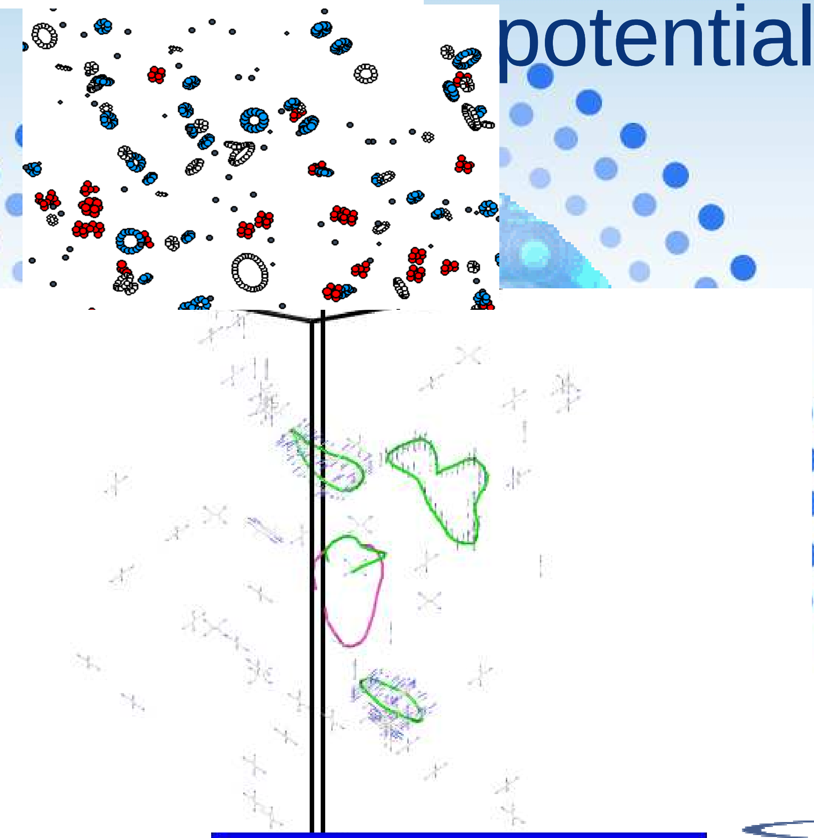
IAEA – Vienna – November 2017

Collisional Cascades Database Technical Meeting

# Cascades by molecular dynamics in metals: interatomic potentials and BCA comparison, statistics




C. Domain[1] , C.S. Becquart[2], P. Olsson[3], A. De Backer[4]

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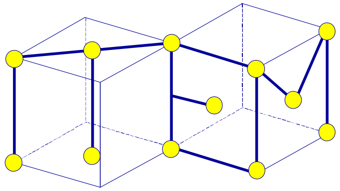
# ITEM Network



- European network
- EDF Coordinator
- 7 technical areas
- 40 members
- 4 years (starting 1/10/2001)
- Objectives:
  - to prepare new simulation tools by solving key problems and by giving some recommendations...
  - to build the European DAtabase for Multiscale modelling (EDAM)

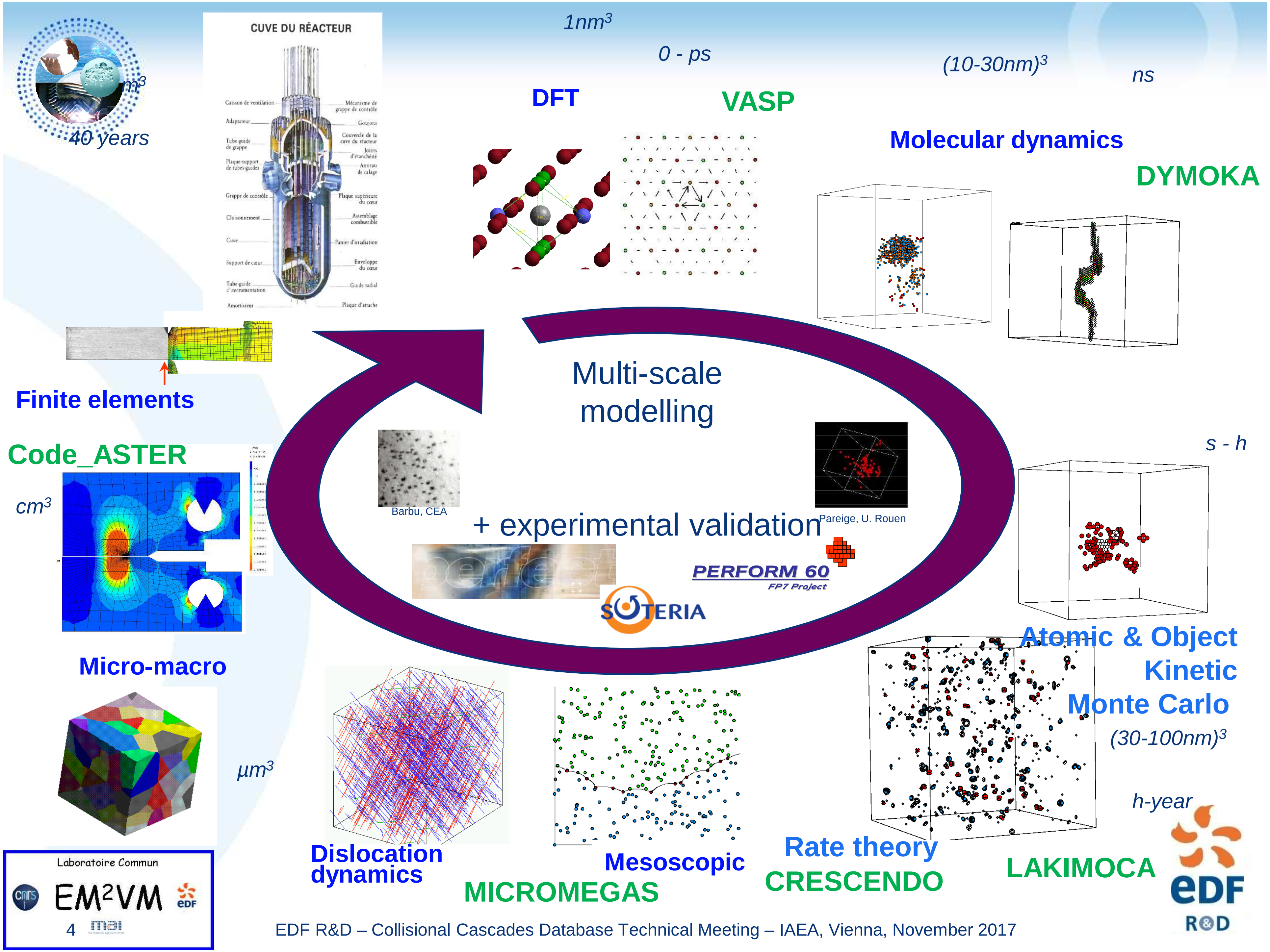
Final report:

