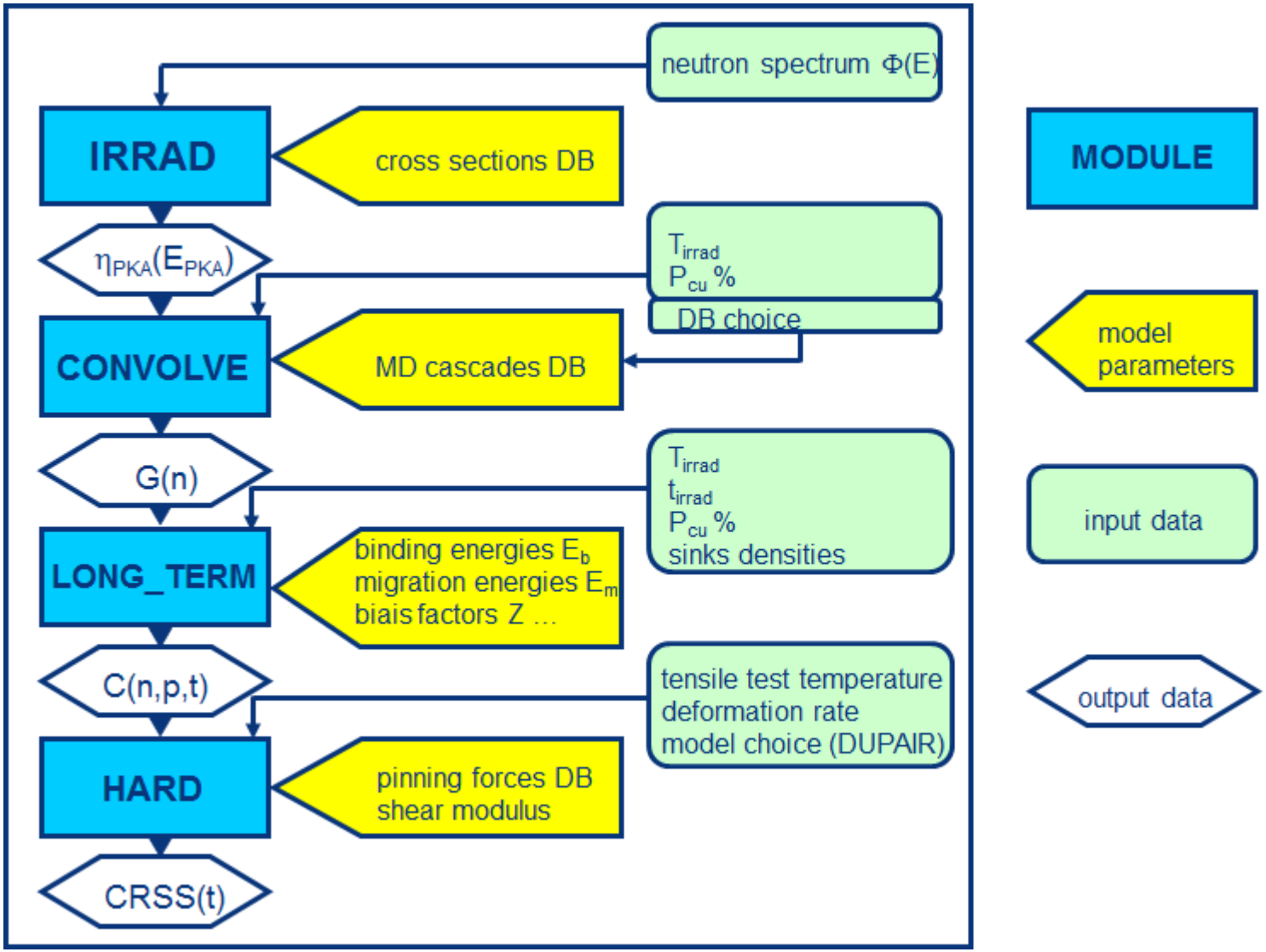
COLLECTIVE EXERCISE ON IRRADIATION AND MICROSTRUCTURE EVOLUTION

J. Vidal (EDF R&D)

This project received funding under the Euratom research and training programme 2014-2018 under grant agreement N° 661913

Summary of the caracteristic simulation sequence



The IRRAD MODULE: concept of PKA

- Upon interaction with a neutron, an atom can be kicked out of its lattice position if the energy transferred is superior to the threshold displacement energy E_d

