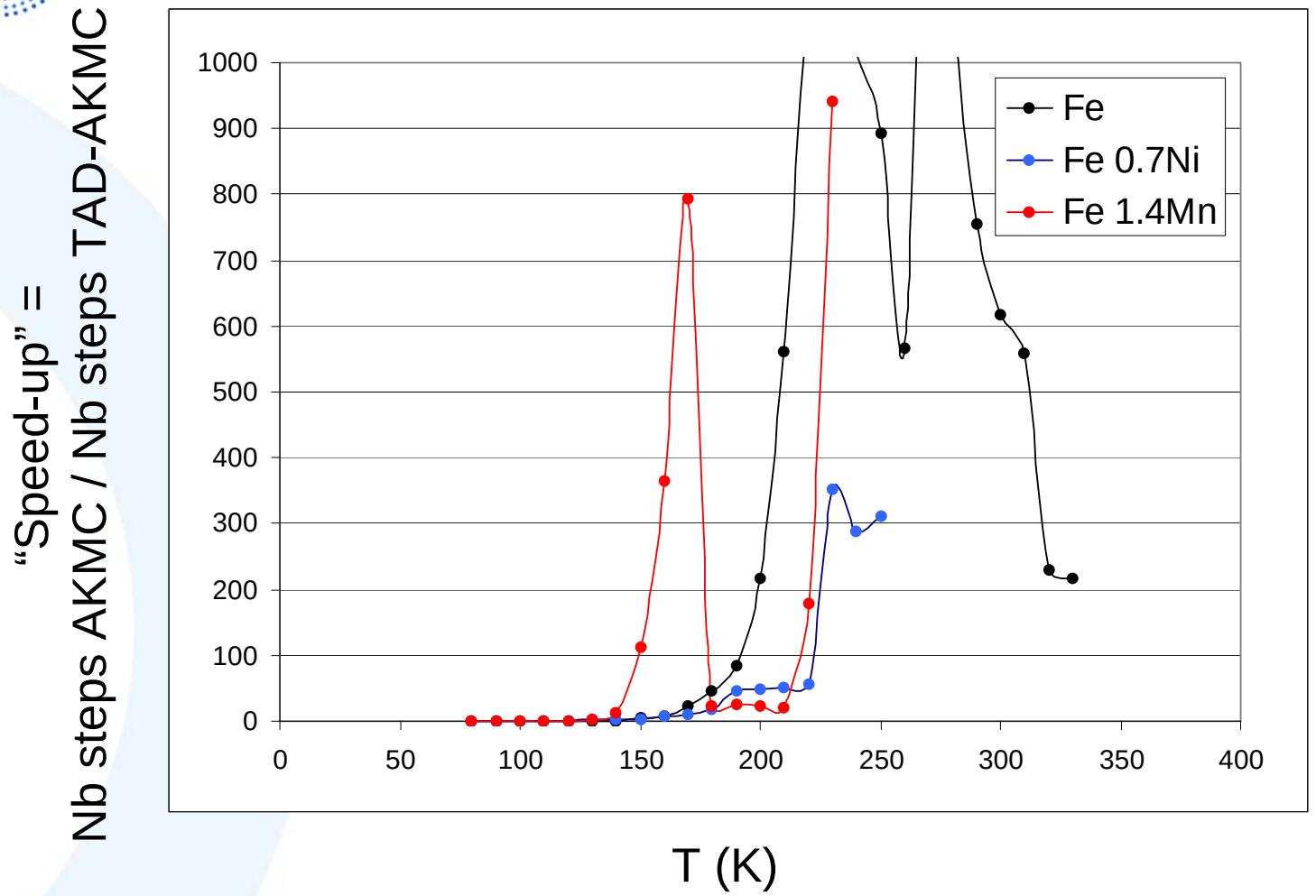
- Every N steps, determination each defect mean free path (MFP)
- If all MFPs are very low
  - Search of the 5 largest jump probabilities ($P_1 > P_2 > P_3 > P_4 > P_5$)
  - If (P_5 / P_1) > 10
  - Choose T_{TAD} in order to have P5/P1 = 10
  - Perform 3 AKMC steps (with adjusted time step)