## Guideline for Multi-scaling Modeling of Irradiation Effects

**FIS5-2001-00031**

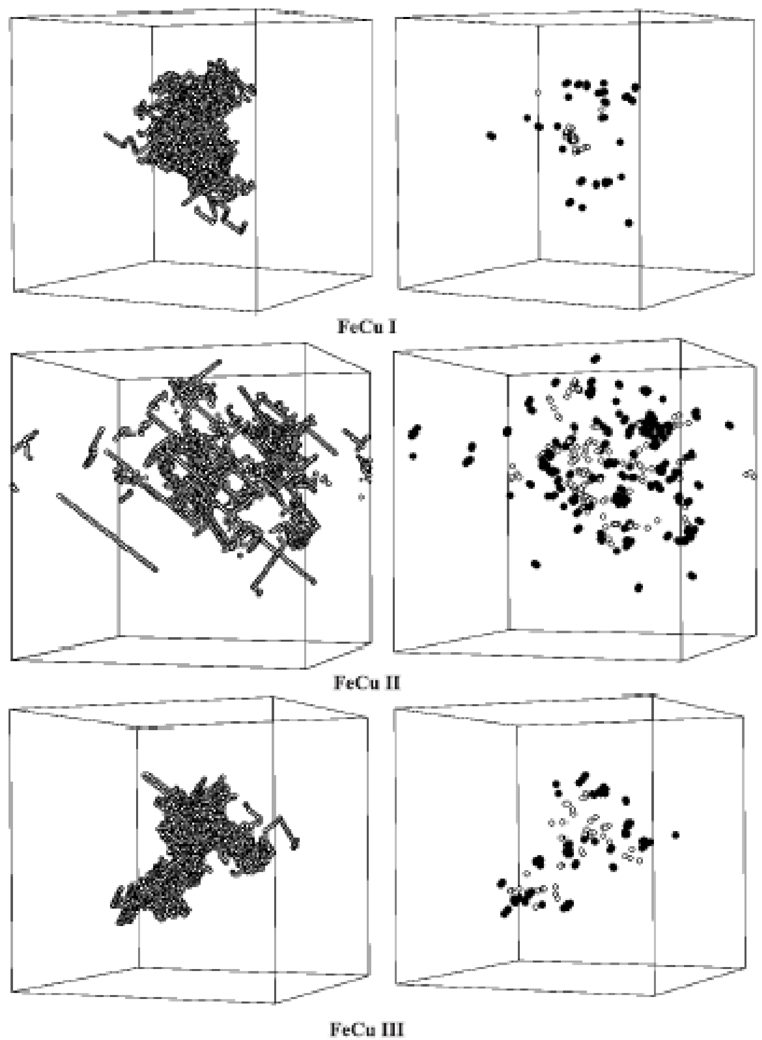
# Microstructure modeling evolution: Towards long irradiation

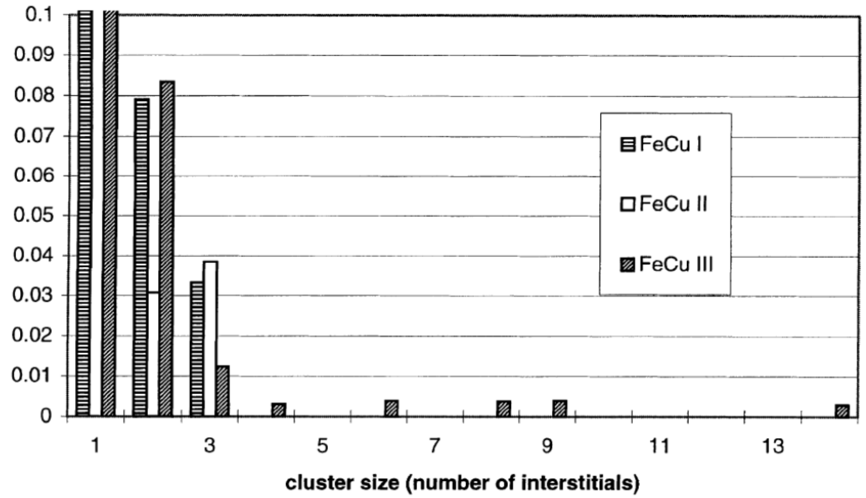
- Modelling complex chemistry + defects (point defects and clusters)
  - → Atomic Kinetic Monte Carlo (AKMC) / OKMC / hybrid / rate theory
    - → Data on defect solute clusters mobility & stability
    - → Primary damage
- Primary damage
  - → Prediction of empirical potentials
    - → Representative
    - → Quantitative
    - → Threshold Displacement Energy