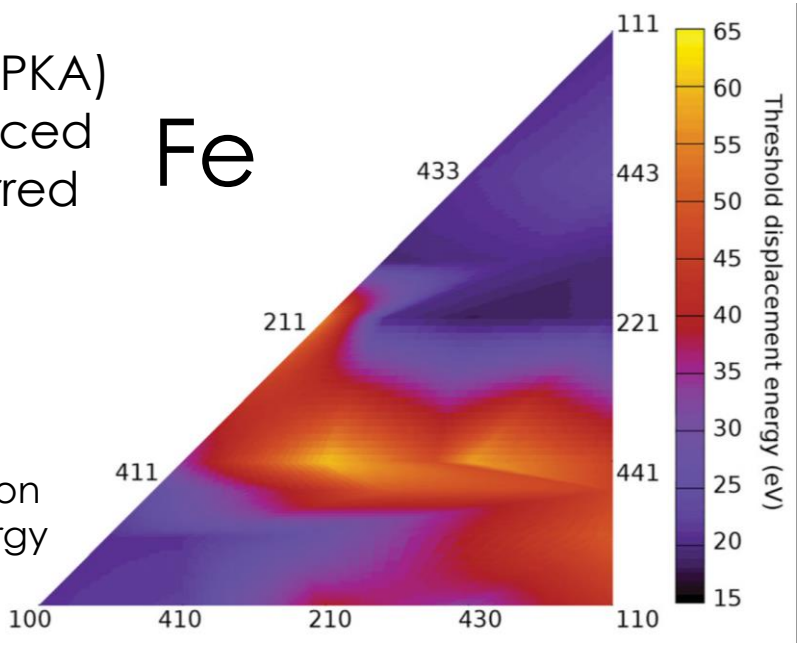
The spectrum of primary knock-on atom (PKA) represents the distribution of atom displaced with respect to its kinetic energy transferred from the neutron.

$$E_{rec} = F_{D,n} + F_{D,e} + F_{D,nr}$$

Damage energy

Electronic deposited energy

Nuclear reaction deposited energy



P. Olsson et al., Material Research Letters, 4,219, (2016)

The IRRAD Module

neutron spectrum

IRRAD

PKA

CONVOLVE

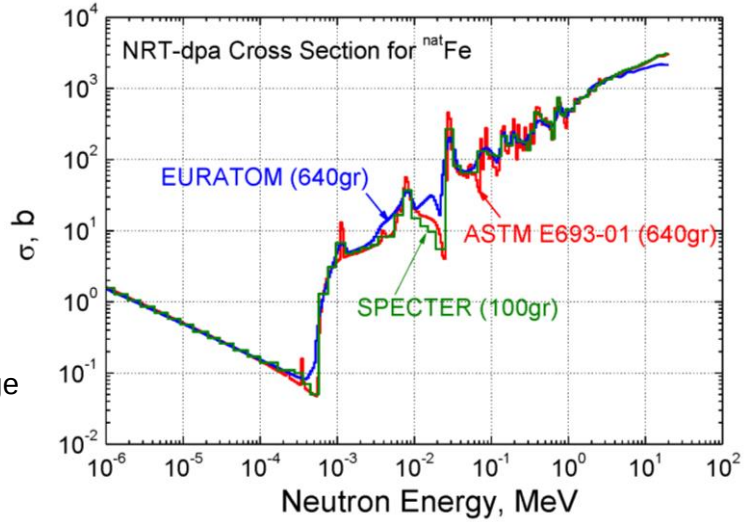
LONG_TERM

HARD

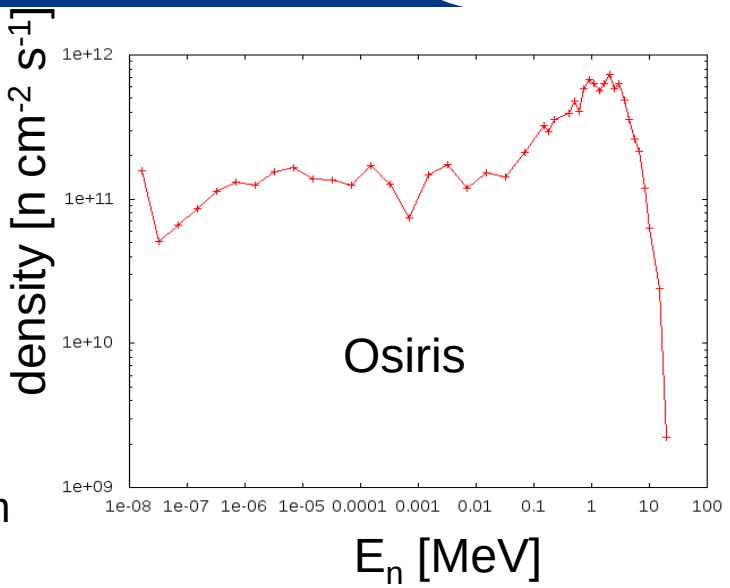
- input : grouped neutron spectrum with E_{max} = 20 MeV