$$\delta t_{ref} = \delta t_{TAD} \exp[E_m / (1 / kT_{ref} - 1 / kT_{TAD})]$$

- back to T_{ref}

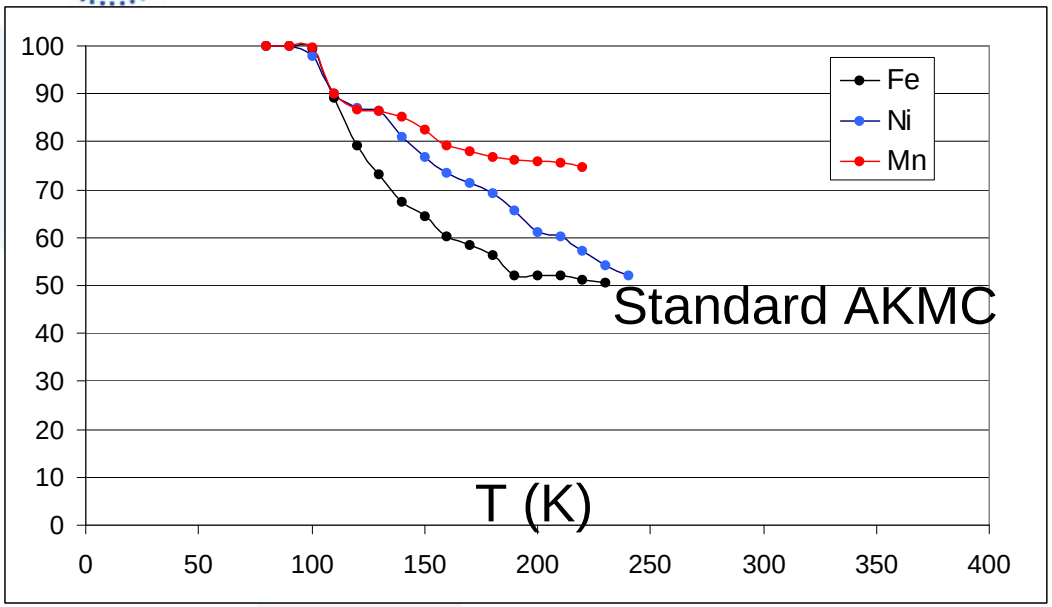


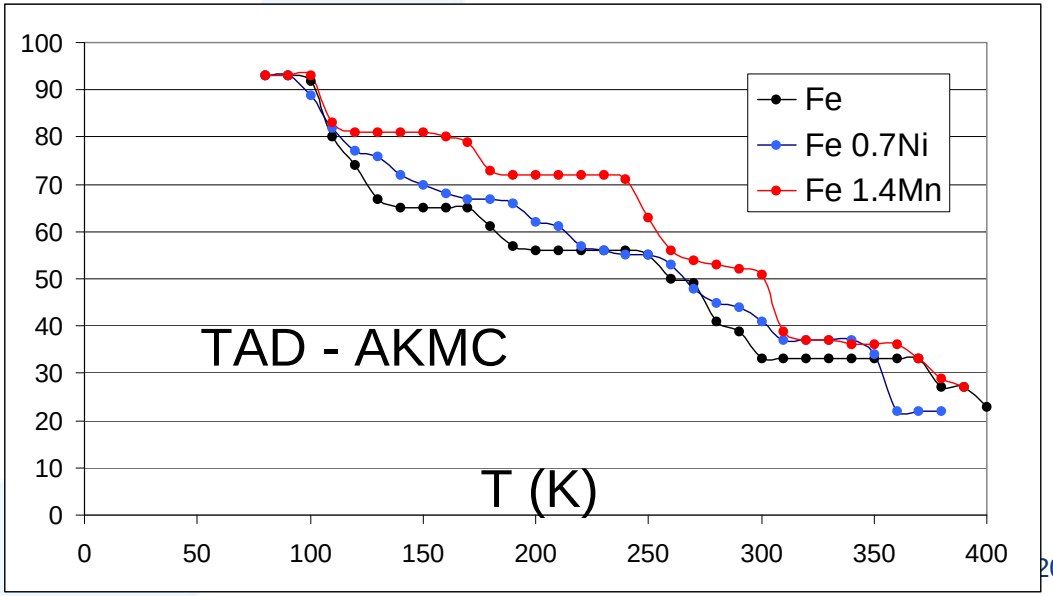
TAD - AKMC: performance improvements



- "speed-up" : 2 order of magnitude
- Simulation with solutes (Ni, Mn) very long due to SIA-solute interactions

TAD - AKMC: preliminary results





- Isochronal annealing: Fe, Fe 0.7%Ni, Fe 1.4%Mn
- Good agreement with experimental results

- standard-AKMC: 1 week CPU
- TAD-AKMC: 12 hours CPU

- Similar physical results (some statistics are required)

Conclusions & perspectives

- AKMC of complex alloys (with simple cohesive models) under irradiation feasible for low doses and high fluxes
- **Massive** Parallelisation is a difficult issue
- TAD method allows to improve the performance of the AKMC tools.
- TAD method validated on isochronal annealing simulation.
- Perspectives:
  - To use TAD for radiation damage simulation under flux.
  - To improve cohesive models