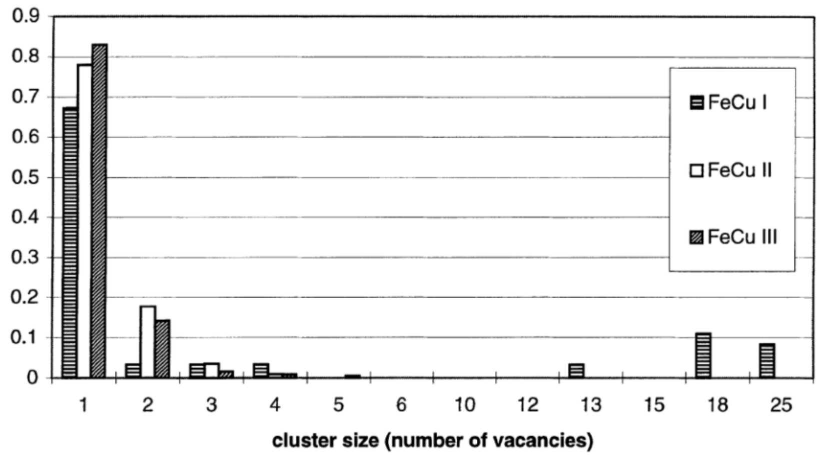

1nm3
0 - ps
(10-30nm)3
ns
40 years
CUVE DU RÉACTEUR
DFT
VASP
Molecular dynamics
DYMOKA
Finite elements
Multi-scale modelling
Code_ASTER
cm3
Barbu, CEA
+ experimental validation
Pareige, U. Rouen
s - h
PERFORM 60
FP7 Project
SOTERIA
Atomic & Object Kinetic Monte Carlo
(30-100nm)3
Micro-macro
μm3
Dislocation dynamics
Mesoscopic
MICROMEGAS
Rate theory
CRESCENDO
LAKIMOCA
h-year
Laboratoire Commun
EM2VM
edf
R&D

# EAM Potential comparison

DYMOKA, NVE, PBC

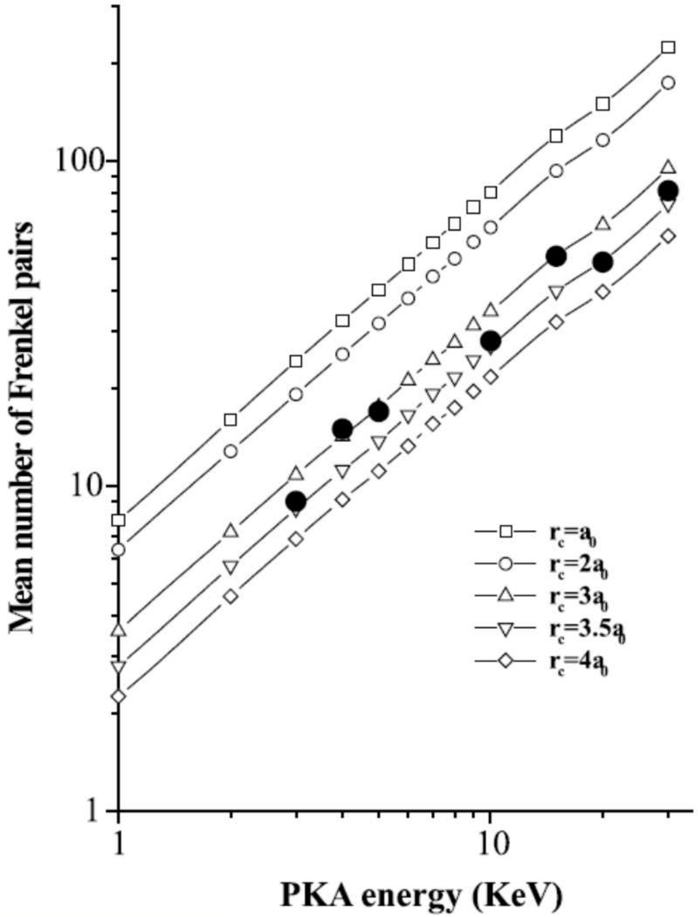


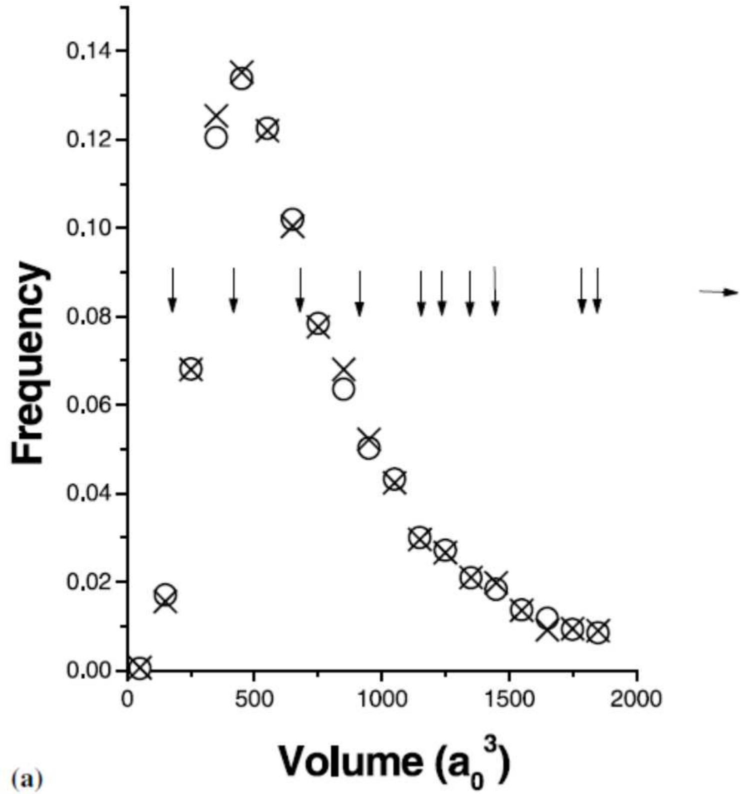




[Becquart JNM2000]