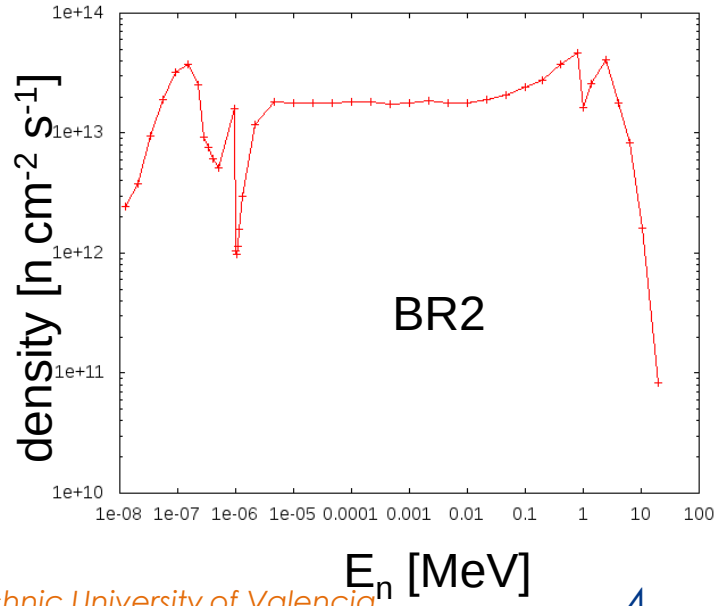
$$\eta_{PKA}(E_{PKA}) = \rho \sum_k \int_{E_{min}}^{E_{max}} \Phi(E_n)\sigma_k(E_n, E_{PKA})dE_n$$

differential cross-section : probability to transfer E_{PKA} to struck atom the incident neutron of energy E_n by reaction channel k



Primary radiation damage in Materials, Report OECD/NEA (2015)





How to measure the irradiation damage ?

- Norgett Robinson Torrens displacement per atom (**NRT-DPA**) measure the level of irradiation considering binary collision model including ballistic processes leading to recombination.[1]

$$N_d(T_d) = \begin{cases} 0 & , \quad T_d < E_d \\ 1 & , \quad E_d < T_d < 2E_d / 0.8 \\ \dfrac{0.8 T_d}{2E_d} & , \quad 2E_d / 0.8 < T_d < \infty \end{cases}$$

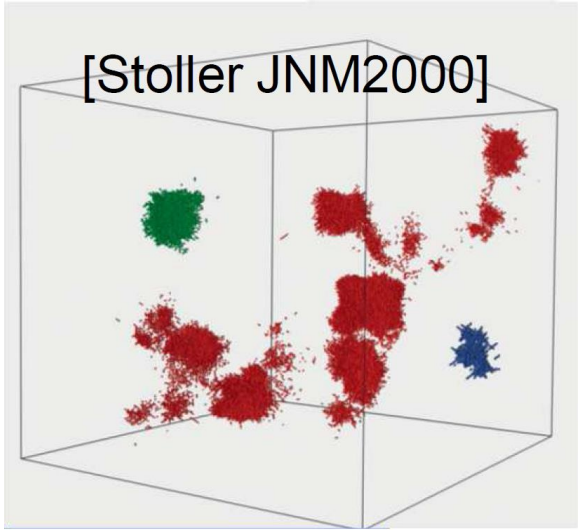
Less damage due to recombination

PKA kinetic energy

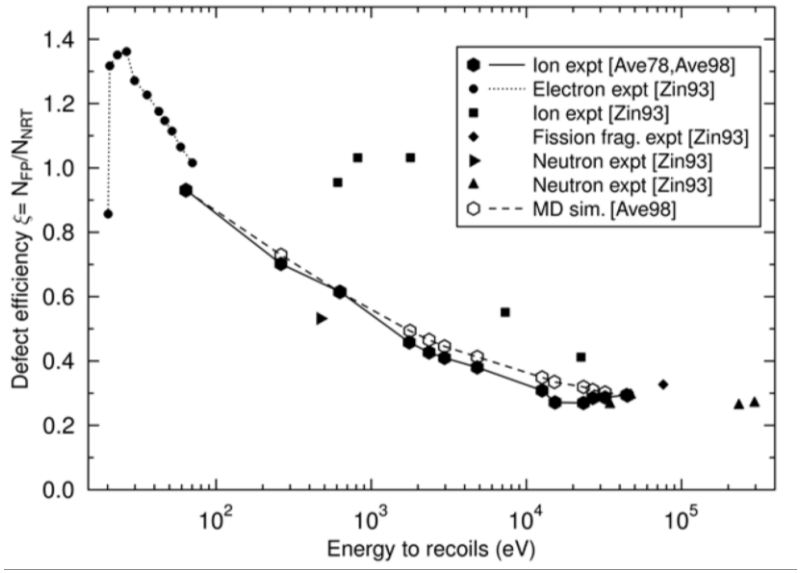
[1] Norgett, M.J., M.T. Robinson and I.M. Torrens (1975), "A proposed method of calculating displacement dose rates", Nucl. Engr. and Design, 33(1):50-54.

