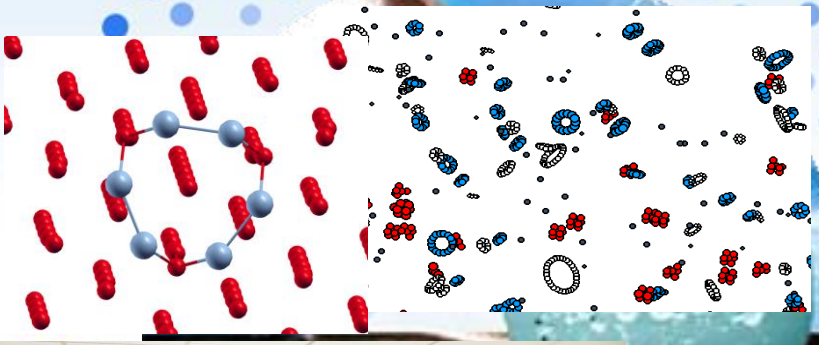
Forum Ter@tec, Ecole Polytechnique, Juillet 2014

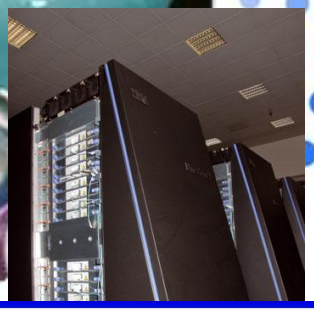
Atelier : Simulation haute performance des matériaux: nouveaux matériaux, usage et tenue en fonction

PERFORM 60

FP7 Project

HPC et modélisation multi-échelle des matériaux de structure des centrales nucléaires





C. Domain[1], G. Adjanor[1], G. Monnet[1]

1 EDF R&D

Dpt Matériaux & Mécanique des Composants

Les Renardieres, Moret sur Loing, France

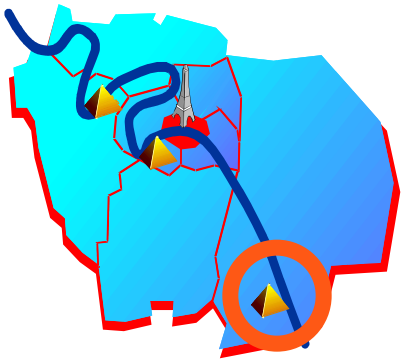
Laboratoire Commun

cnrs EM²VM EDF

mai

EDF R&D

HPC et modélisation multi-échelle des matériaux de structure des centrales nucléaires



EDF R&D - département Matériaux et Mécanique des Composants

Laboratoire Commun:

EM2VM: Etude et Modélisation des Mécanismes de Vieillissement des Matériaux

EDF R&D (MMC)

GPM (Univ Rouen) [C. &P. Pareige, B. Radiguet, H. Zapolsky]

UMET (Univ Lille1) [A. Legris, C. Becquart, L. Thuinet]

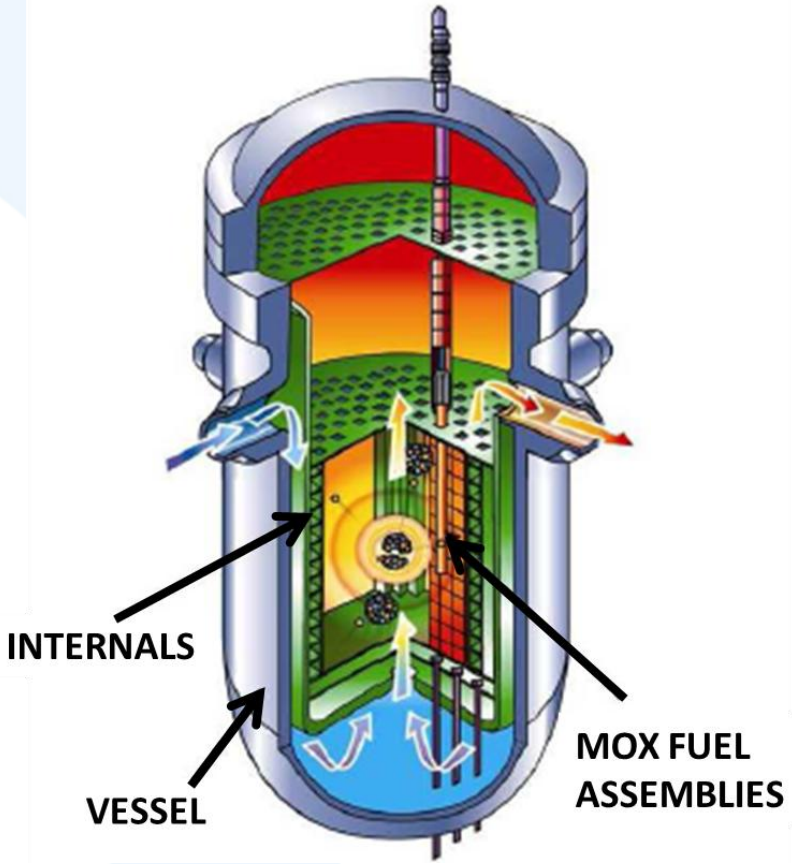
ATHOS Intel Xeon cluster with 18144 cores (353 TFlop/s)

113th @ June 2014 top500.org list

Zumbrota - BlueGene/Q (IBM) with 65536 cores (715 Tflop/s)

55th @ June 2014 top500.org list

Lifetime extension: Materials ageing prediction



- To improve quantitative predictions of ageing of irradiated structural materials in nuclear power plants in order to gain margins.
- Challenge: to predict the evolution of hundred of tons over more than 40 years based on physical phenomena occurring at the nanometer scale and picosecond times (10^{-12} s)
- Construction and improvement of multiscale modelling methods allowing to better take into account the material composition and radiation damage

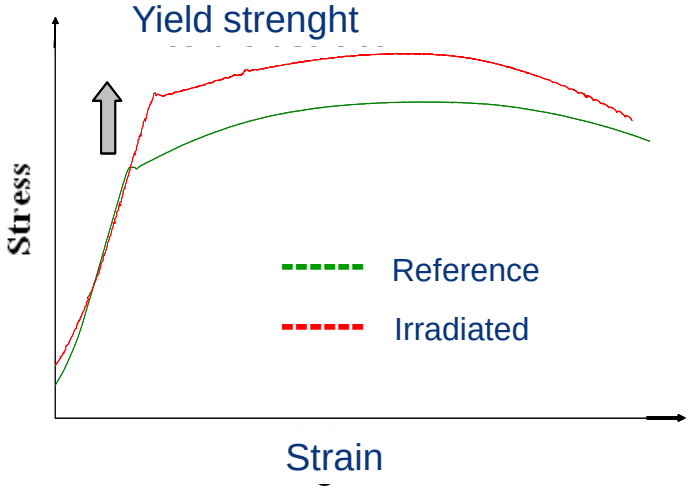
Laboratoire Commun
EM²VM

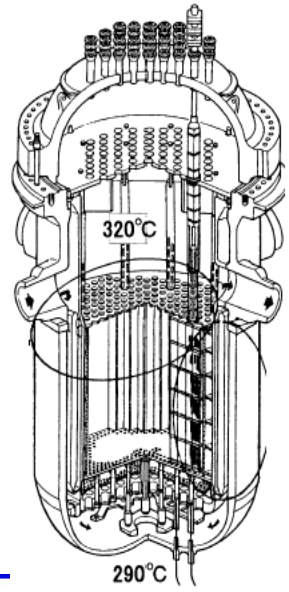
the materials ageing institute

EDF R&D

Reactor Pressure Vessel
Alloy composition

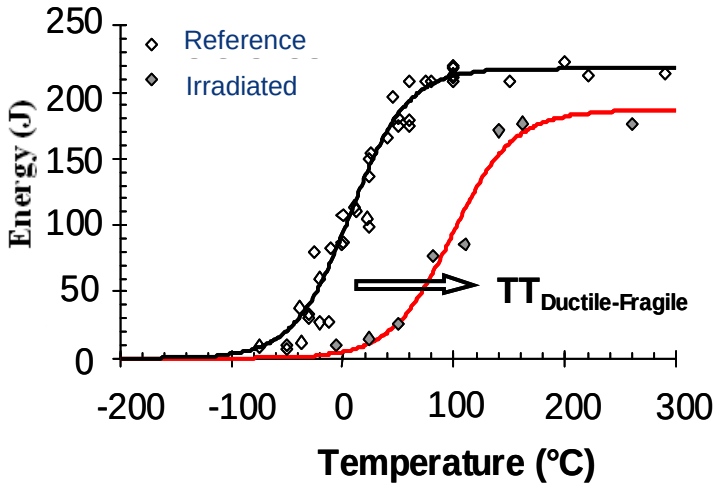
- Low Alloy Steel
- Max. End of Life Dose: <0.1 dpa
- Max. Temperature: 290 °C
- Hardening
- Degradation of Fracture Toughness





RPV steel (%w)

C	0.036
Co	0.027
P	0.005
Si	0.44
Cr	0.12
Mo	0.10
Mn	0.72
Ni	0.65
Cu	0.051

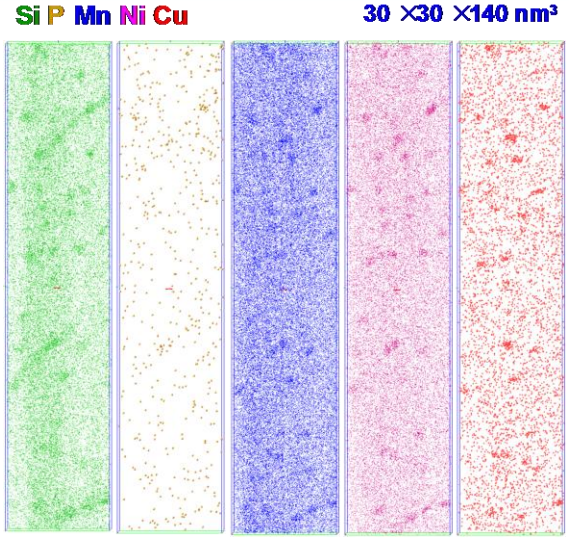


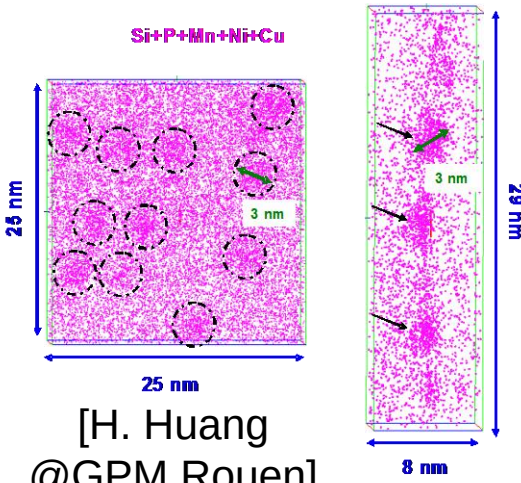
Microstructure evolution of Fe alloys under irradiation

RPV Fe ferritic alloys

- microstructure modelling
  short & long term evolution

- plasticity

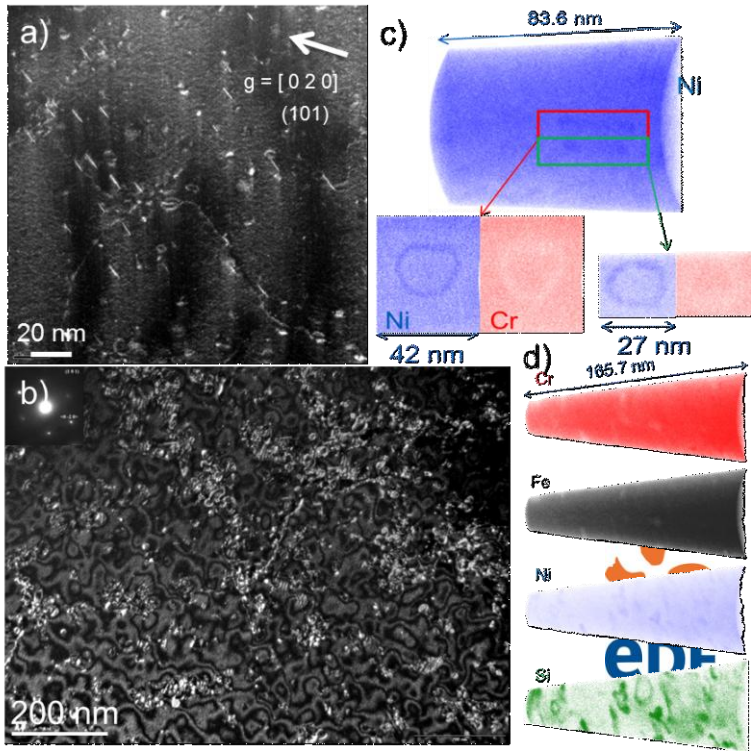




[H. Huang @GPM Rouen]

Austenitic alloys

- FeNiCr AKMC RIS modelling



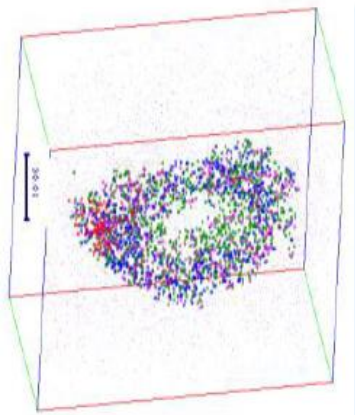
[A. Volgin @GPM Rouen]