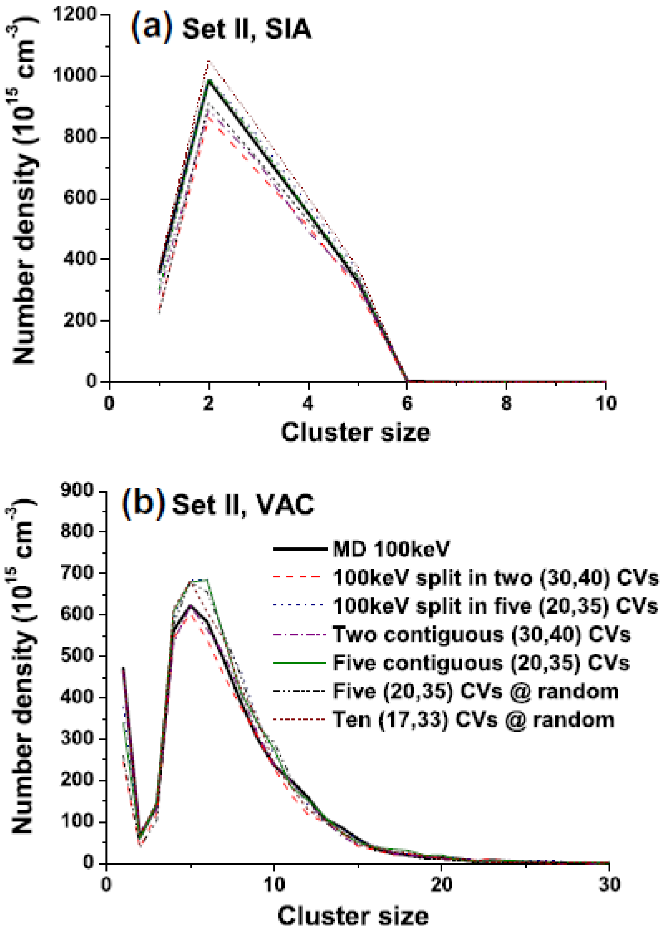
# BCA (Marlowe) – MD cross comparison

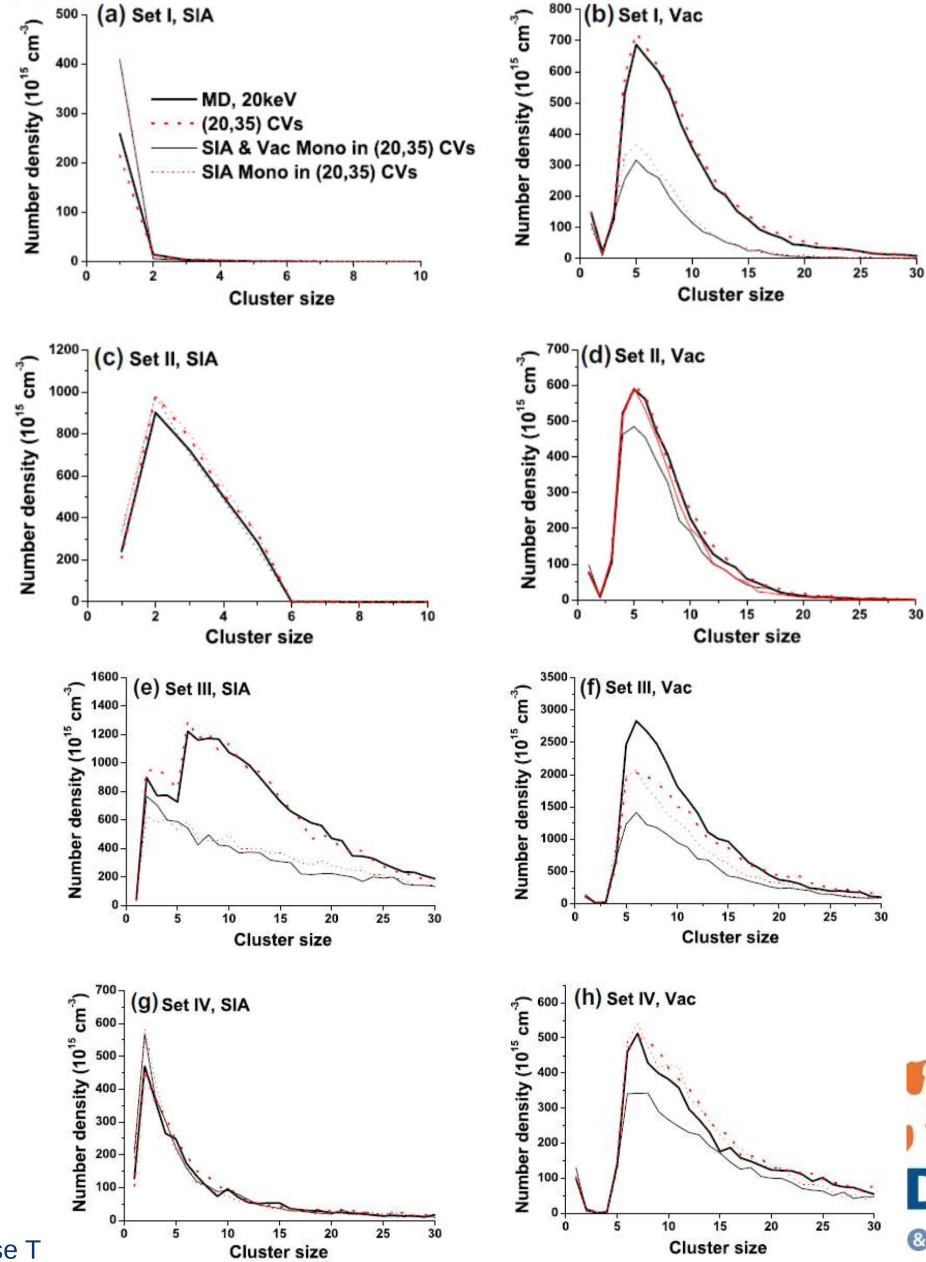



[Souidi JNM2001]