Towards a realistic representation of primary damage

Damage produces during irradiation is significantly lower than the one predicted by NRT dpa.



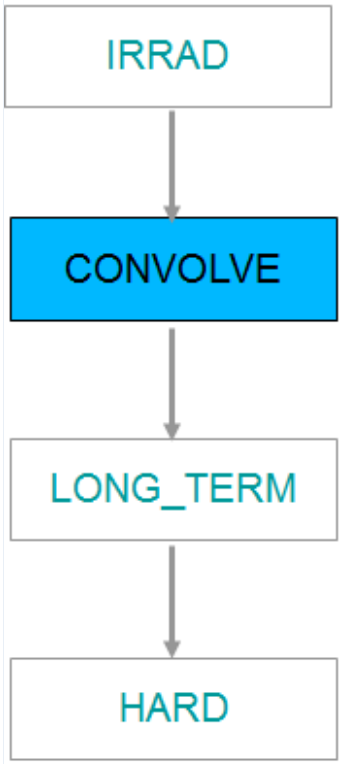
→ Molecular Dynamics calculation



Primary radiation damage in Materials, Report OECD/NEA (2015)

- 200 fs: creation of large amount of damage corresponding to NRT dpa.
- Few ps: Heat spike creating a liquid-like region of high kinetic energy followed by recrystallisation → athermal recombination fewer defect
- Several s: cascade annealing perform with Kinetic Monte Carlo to account for thermal recombination of defects: cascade escape.

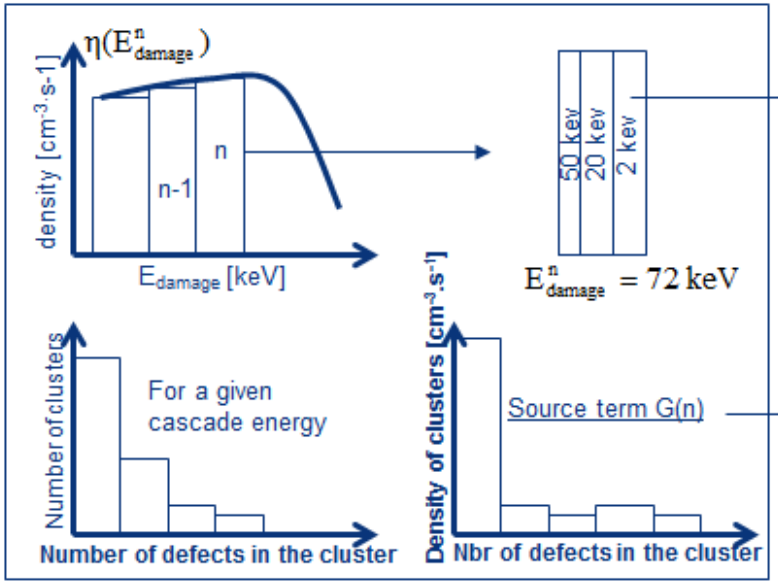
The Convolve module



- PKA-spectrum → damage energies spectrum : Lindhard model for electronic losses

$E_{dam} = E_{PKA} \cdot \xi$,
$\xi = f(A_1, A_2, Z_1, Z_2)$, 1: PKA atom, 2: target atom
semi-classical model whose results are given in the documentation

- cascade database → 4 choices for "cascade_origin " RPV-1, RPV-2, BCA, SCK_AMS
  → $E_{cascade} \in$ {5 keV, 10, 20, 30, 40, 50, 100 keV} for RPV-2 DB
  → T ∈ {333 K, 423 K, 573 K}, but weak influence for α-iron