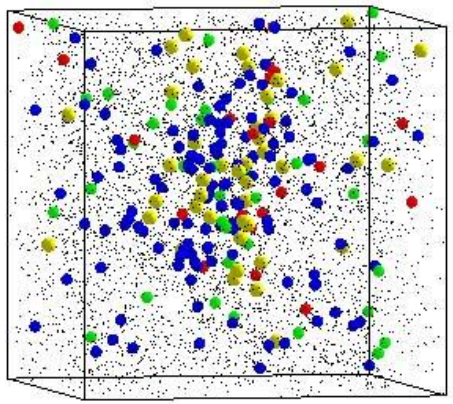
Radiation damage

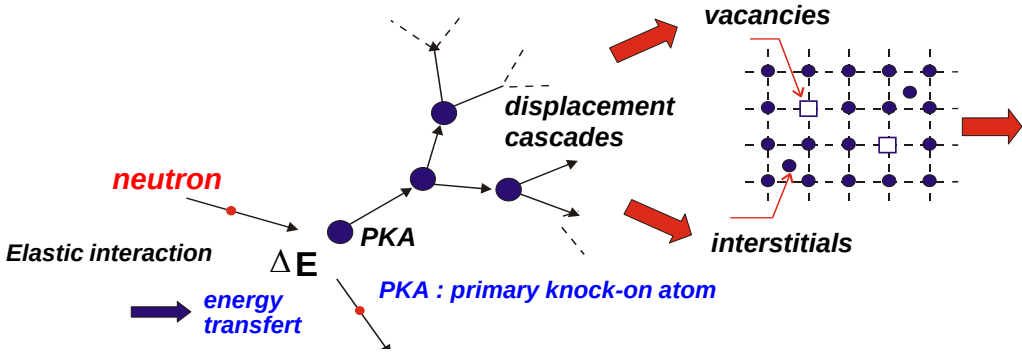
Material:
Fe
+ alloying elements: Cu, Ni, Mn, Si, …
+ carbon, nitrogen

+ dislocations

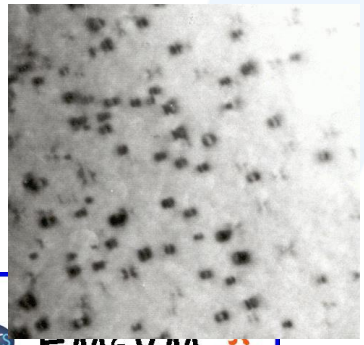
Irradiation:
Electron:
Frenkel pairs
Ion and neutron:
displacement cascades (10 - 100 keV)
vacancies and interstitials:
isolated and in clusters



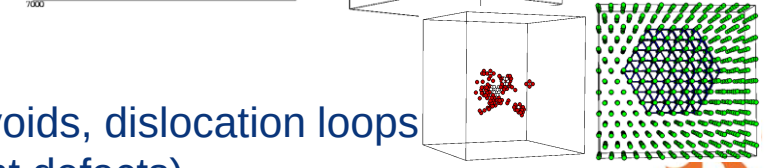




TAP, Pareige, U. Rouen

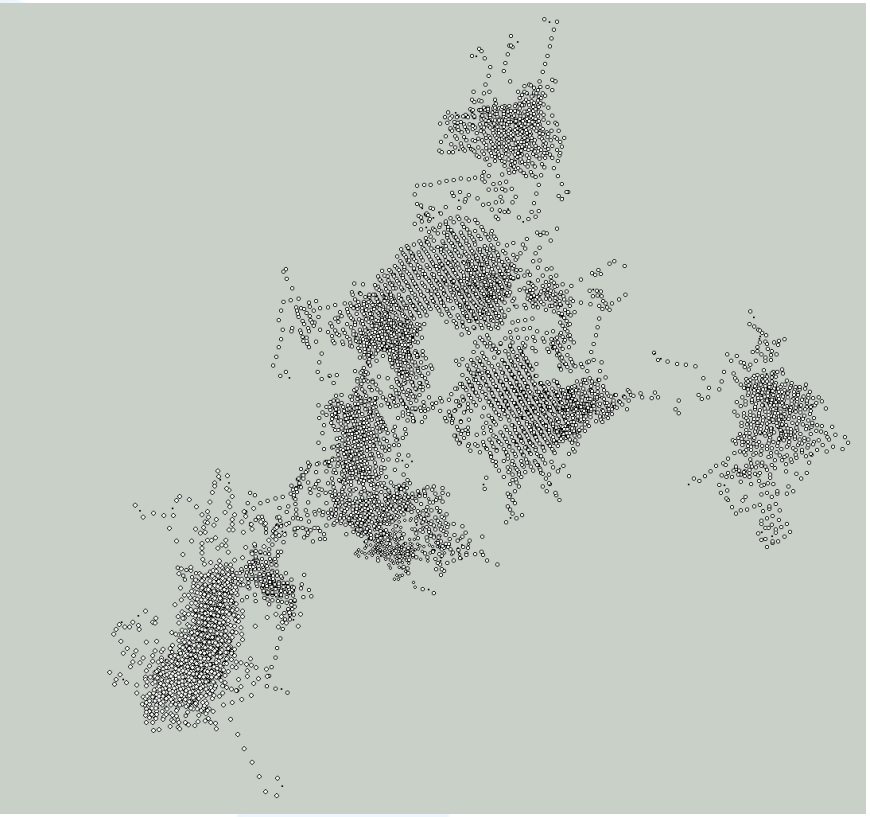


TEM, Barbu, CEA

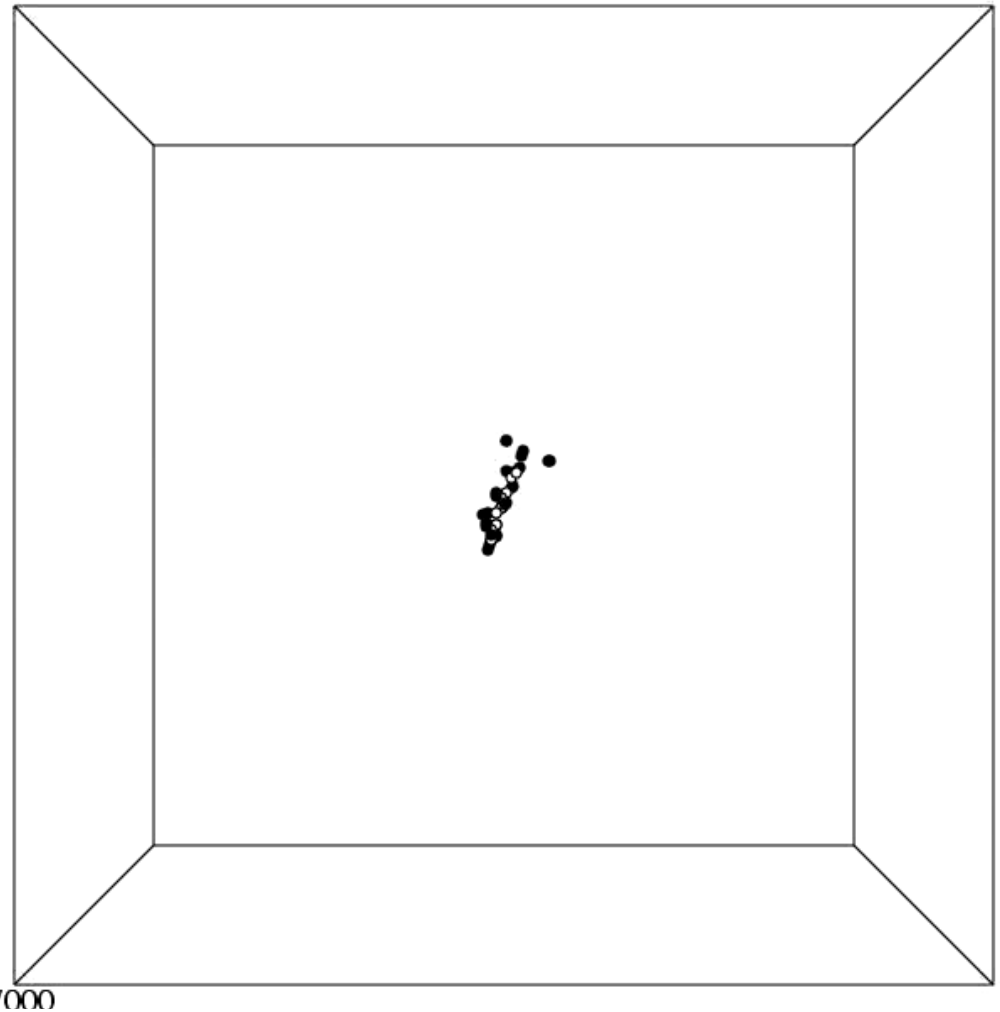


Microstructure evolution:
point defect clusters: nanovoids, dislocation loops
solute clusters (# or \# point defects)

Displacement cascades (Classical Molecular Dynamics)



30 keV in fcc Ni



$$\frac{d}{dt}(m_i \boldsymbol{v}_i) = \boldsymbol{F}_i = -\nabla V \qquad \frac{d\boldsymbol{r}_i}{dt} = \boldsymbol{v}_i$$

$$U = \sum_{ij} V(r_{ij}) + F_i[\sum_{j} \phi(r_{ij})]$$

20 keV in Fe
box $(40a - 80)^3$
~few 1.000.000 atoms
10 - 20 ps

DYMOKA EDF code

Relevant phenomena and appropriate computational methods for microstructure evolution

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

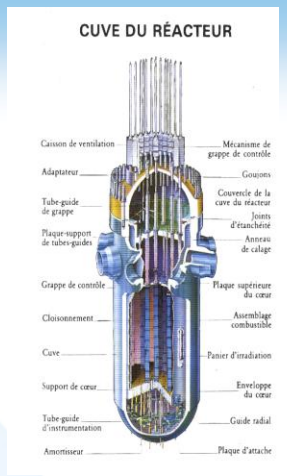
10^{-7} m

10^{-6} m

$> 10^{-3}$ m

m³

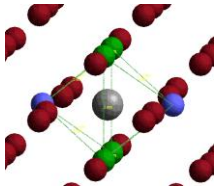
40 years

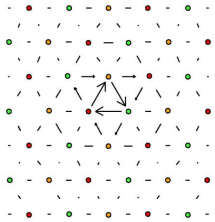


1nm³

0 - ps

ab initio

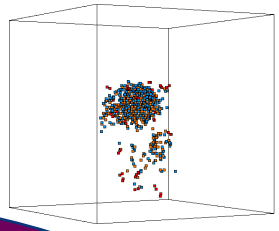


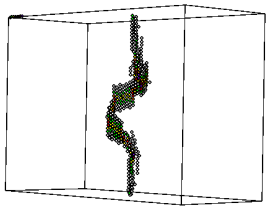


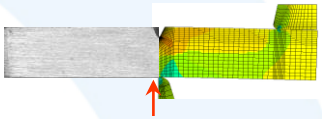
(10-30nm)³

ns

Molecular dynamics

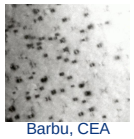




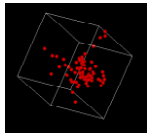


Finite elements

Multi-scale modelling



Barbu, CEA



Pareige, U. Rouen

+ experimental validation

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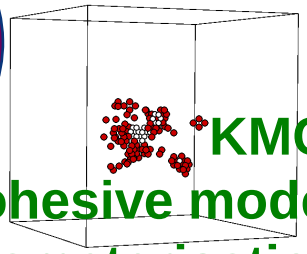
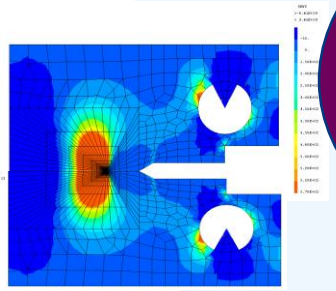
s - h

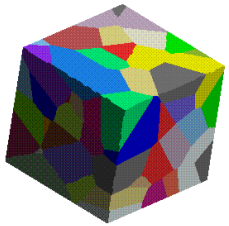


KMC cohesive model & parameterisation

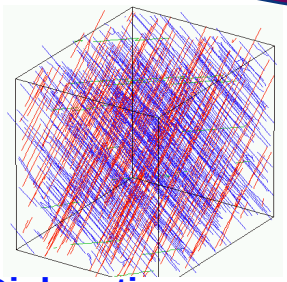
cm³



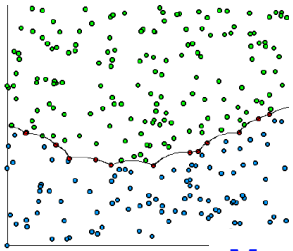
Micro-macro



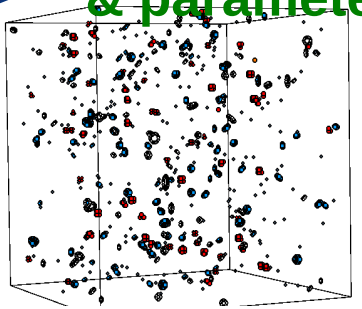
µm³



Dislocation dynamics



Mesoscopic



(30-100nm)³

h-year

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EM²VM

EDF R&D

Simulation tools

Prog. de surveillance

Positon annhilation

SANS

Microscopy and chemical analysis

Time

h-year

s - h

ns

0 - ps

Tomographic atom probe

Finite Elements

Mesoscopic
(grain, set of grains)

Dislocation Dynamics

Kinetic Monte Carlo (diffusion) [Rate theory/cluster dynamics]
(cf. T Jourdan)

Classical Molecular Dynamics
(atomic forces derived from empirical potentials)