# Microstructure evolution: importance of source term (OKMC)

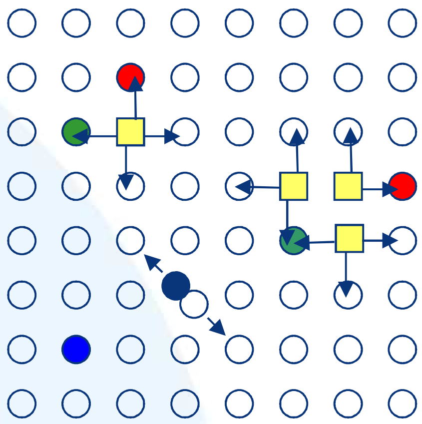


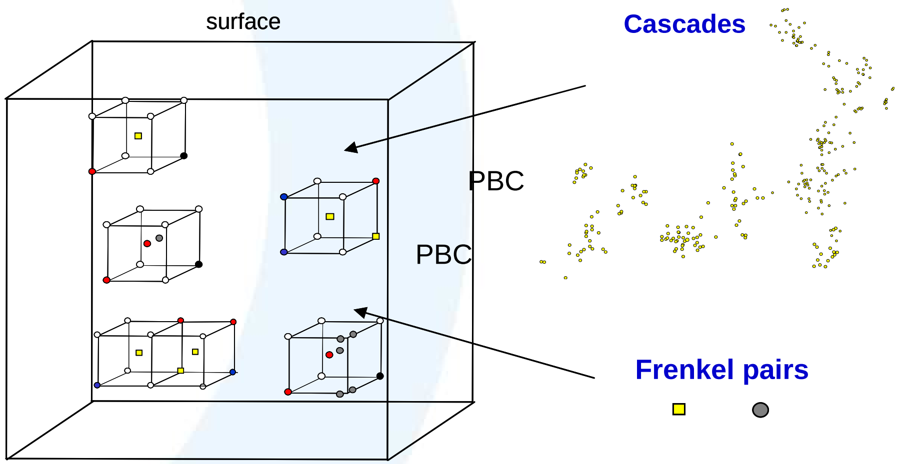




[Souidi JNM2011]

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

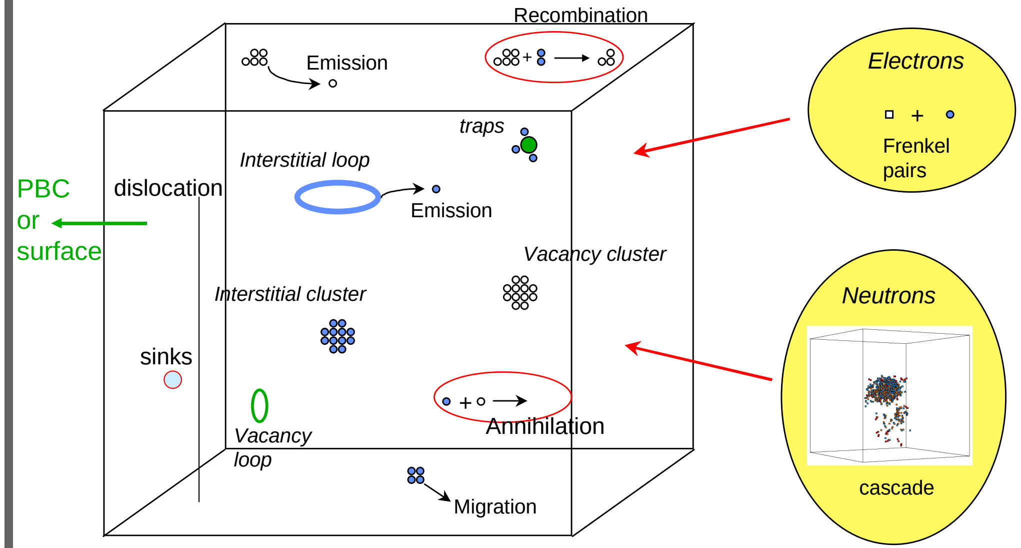
## Atomic KMC






**Ageing (one single vacancy)**

## Object KMC




Box size ≈ 30 - 100 nm

V ≈ $10^{-4}$ µm$^3$

t ≈ h to yr (T, G dependent)

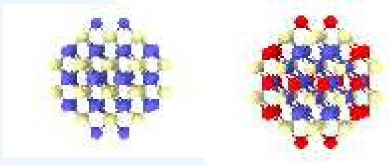
$$\Gamma_X = \nu_X \exp\left(-\frac{Ea}{kT}\right)$$

[JNM 335 (2004) 121–145]

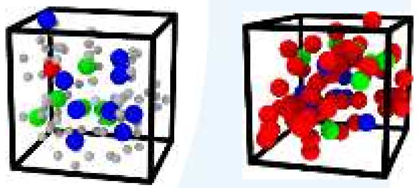
# Medium / long term microstructure evolution modelling KMC simulation of irradiation (n, ion)

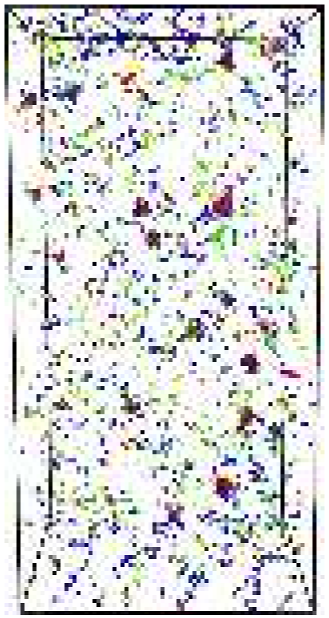
**Atomic** KMC

Rigid lattice cohesive model based on DFT calculations



Hybrid AKMC / OKMC

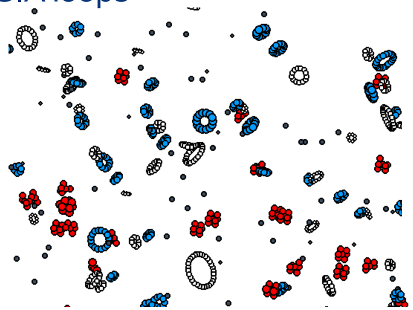




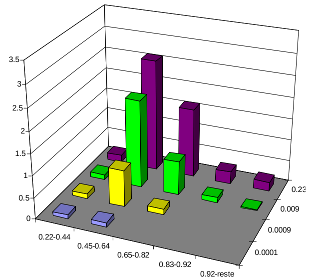
[Pannier PhD 2017]