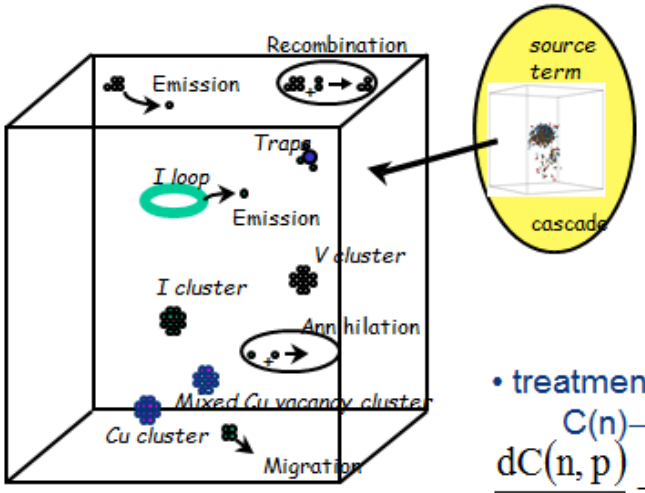


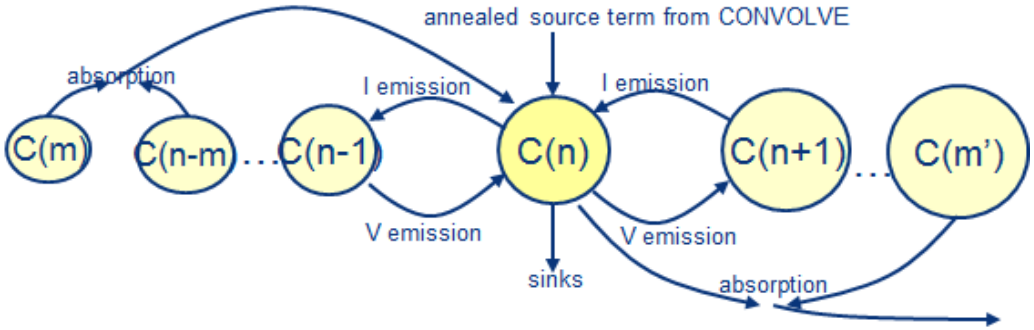
→ the remaining 2 keV are assumed to produce Frenkel pairs only, according to the Bacon-Calder model :
$N_{FP} = \alpha E^{\beta}$

→ the "MD"-damage rate G_{MD} is obtained by $G_{MD} = \sum_{n>0} n \cdot G(n)$

→ comparison with G_{NRT}
calculate the ratio
calculate dpa cross-section

Rate Theory and CRESCENDO Sub module





- treatment of mixed cluster in MFVISC and CRESCENDO :
  C(n)→C(n, p) , p: nbr of solute atoms in the cluster

$$\frac{dC(n,p)}{dt} = G_n - B((n,p),(\pm 1,0/1)\cdot C(n,p) + B((n\pm 1,p),(\pm 1,0/1))\cdot C(n\pm 1,p) + \sum_{all(m,q)} A((n-m,p-q),(m,q))\cdot C(n-m,p-q)\cdot C(m,q) - \sum_{all(m,q)} A((n,p),(m,q))\cdot C(n,p)\cdot C(m,q) - sinks$$

- solute species can only be mobile if associated to a single defect → (1,1) and (-1,1)
- consistently, only single defect or single defect-solute pairs can be emitted

Rate Theory and CRESCENDO Sub module

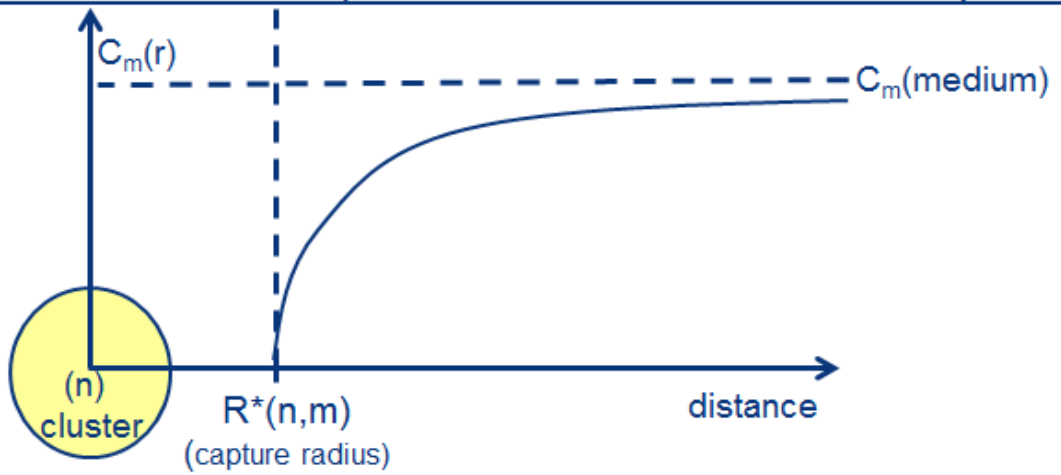
IRRAD

CONVOLVE

LONG_TERM

HARD

calculation of the absorption coefficient B of an m-cluster by an n-cluster:



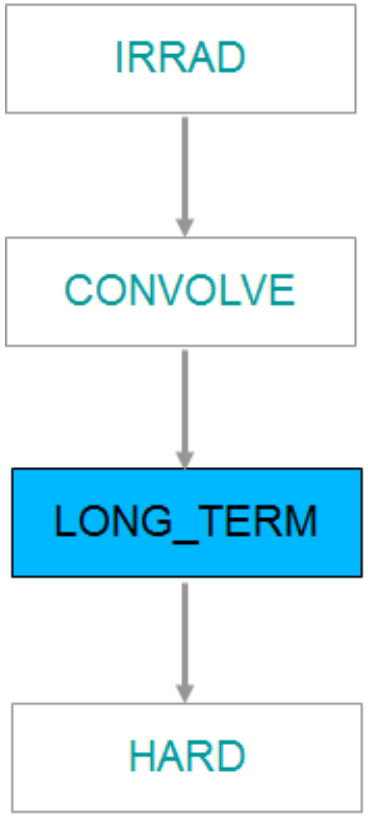
solving diffusion eq. in the stationnary state

m-clusters current: $\vec{j} = -D \cdot \mathrm{grad}(C_m)$

m-clusters flux at the capture radius R*: $\varphi = \int_{S(r^*)} \vec{j} \cdot d\vec{S} = 4\pi R^* D_m C_m(\mathrm{medium})$

- absorption coefficient depends on the capture radius and the diffusion coefficient
  $B(n,m) = 4\pi R^* D_m$
- a common model for capture radius is $R^*(n,m) = Z_6[R(n)+R(m)+R_0]$,
- Arrhenius' law $D = D_0 \exp\left(-\frac{E_m}{kT}\right)$ ⇒ need of migration energies
- emission coefficient are Boltzmannian : $A(n,m) = \rho\, B(n,m) \exp(-E_B(n-m, m)/kT)$
  ⇒ need of binding energies

Rate Theory and CRESCENDO Sub module

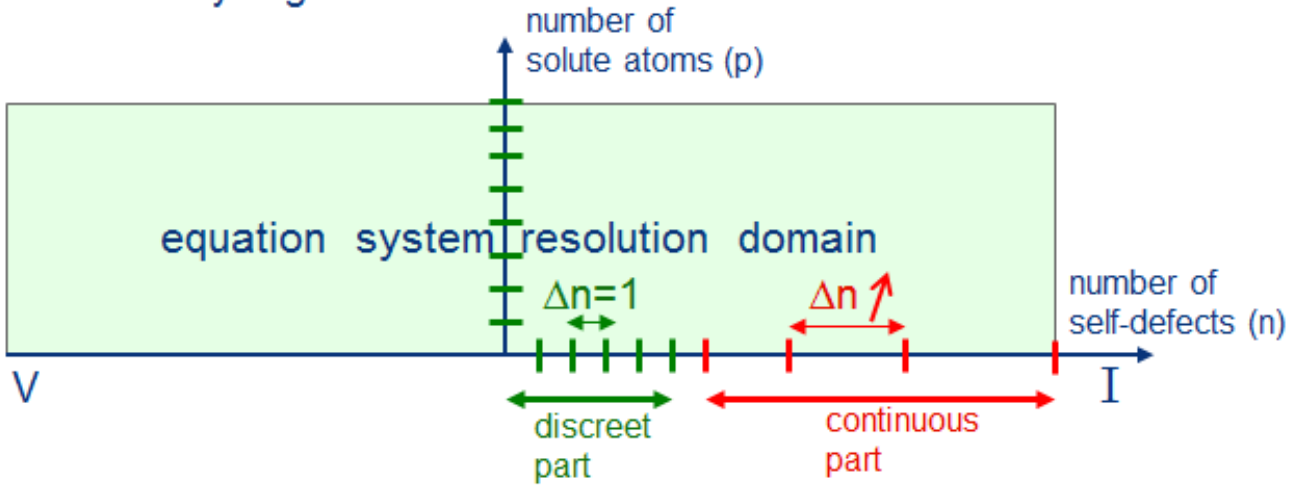


- for binding energies (needed for emission rates) of clusters it uses *ab initio* results for small clusters and extrapolation for large ones
- size of resolution domain for a mixed cluster calculation =