Elementary Mecanisms

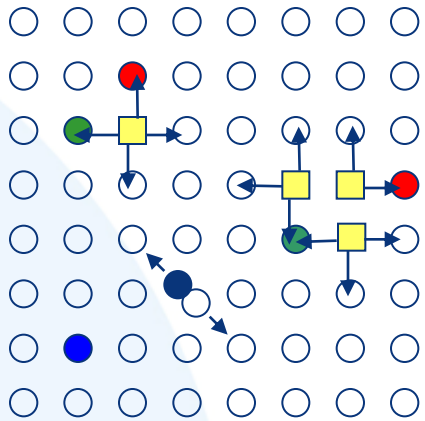
ab initio (forces and energies determined from the electronic structure -- Density Functional Theory (DFT))

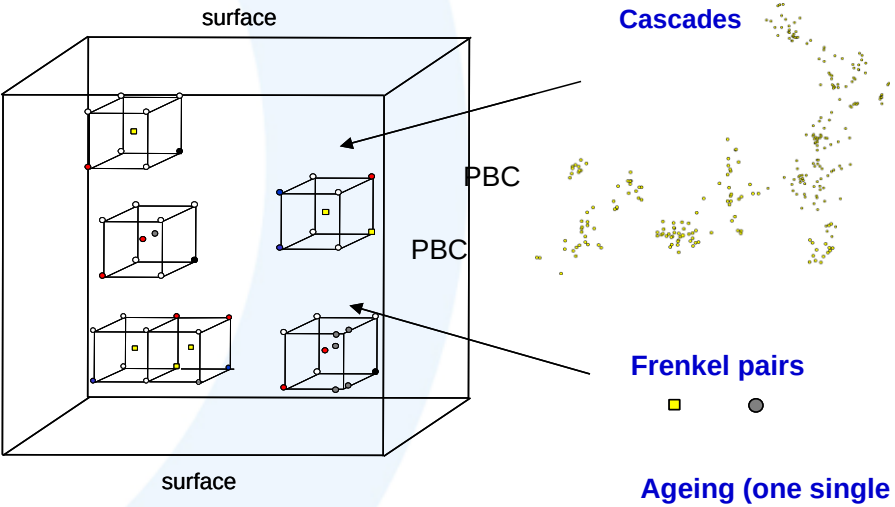
System size

$1nm^3$ $(10\text{-}30nm)^3$ $(30\text{-}100nm)^3$ μm^3 cm^3

Medium / long term microstructure evolution modelling
Kinetic Monte Carlo (KMC) simulation of irradiation

Atomic KMC





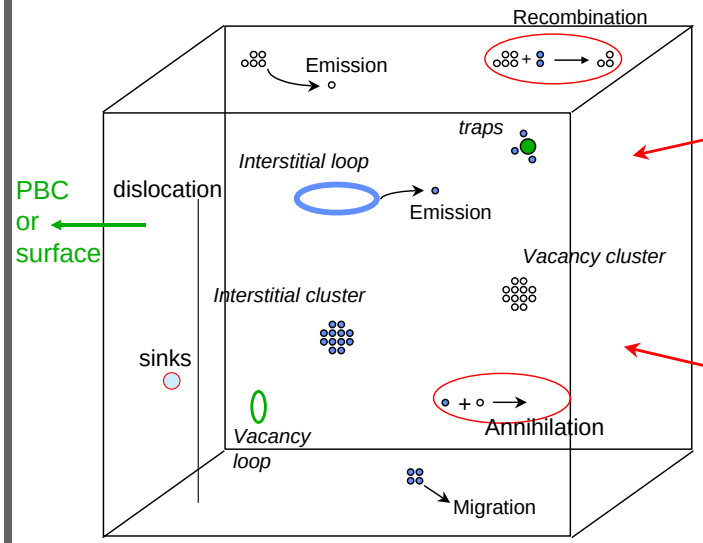
Cascades

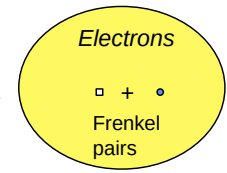
Frenkel pairs

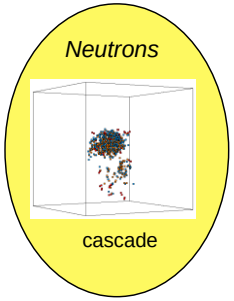
Ageing (one single vacancy)

$$\Gamma_X = \nu_X \exp\left(-\frac{Ea}{kT}\right)$$

Object KMC







Box size ≈ 30 - 100 nm
V ≈ 10^{-4} µm^3
t ≈ h to yr (T, G dependent)

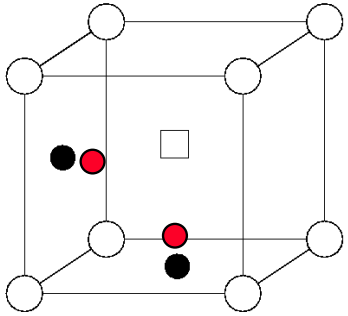
LAKIMOCA EDF code

[JNM 335 (2004) 121–145]

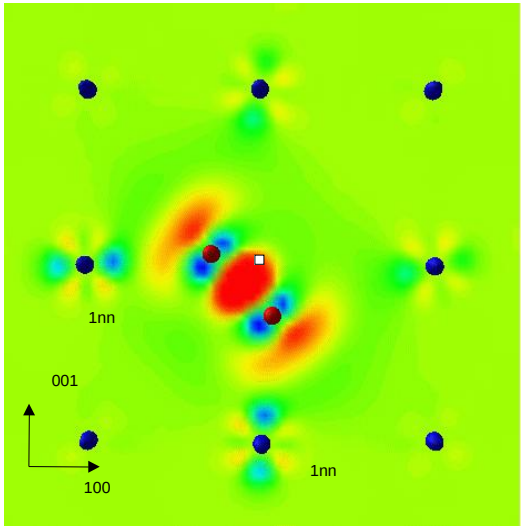
Density Functional Theory: point defect & point defect cluster properties (stability & mobility)

Fe-C

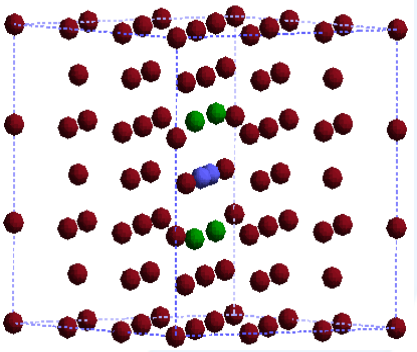
Strong Vacancy-C2 complex

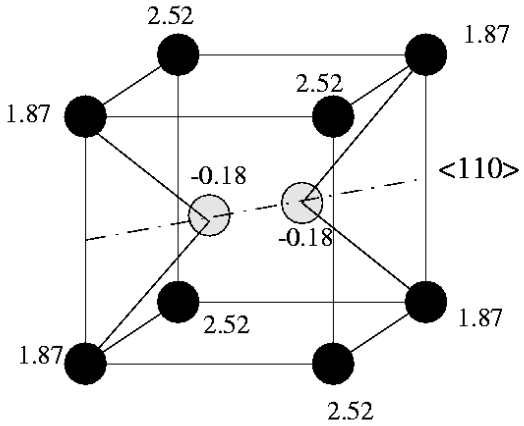


Phys. Rev. B 69 (2004) 144112

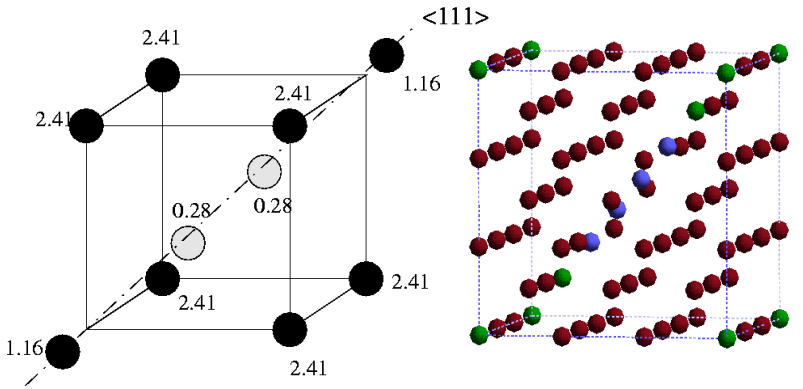


Fe: stable interstitial configuration





Phys. Rev. B 65 (2002) 024103



Local magnetic moment (μB)

VASP code

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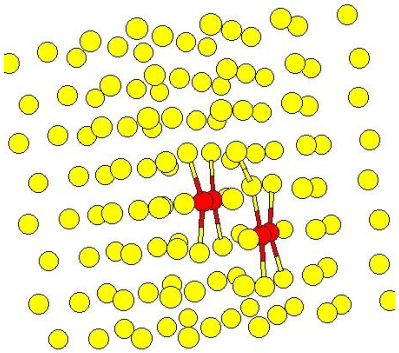
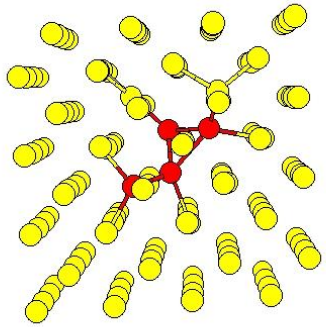
Nucl. Inst. Meth. Phys. Res. B: 228 (2005) 137-141

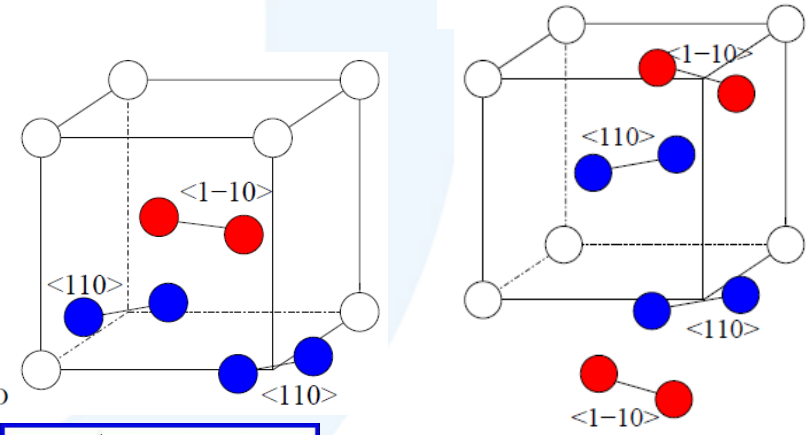
Density Functional Theory: point defect & point defect cluster properties (stability & mobility)

Fe: from interstitial clusters to interstitial loops

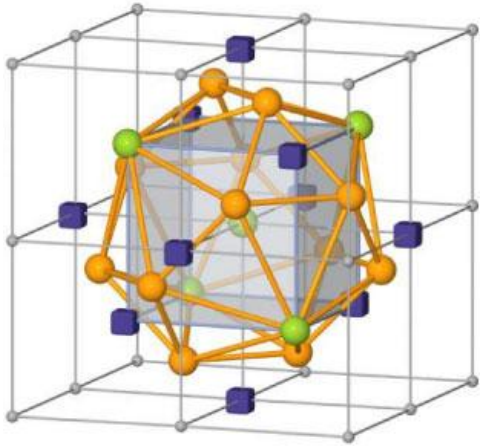
I2 - I4 clusters





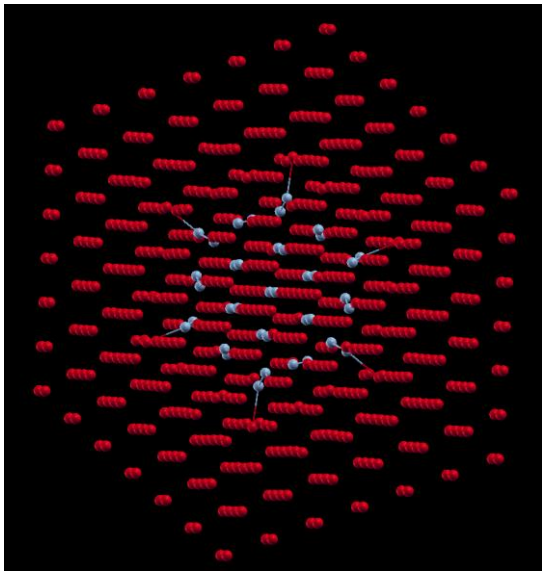


C15 clusters



[Marinica et al PRL 2012]