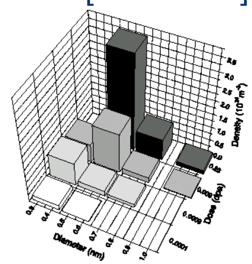
**Object** KMC

SIA loops

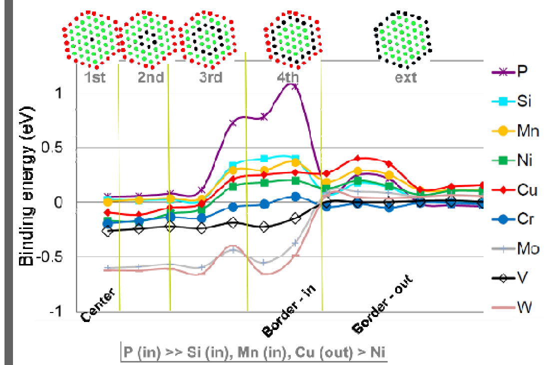


[JNM 2004]



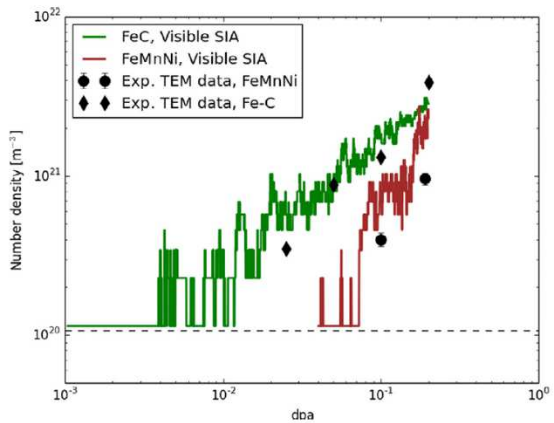


OKMC ← vac → PA exp




solute – <111> SIA loop DFT

[Domain JNM 2018]




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

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

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

[Chiappetto NIMB 2015]

# TDE from first principles

- **TDE simulation characteristics:**
- Non-cubic supercells: 504 atoms (6x6x7 bcc cells)
- Born-Oppenheimer MD: electronic convergence for each MD step
- Time step: 2 – 3 fs
- TDE energy discretisation: 1 eV
- On 2048 cores (IBM BlueGene Q) and 1024 cores (Cray XE6)
- need up to ~2 ps simulated time
- very, very core-hour expensive!!!

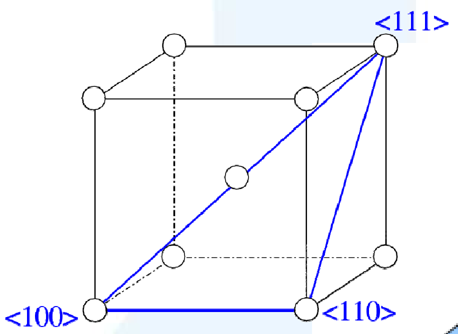
Standard minimal potentials

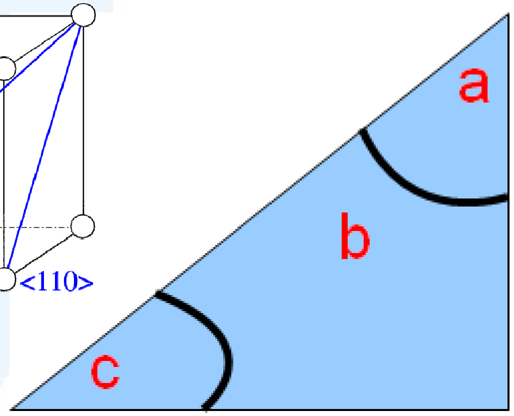
- $Fe_{sd}$= $Ar4s^1 3d^7$

and the semi-core potentials

- $Fe_{psd}$= $Mg3p^6 4s^1 3d^7$

| $E_f$ (eV) | $Fe_{sd}$ | | $Fe_{psd}$ | |
|---|---|---|---|---|
| Config | 250 | 1024 | 250 | 1024 |
| Vac | 2.16 | 2.06 | 2.16 | 2.09 |
| ⟨110⟩ | **4.05** | **3.97** | **4.31** | **4.25** |
| ⟨111⟩ | 4.79 | 4.64 | 5.12 | 4.98 |
| ⟨100⟩ | 5.18 | 5.02 | 5.54 | 5.42 |
| ⟨110⟩-⟨111⟩ | 0.74 | 0.67 | 0.81 | 0.73 |
| FP | 6.21 | 6.05 | 6.47 | 6.34 |