2 x max_nbr_of_self_defects_in_clusters x max_nbr_of_solute_atoms_in_clusters

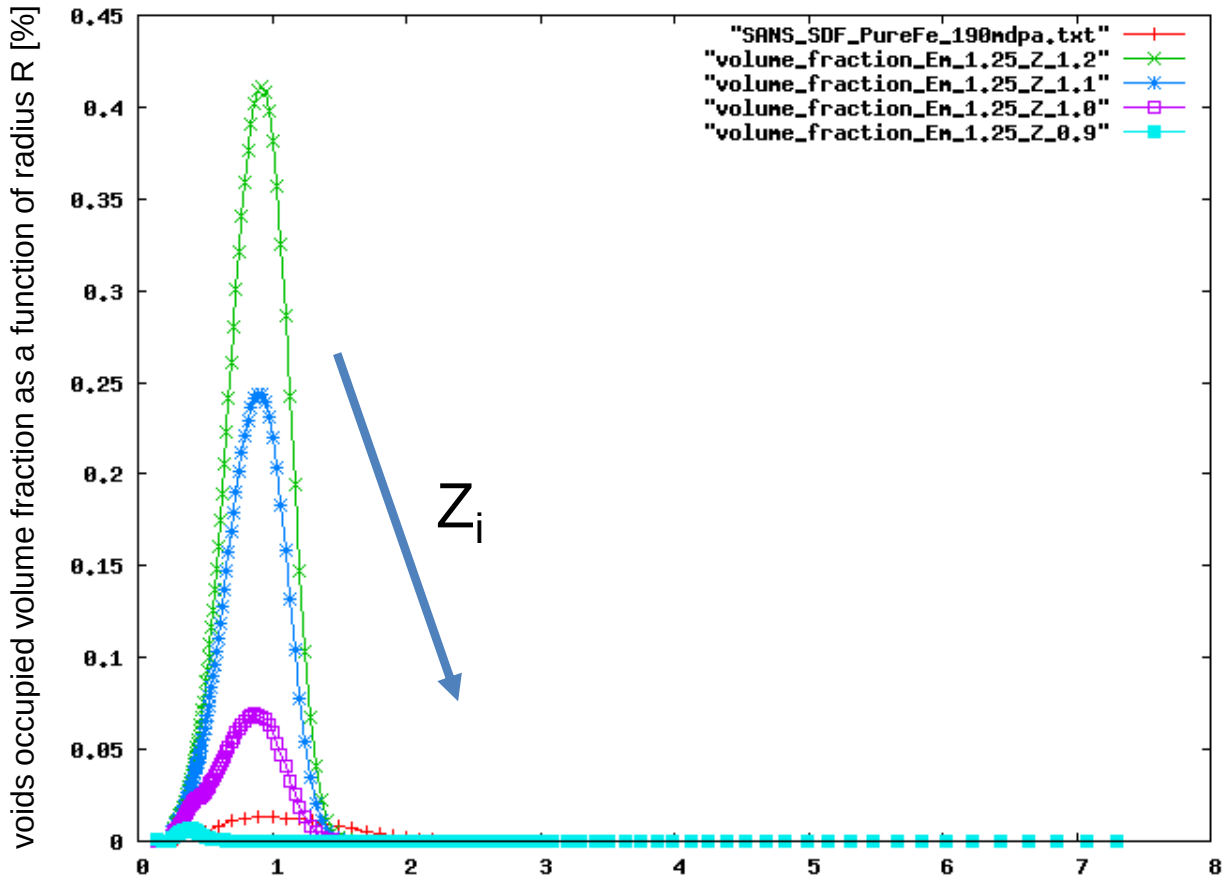
→ far too large, if we want to treat some hundreds of thousands of self-defects mixed with some hundreds of solutes

→ uses of Fokker-Planck formalism to discrete and continuous solving of the equation for very large clusters



→ some parameters related to this transformation and to the resolution numerical scheme can ne changed by (very) expert users