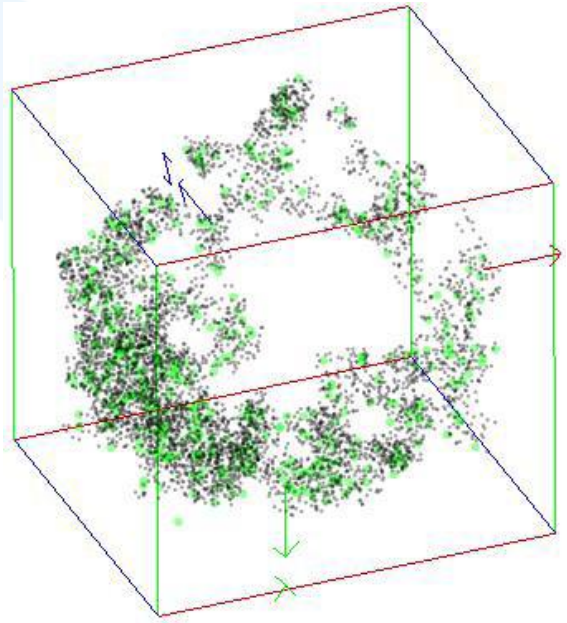
<111> loops

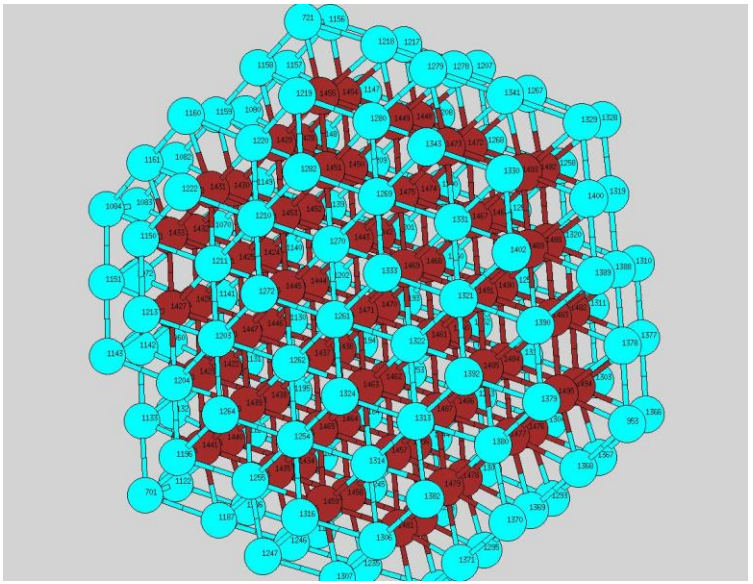


686+19 Fe atoms
PAW GGA
400 eV - 1 kpoints

VASP code

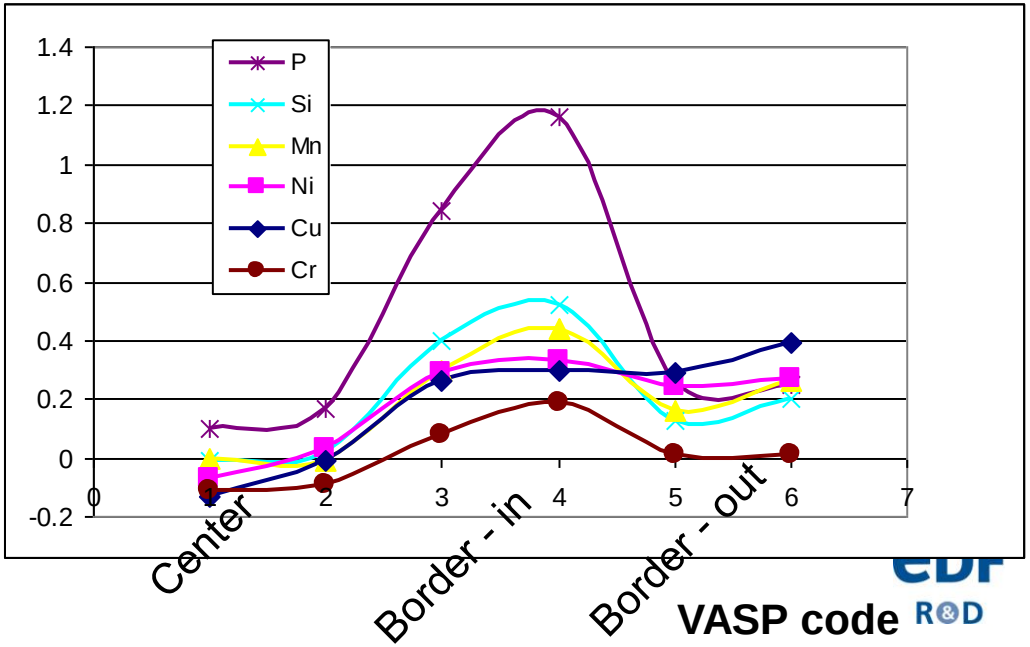
Density Functional Theory: Solute segregation on interstitial loops





1500 atoms Fe
bcc - magnetism

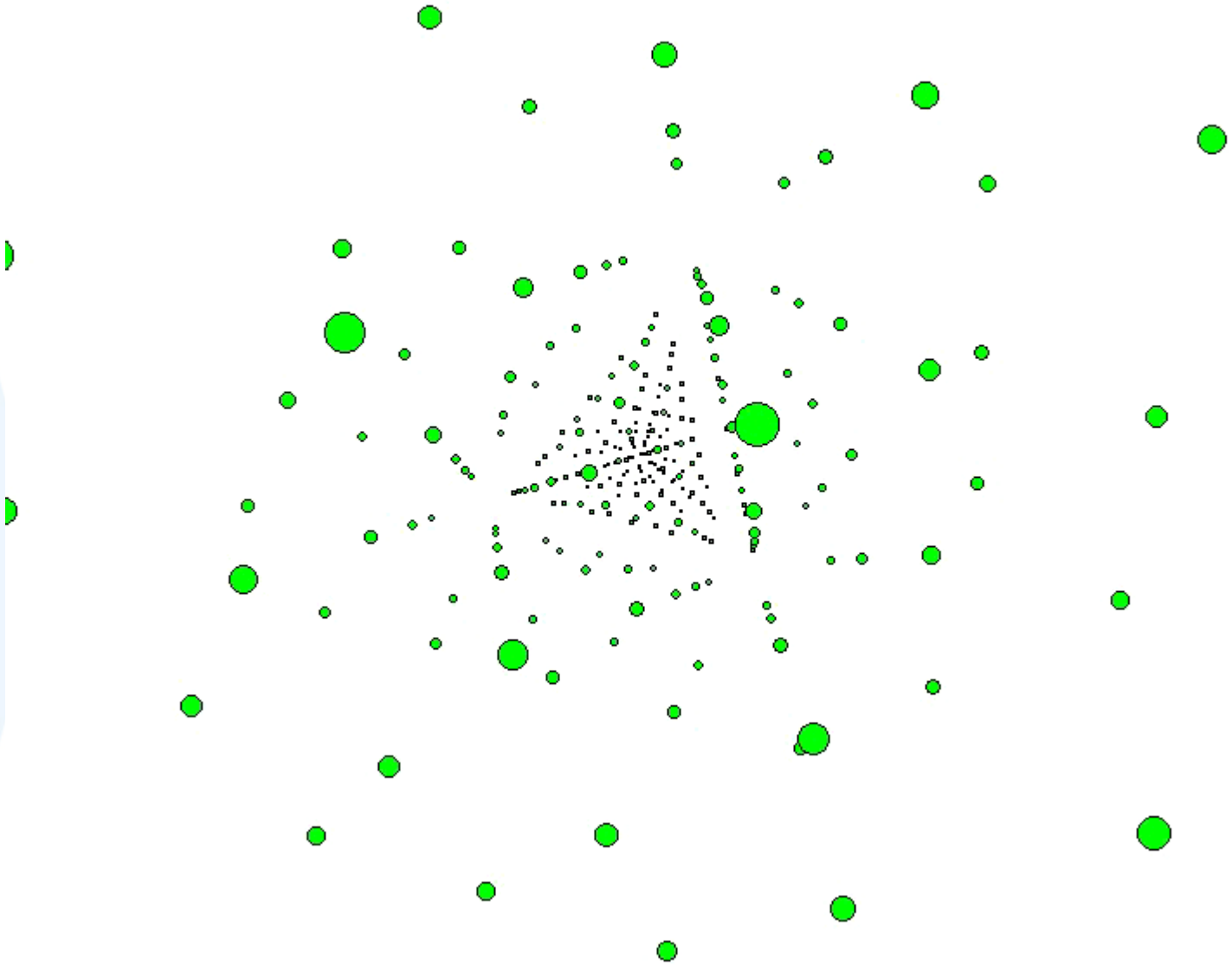
Solute segreg on loop
Exp. Atom probe
[GPM Rouen]



VASP code

Density Functional Theory: Dynamic simulation of defect creation

- DFT simulation of 40 eV knock-on in <110> direction
- BO-DFT
- Green: Fe
- White: Vacancy



AKMC irradiation simulation conditions

For electron irradiation:

Frenkel Pair (FP) flux

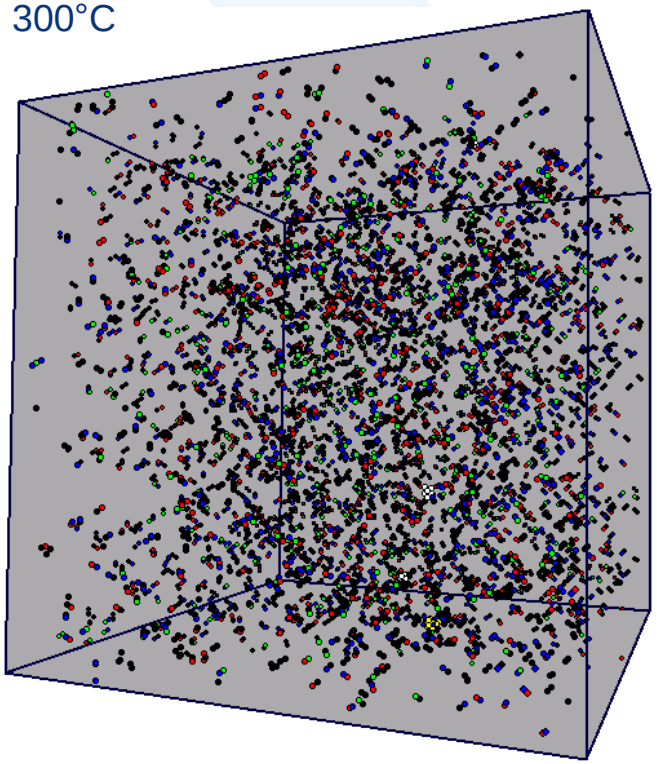
For neutron irradiation:

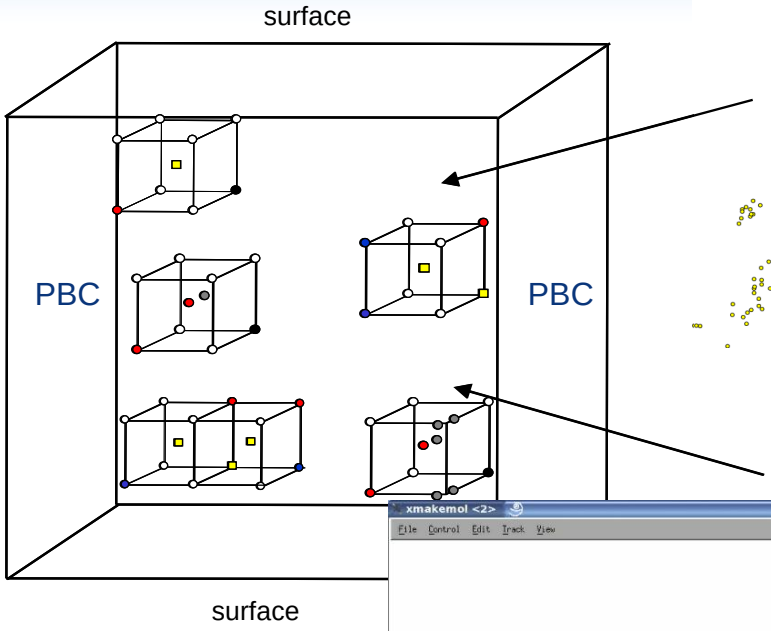
flux of cascades (and FP)

box: 10 x 10^6 atoms

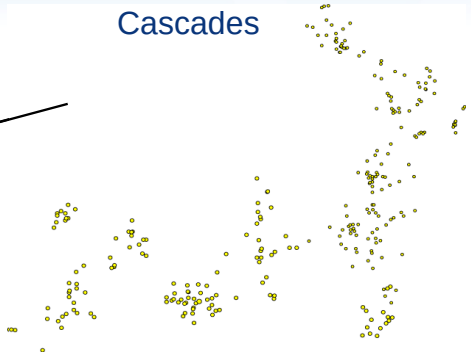
Fe-0.2Cu-0.53Ni-1.26Mn-0.63Si (at.%)