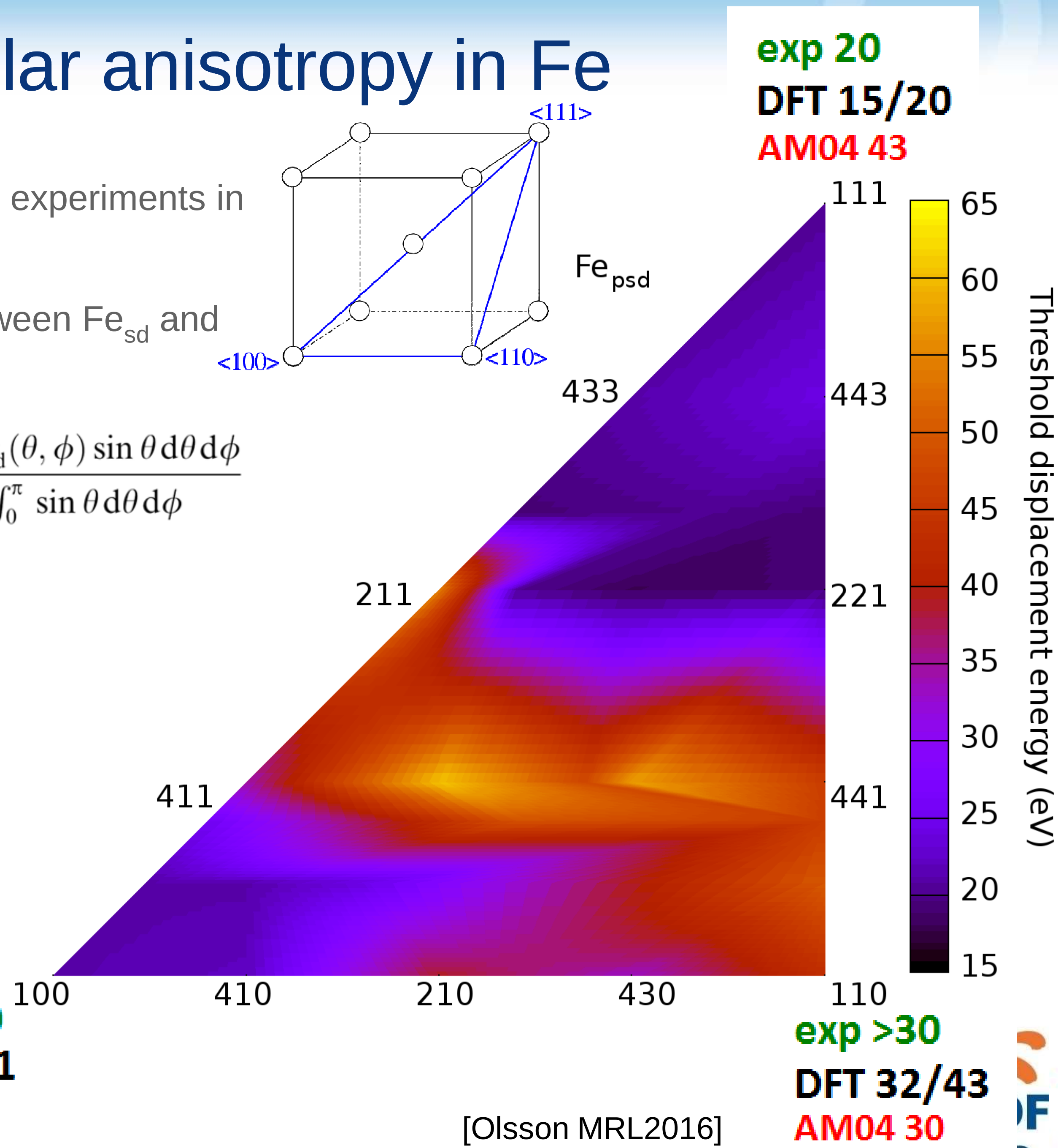

[Olsson MRL2016]

# TDE angular anisotropy in Fe

- Very good agreement with experiments in high-symmetry directions
- About 5 eV difference between $Fe_{sd}$ and $Fe_{psd}$

Average TDE: $$E^{\mathrm{av}}_{\mathrm{d,ave}} = \frac{\int_0^{2\pi}\int_0^{\pi} E^{\mathrm{l}}_{\mathrm{d}}(\theta,\phi)\sin\theta\,\mathrm{d}\theta\,\mathrm{d}\phi}{\int_0^{2\pi}\int_0^{\pi}\sin\theta\,\mathrm{d}\theta\,\mathrm{d}\phi}$$

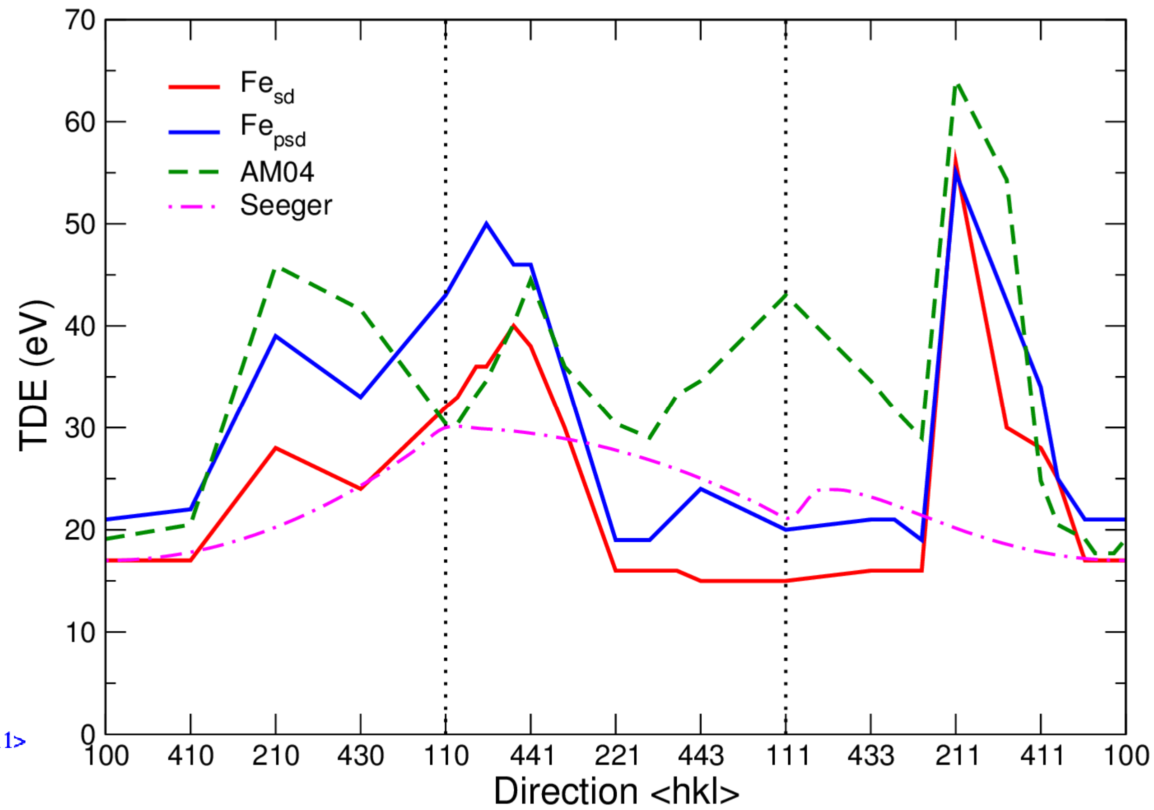
- $Fe_{sd}$: 29 eV
- $Fe_{psd}$: 32 eV
- ASTM: 40 eV
- AM04: 39 eV