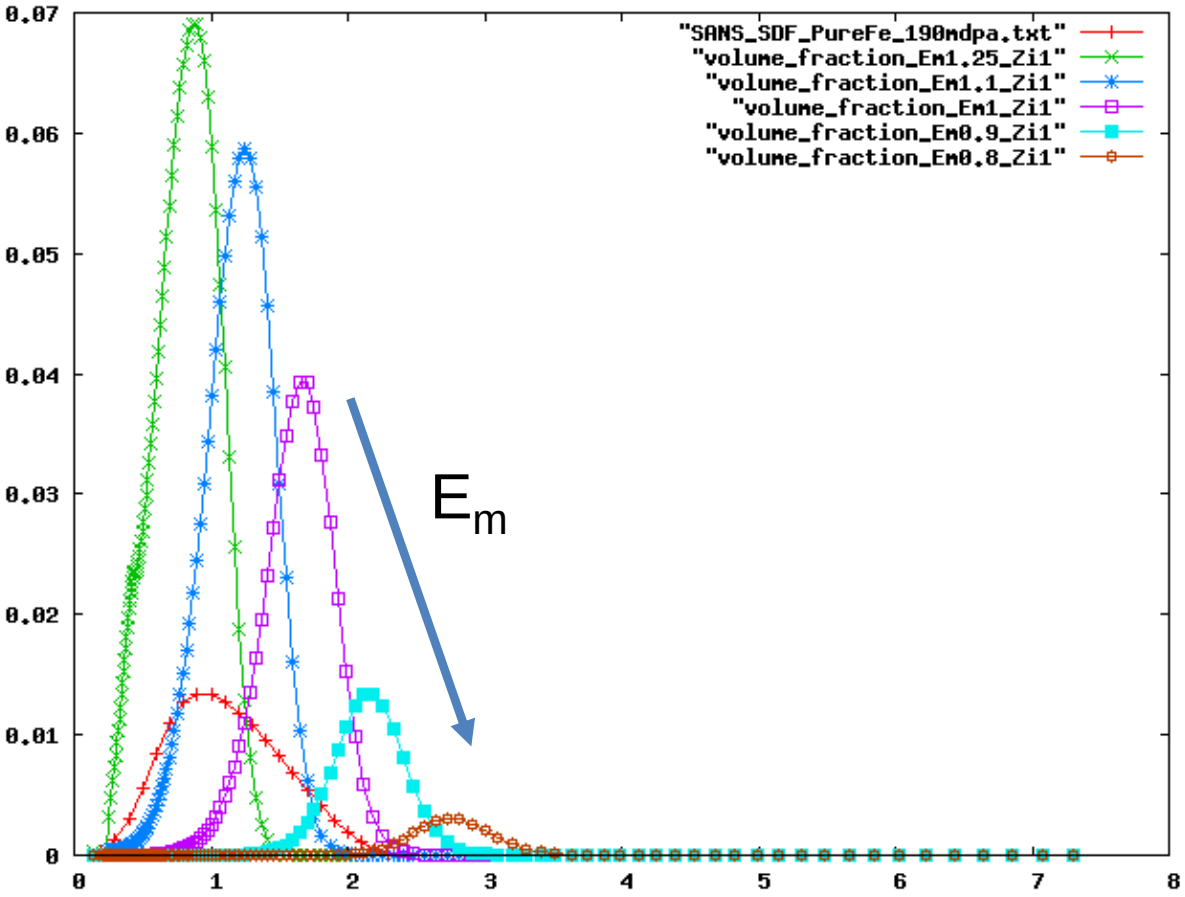
Tuning Rate Theory effective parameters



Behaviour for Zi ↓ :

Zi ↓ ⇒ abs of mI by I-clust ↓ ⇒ Ci ↑ ⇒ abs of mV by I-clust ↑ ⇒ C(nV) ↓for all n (4πRDCiC(nV) ↑)

Tuning Rate Theory effective parameters



Behaviour for $E_m \downarrow$:

$E_m \downarrow \Rightarrow$ abs of V by V-clust $\downarrow \Rightarrow$ n $\uparrow$ and C(nV) $\downarrow$

Obtain Critically Resolved Shear Stress (CRSS) from microstructural data

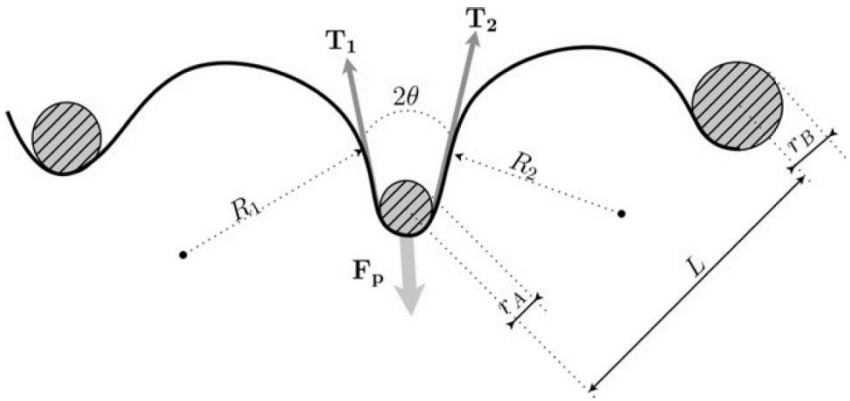
Orowan Bacon model for impenetrable obstacles accounting for dipole interaction between bending dislocation lines.

$$\tau_{OB} = \left(\frac{\ln D'/b}{\ln l/b}\right)^{3/2} \frac{\mu b}{l} \frac{\ln(l/b)}{2\pi},$$

D: diameter of obstacle.
C: concentration of obstacle.
l is defined as $1/\sqrt{(DC)}$

$$\tau_{total} = \sqrt{\sum \tau_{OB,i}^2}$$

i running over all interstitial and vacancy clusters



G. Adjanor, et al., Journal of Nuclear Materials,406, 175 (2010)

- all clusters are Orowan precipitates (with a self and mutual dipole interaction correction from the Bacon et al. model). Note that this assumption may lead to an overestimation of the pinning force in the case of copper precipitates and interstitial clusters and to an underestimation in the case of voids which seem to constitute the major source of hardening in typical irradiation conditions,
- the diameter of the clusters *D* is taken as spherical in all cases. This is actually the case for cavities, precipitates and heterogeneous precipitates, which are known to form atmospheres around cavities, but it is not the case for interstitial loops. Nevertheless, this approximation may not be too severe as their number density is small compared to that of cavities, and, again, because loops are also much weaker obstacles than cavities.

G. Adjanor, et al., Journal of Nuclear Materials,406, 175 (2010)