300°C

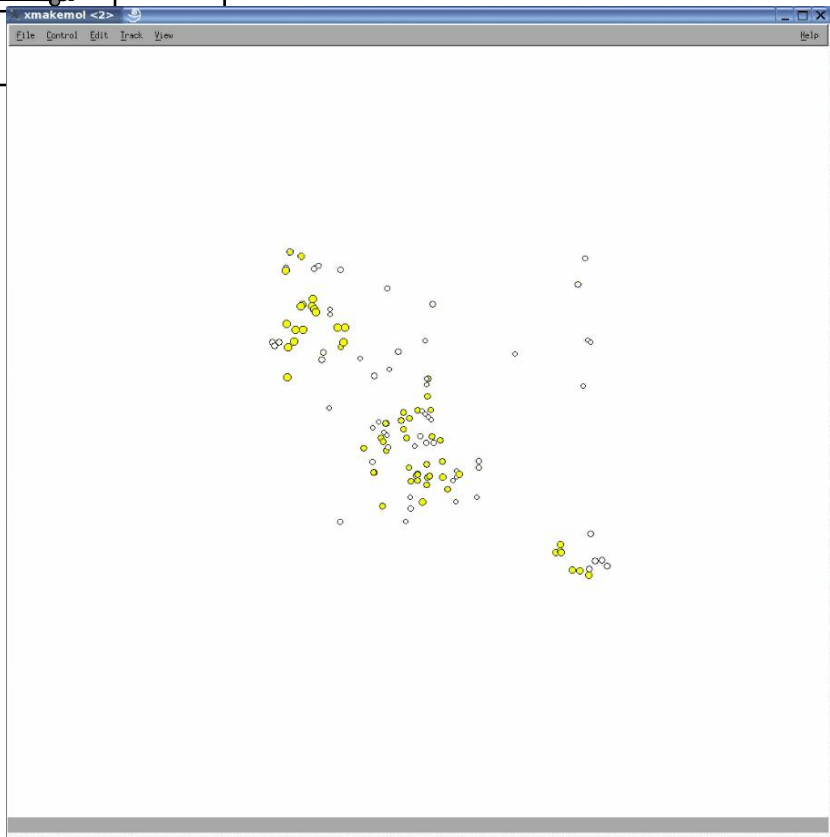




Cascades



Frenkel pairs



Fe-CuNiMnSi

Cu Ni

Si V

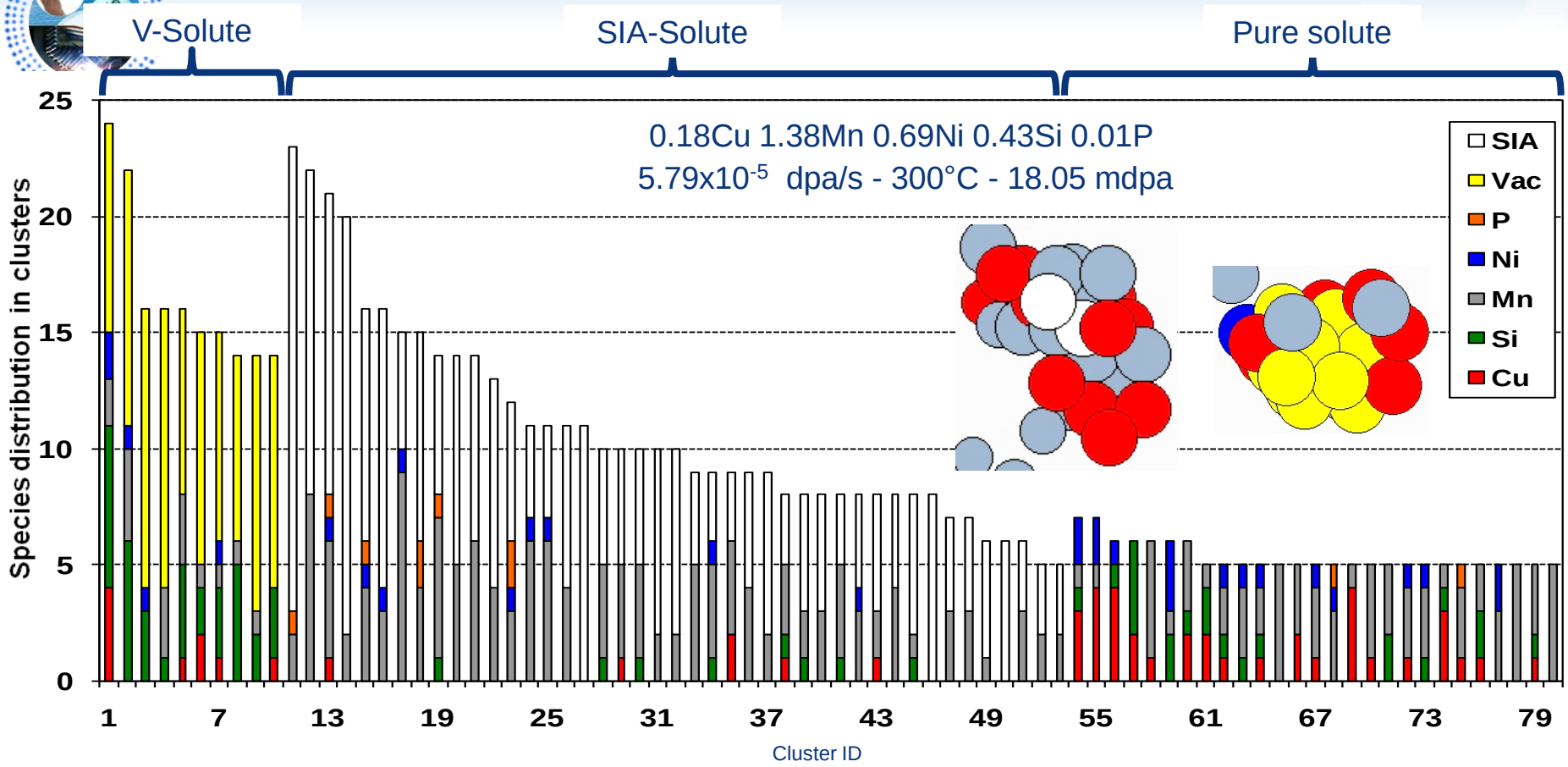
Mn SIA

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

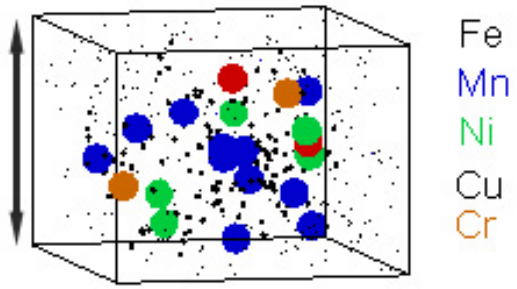
Dose: 1.3 10^{-3} dpa

X, Juillet 2014

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**

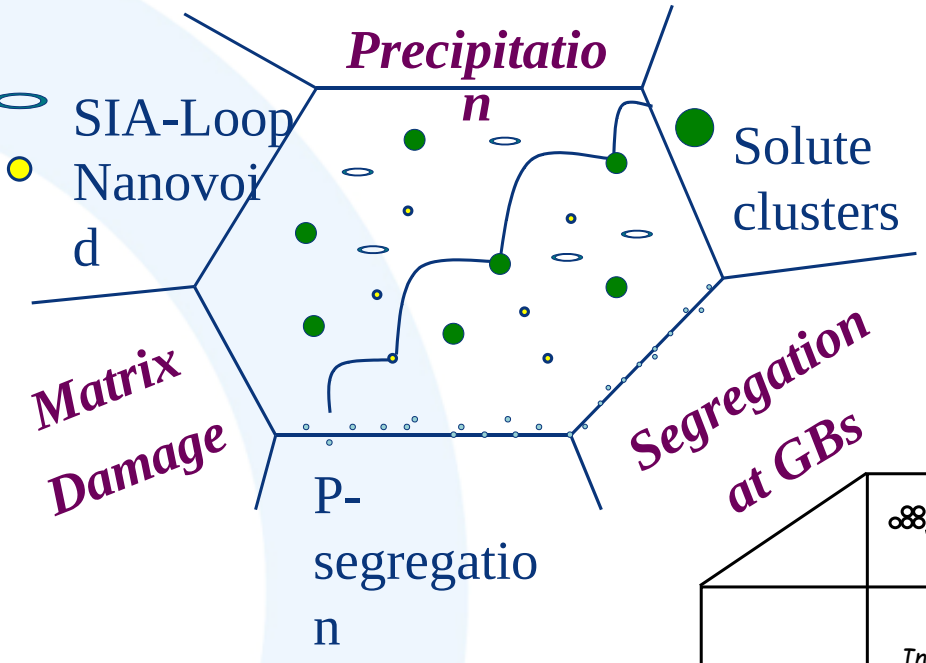


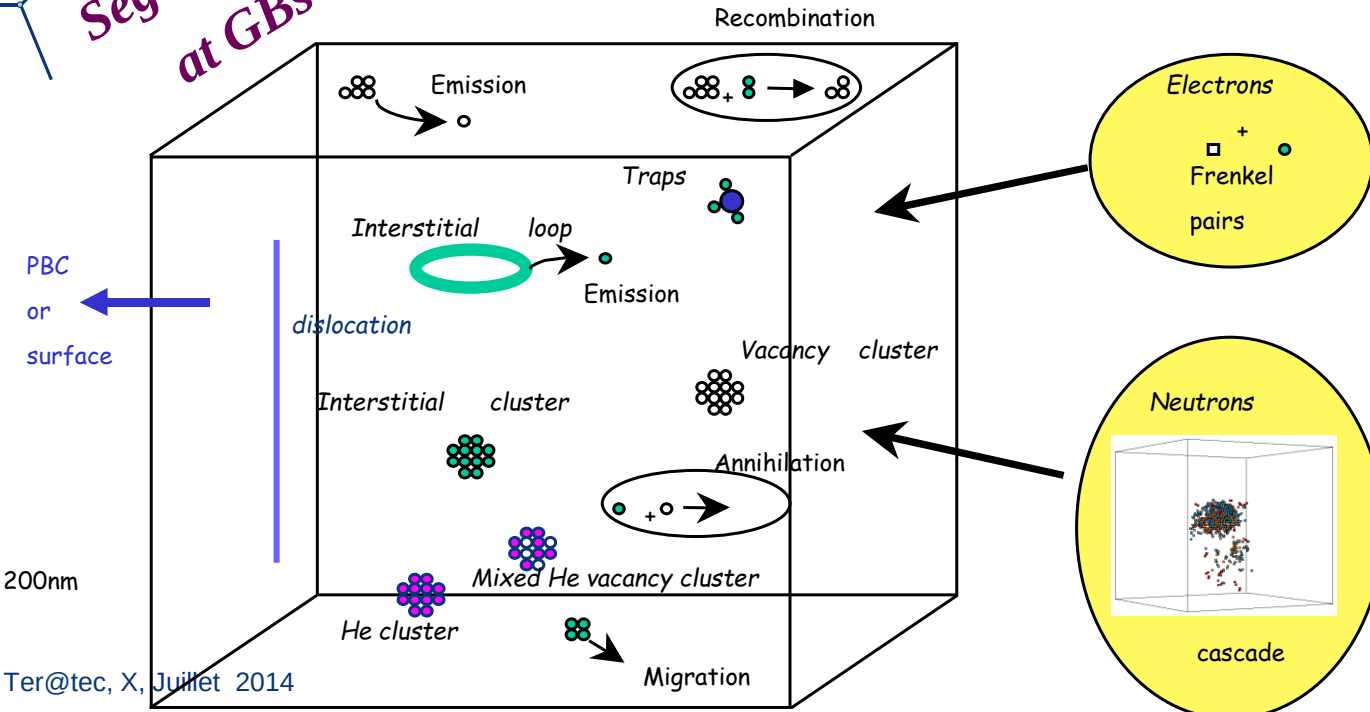
TAP [E. Meslin] [GPM Rouen]

Long term microstructure modelling Object Kinetic Monte Carlo

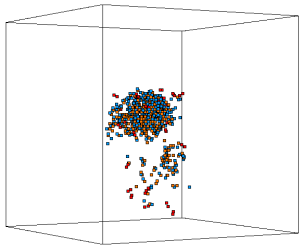
Objects:

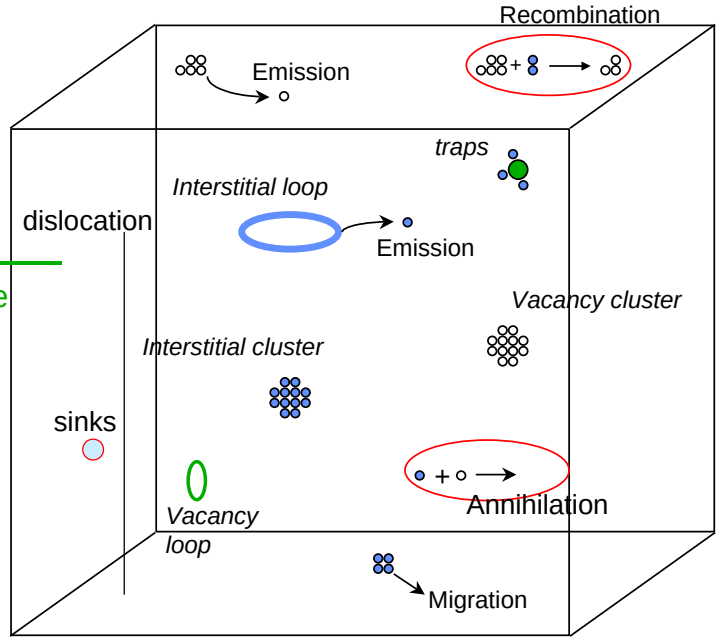
- vacancy
- self interstitial
- dilute solute (with vacancy interactions)
- sink (e.g. grain boundaries, …)
- trap (e.g. impurities, …)
- dislocation
- foreign interstitial atoms
  - He in austenitic alloys
  - C or N in ferritic or austenitic alloys

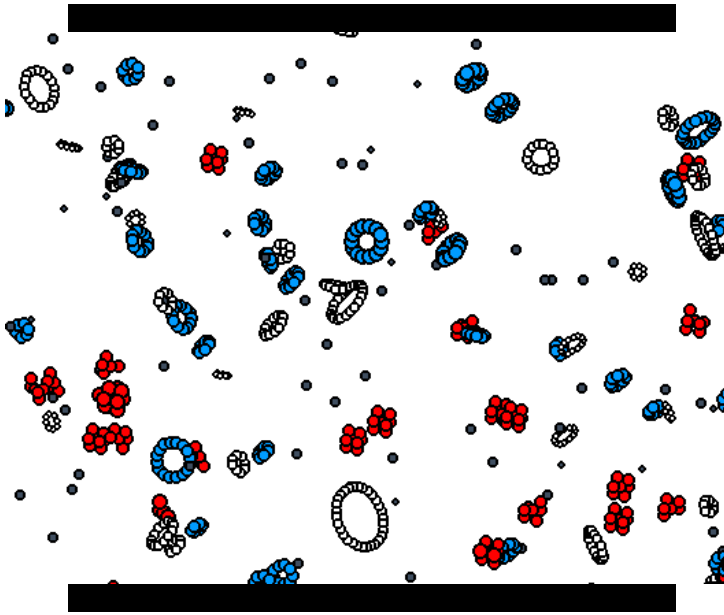




Long term simulation of the microstructure under irradiation of Fe by object kinetic Monte Carlo

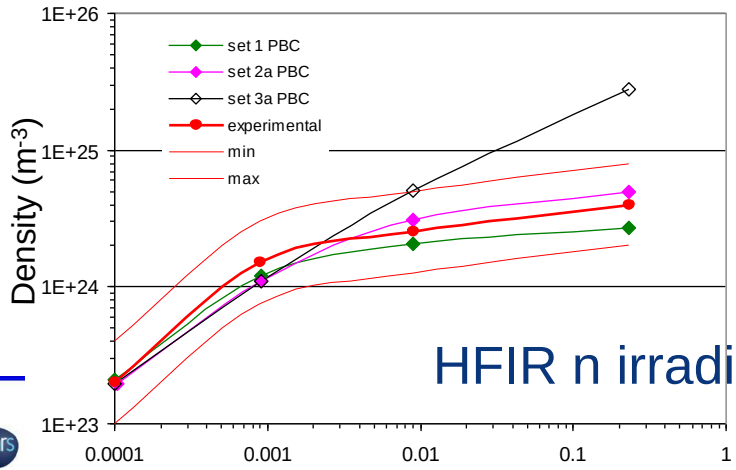




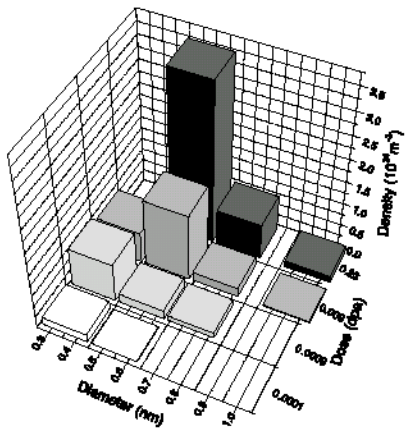


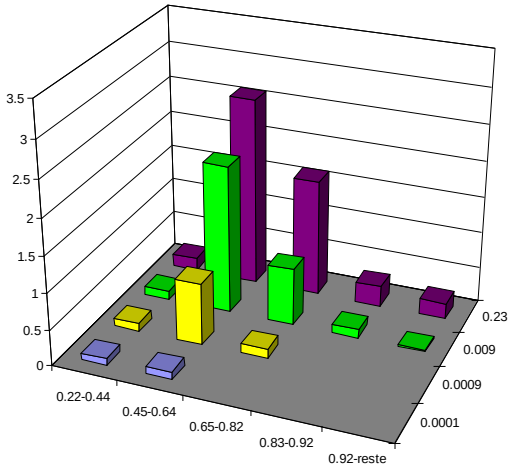
Input required: Mobility: diffusion coefficient

Local interaction rules: Interaction and binding energies



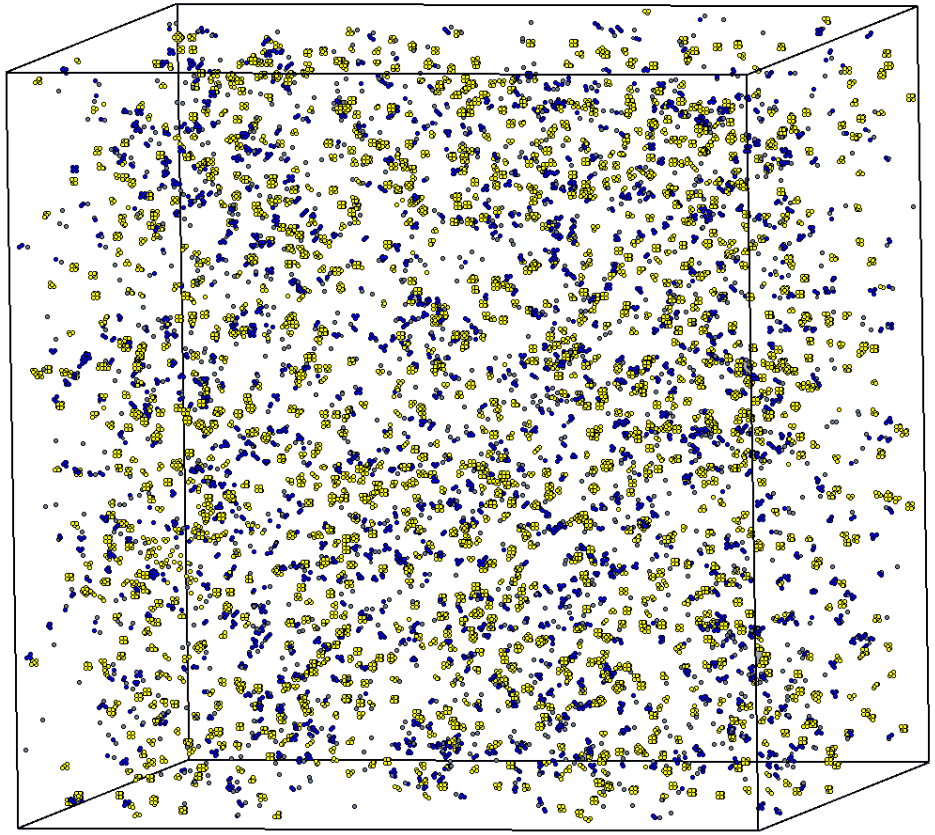
HFIR n irradiation





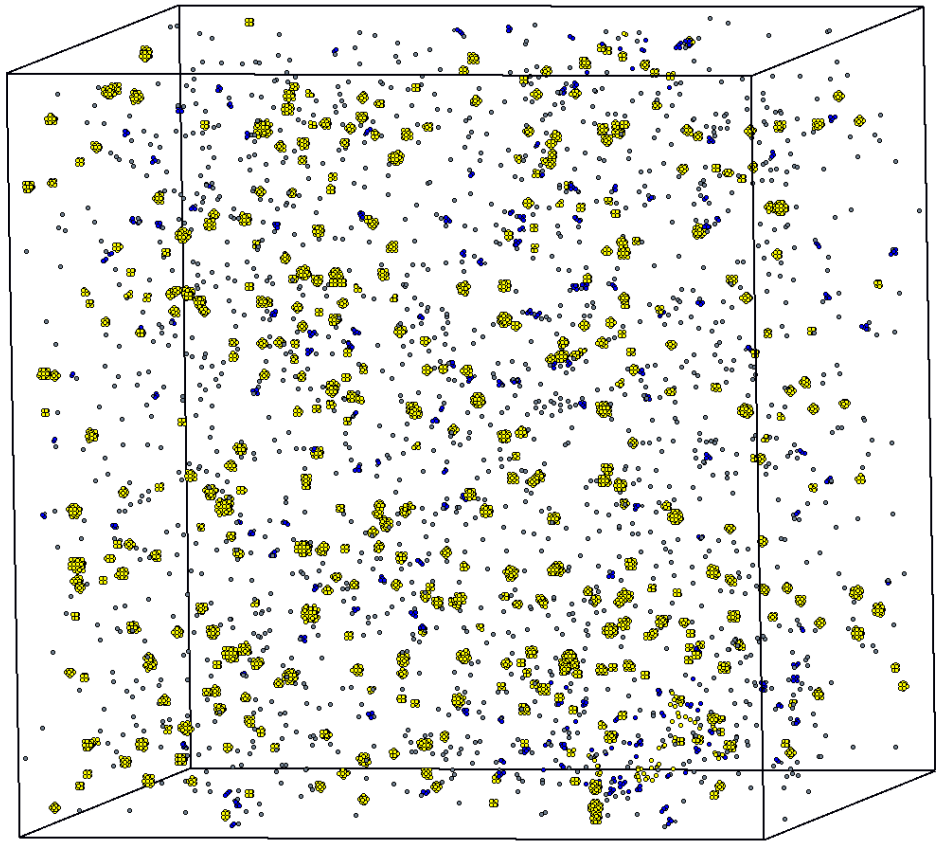
Long term simulation of the microstructure: Application example: flux effect study in bcc Fe

DEFECT POPULATION at 0.1 dpa



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

343K



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

(param Set II)

Mesoscale methods: MFRT

Cluster Dynamics (CD) or Mean Field Rate Theory (MFRT) [CRESCENDO - co-developement EDF - CEA (SRMP)]

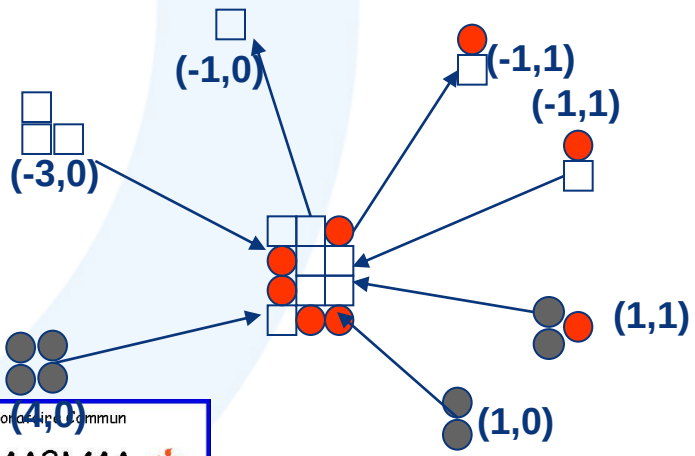
Example for single vacancy concentration:

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

- K_V: Vacancy production rate
- $k_V^2 D_V c_V$: Disappearance of vacancies at sinks
- $\alpha c_I c_V$: Vacancy-SIA recombination rate

Coupling with SIA concentration equation

k^2_v, D_v and α : theory, atomic simulation, phase field



- Vacancy
- SIA
- Solute atom

C(n,p)

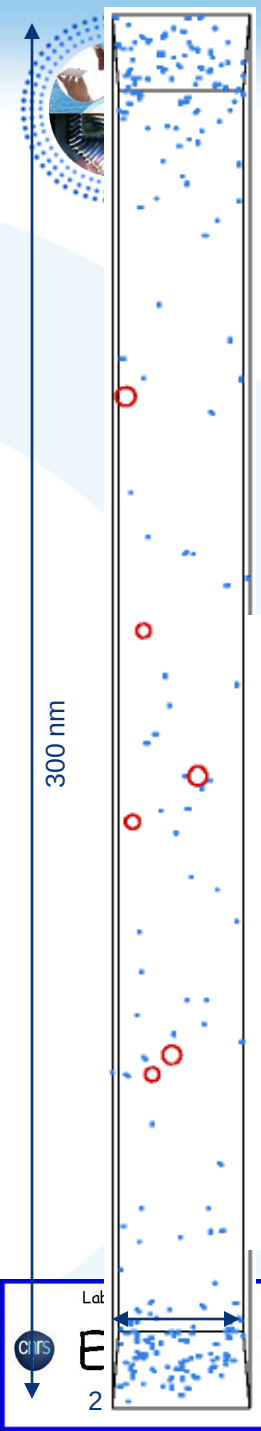
- n : nb de défauts ponctuels
- p : nb de d'atomes de solutés

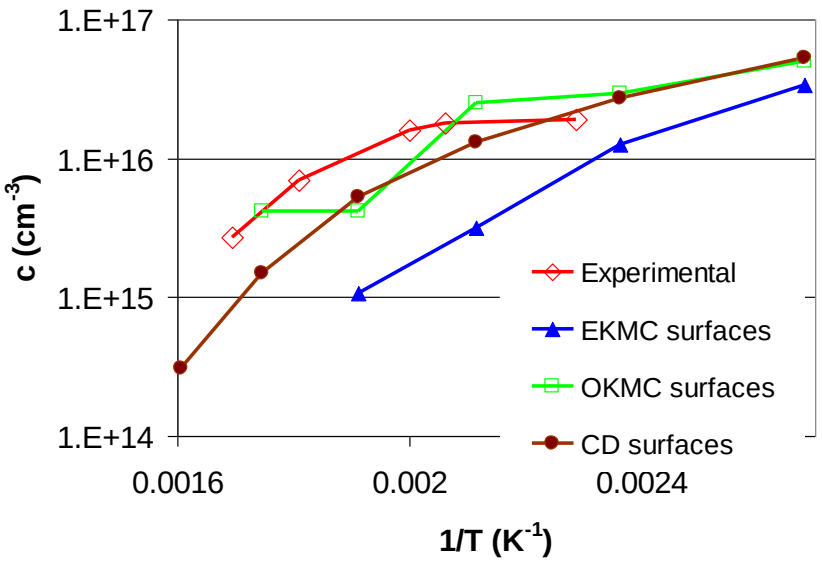
Irradiation d'une lame mince (OKMC / MFRT)

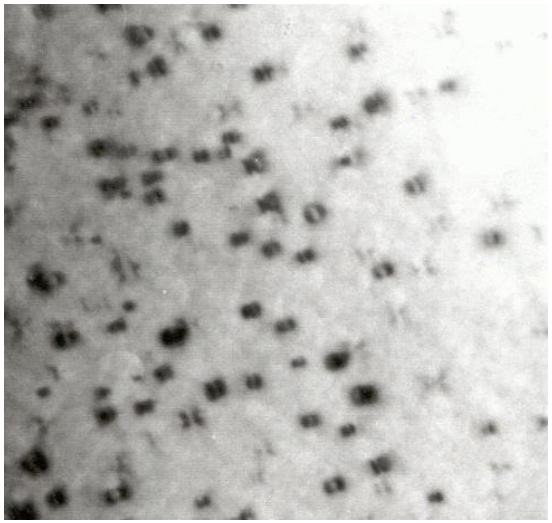
Irradiation aux électrons

150°C, 0.1dpa, 1000 s

Lame mince de microscope



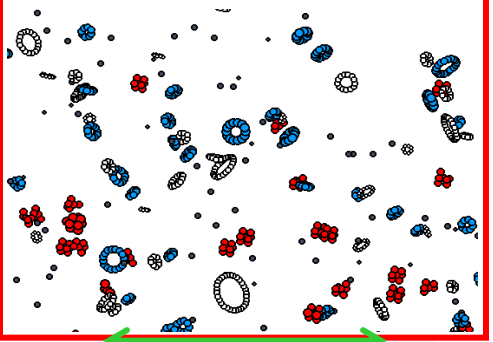




Multiscale modeling of plasticity: phenomenological scales

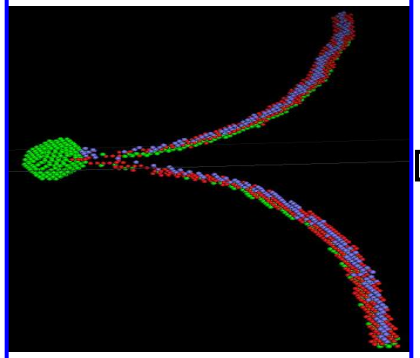
Physics modeling

Irrad. microstructure



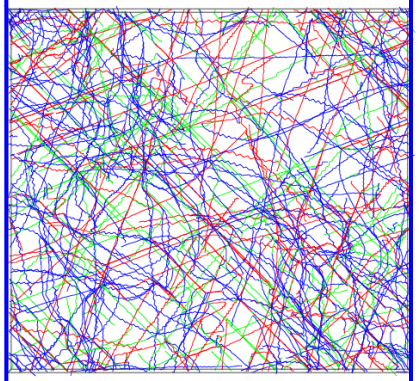
10 nm

Dislocation-defect



10 µm

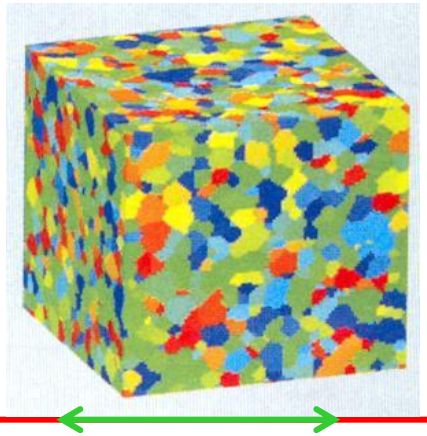
Collective dislocation behavior



10 µm

Mechanical properties

RVE mechanics



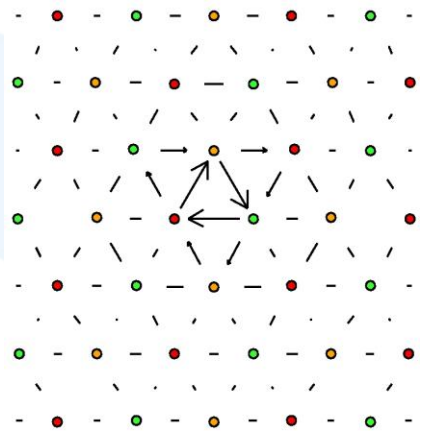
Atom-meso transition

Meso-continuum transition

Homogenization

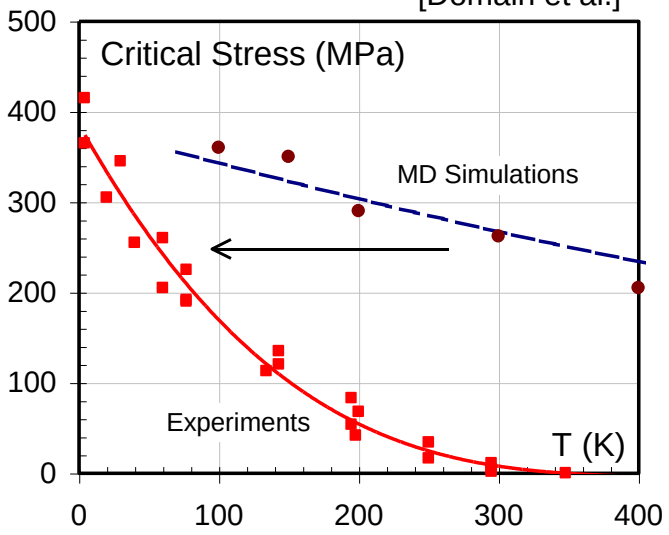
Multiscale approach

Dislocation at the atomic scales



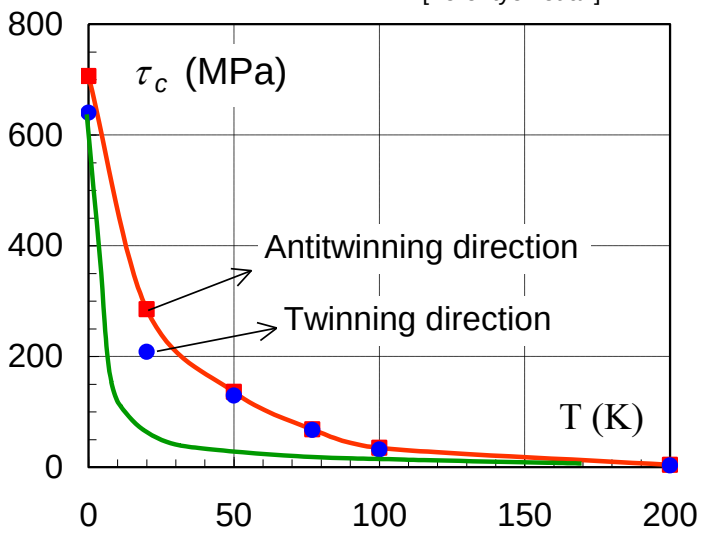
Screw core structure: compact
ab initio
EAM: Mendelev03
EAM: Ackland04

[Domain et al.]

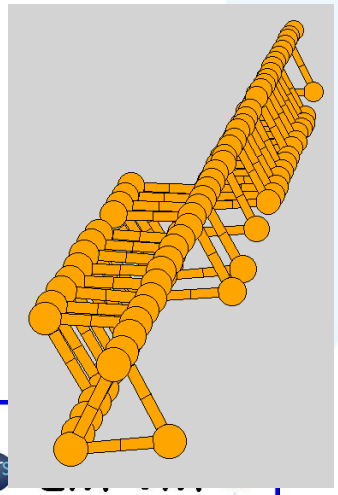


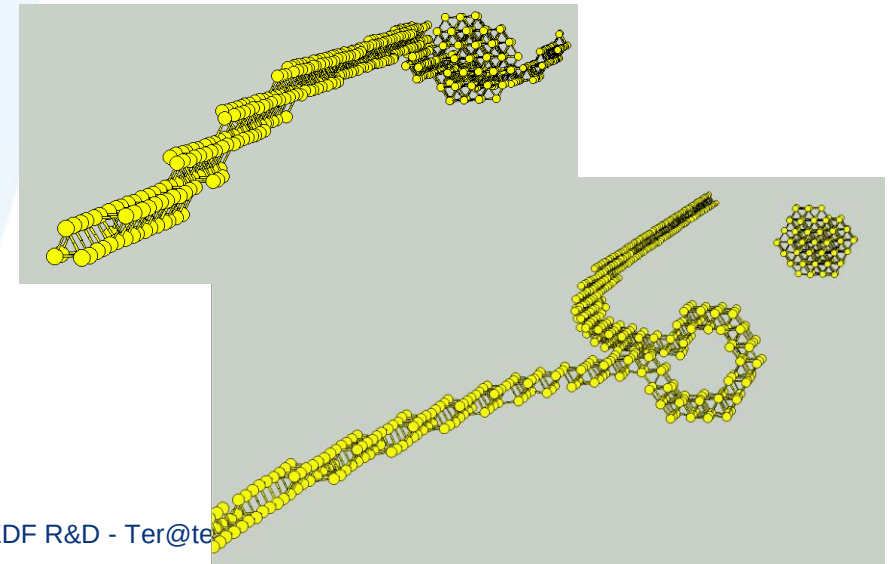
Critical stress for (110) screw dislocation
(temperature, strain rate)

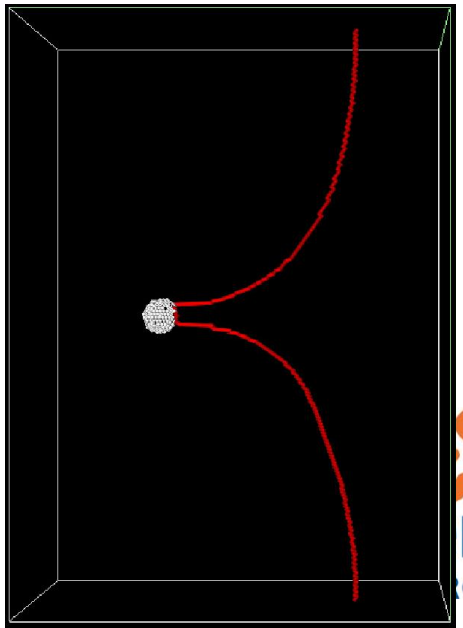
[Terentyev et al.]



Critical stress for (112) edge dislocation
(temperature, strain rate)

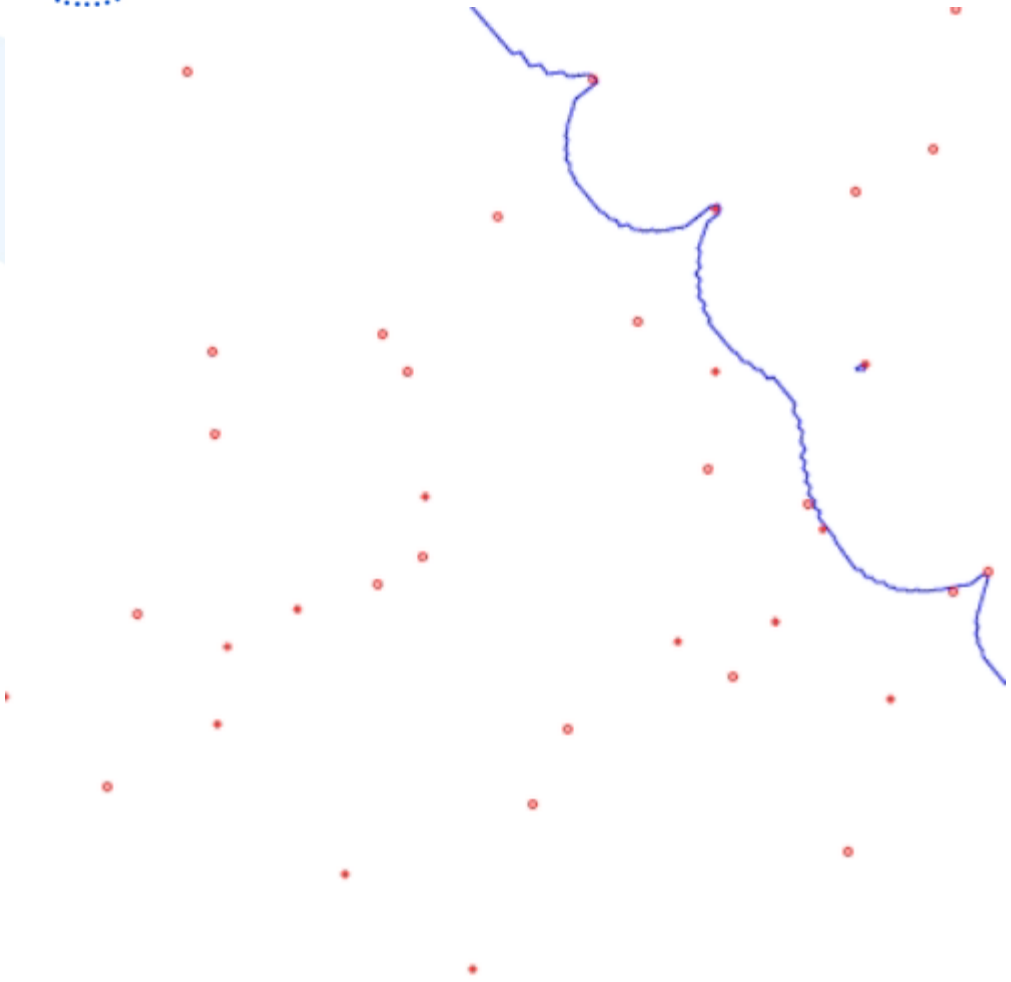


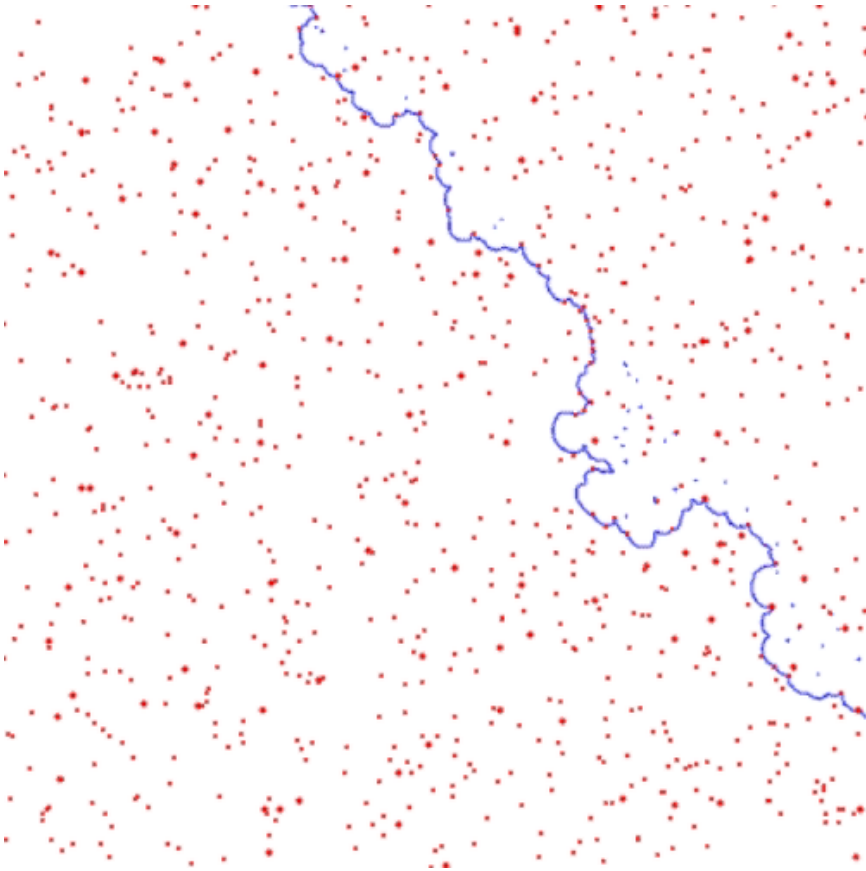




Screw motion by DK

Defect hardening by dislocation dynamics





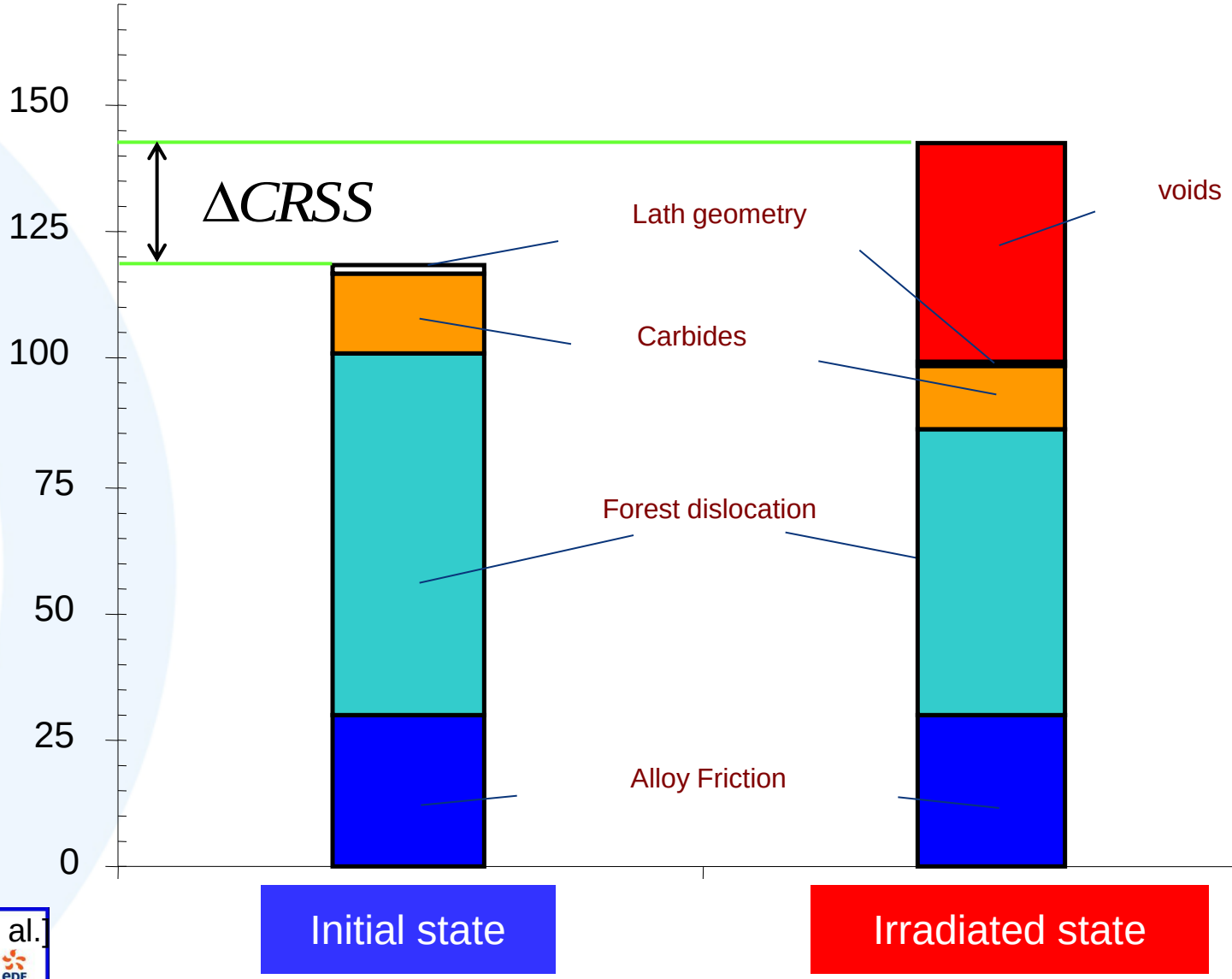
Hardening contribution of each kind of defects

Dislocation dynamics (G. Monnet)

MicroMegas coll B. Devincre (CNRS-ONERA)

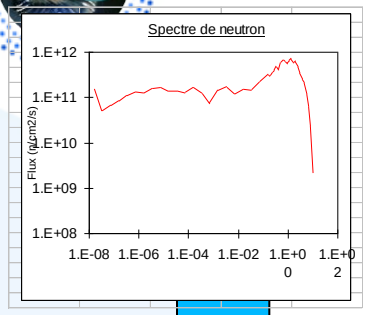
[several days/weeks on 1 CPU]

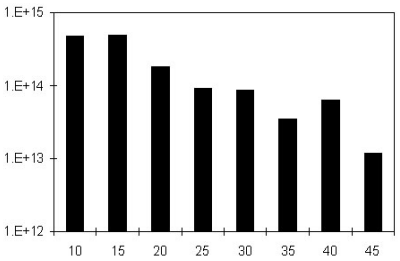
Irradiation strengthening in RPV

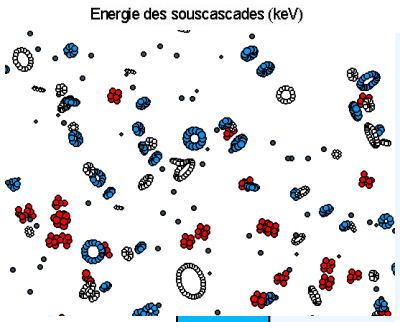


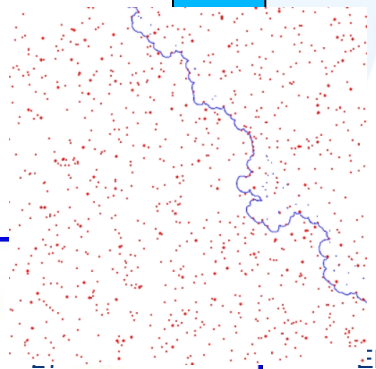
[Queyreau et al.]

Integration: RPV & INTERN plateforms









neutron spectrum

IRRAD

pka spectrum

temperature
+ composition

CONVOLVE

source term

composition
+ mobility rules and diffusion coefficients
+ energetics of clusters
+ sinks densities
+ time steps and total irradiation time

LONG_TERM

clusters distributions f(t)

pinning forces of the clusters
+ slip system
+ shear modulus

HARD

$\Delta\tau(t)$

RPV-2
INTERN-1

PERFORM 60
FP7 Project

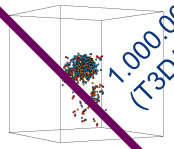
Material modelling roadmap: molecular dynamics and ab initio

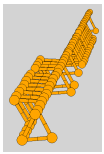
Classical molecular dynamics

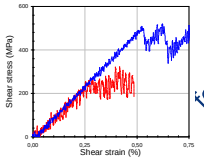
MD few 100 atoms - qq 100 steps - 1 ps

MD few 10.000 atoms - few 10.000 steps - few 10 ps

1.000.000 atoms - 50.000 steps - few 10 ps (T3D/T3E Grenoble)

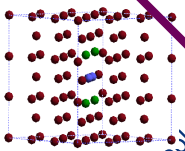


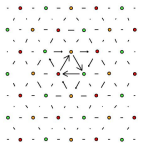


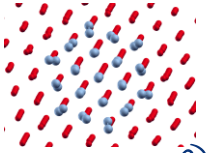


few millions atoms, **few millions** steps - few ns

1960 1990 1995 2000 2006 2010 2015







Ab initio

Static calculation few 10 atoms (T3E Grenoble)

Static calculation - 250 atomes (tantale (CRT1)

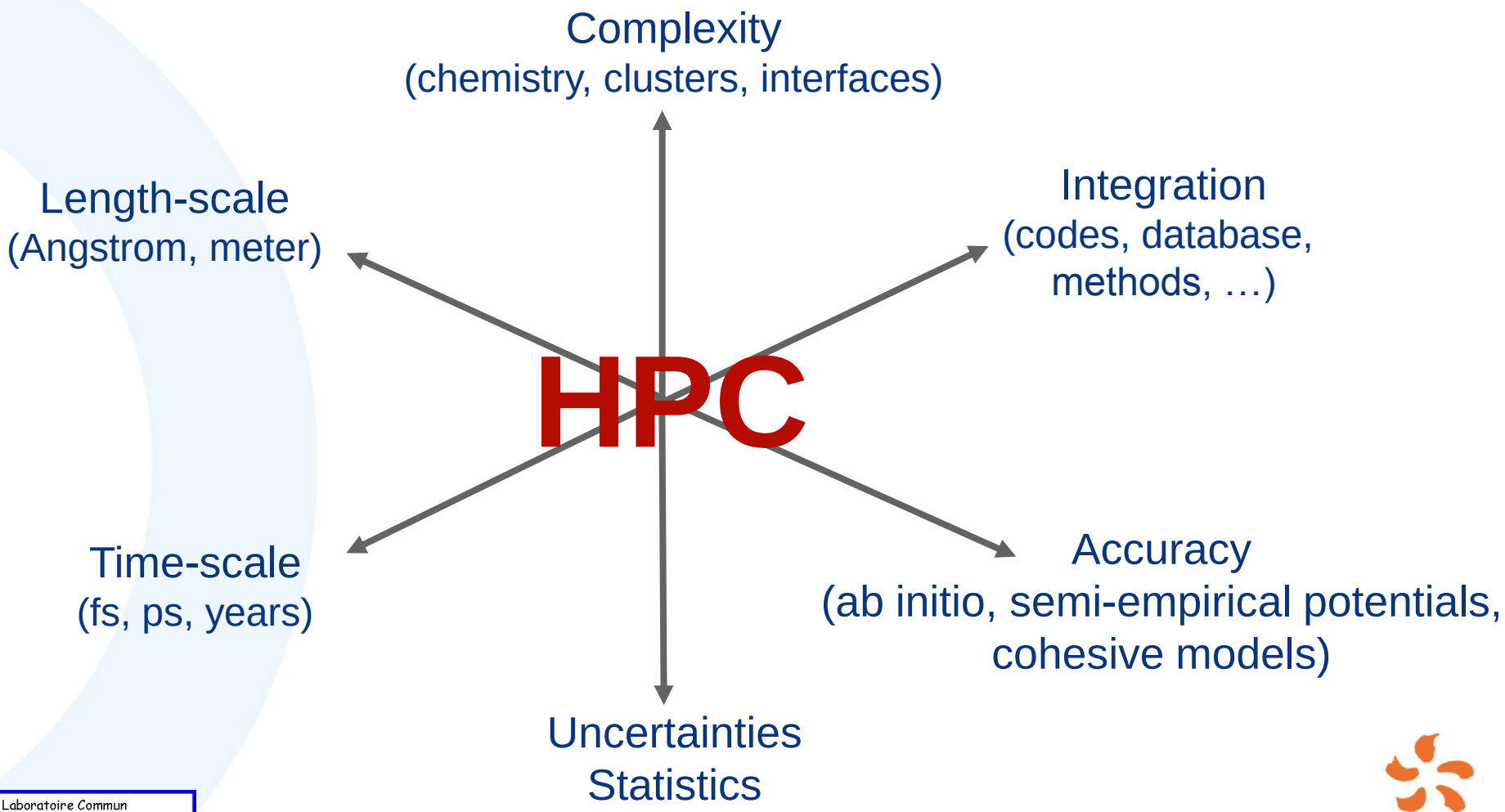
Static calculation 1000 atoms (EGL)

Static calculation - few 1000 atoms (BGP)

Dynamical cacl. **ab initio few 100 to 1000 atoms - few 1000 steps**

Dynamic calculation (MD) few 10.000 atoms - **few 10.000 steps - few 10 ps**

Material Multiscale Modeling Challenge



Conclusions & perspectives

- A multi-scale modelling approach is developed for more than 15 years (e.g. through internal & EURATOM European projects & ANR).
- Improvement of the knowledge elementary properties allow to better predict material evolution.
- Important progress thanks to the use of HPC machines.
- The prediction of the evolution of the mechanical properties requires to know the plasticity of the materials.
- The prediction of the evolution of the irradiated microstructure requires as input physical parameters the properties of each point defect clusters (mobility and stability).
- **Parallelisation & HPC**
  - **Classical Molecular dynamics (MD), ab initio (DFT), dislocation dynamics (DD), phase field: OK**
  - **kinetic Monte Carlo: difficult**