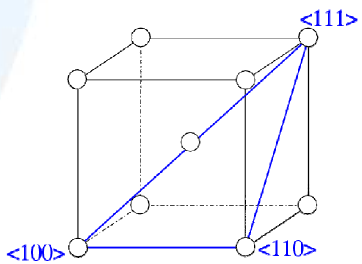



[Olsson MRL2016]

# TDE angular anisotropy in Fe

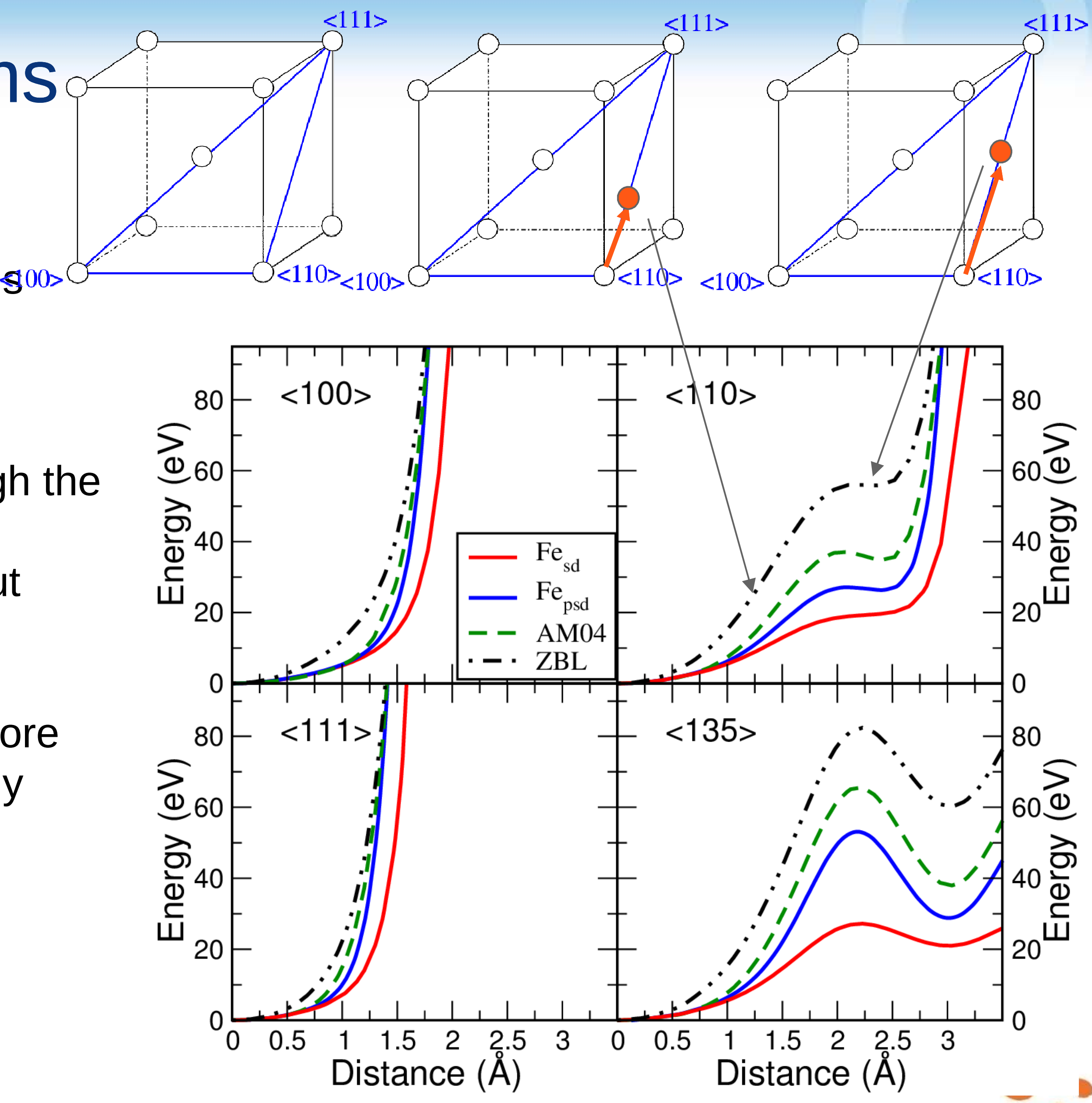
- Very similar topology for $Fe_{sd}$ and $Fe_{psd}$
- Not so similar to EAM (nor the analytical model of Seeger)
- ⟨110⟩ is hyperbolic in DFT, minimal in EAM and maximal in Seeger
- ⟨111⟩ is strongly maximal in EAM




[Olsson MRL 2016]

# Drag atoms




Quasi-static drag simulations show difference between methods

One atom is dragged through the lattice and the energetic response is recorded without relaxation

ZBL, AM04 and $Fe_{psd}$ are more or less in agreement (equally stiff) for the close packed directions

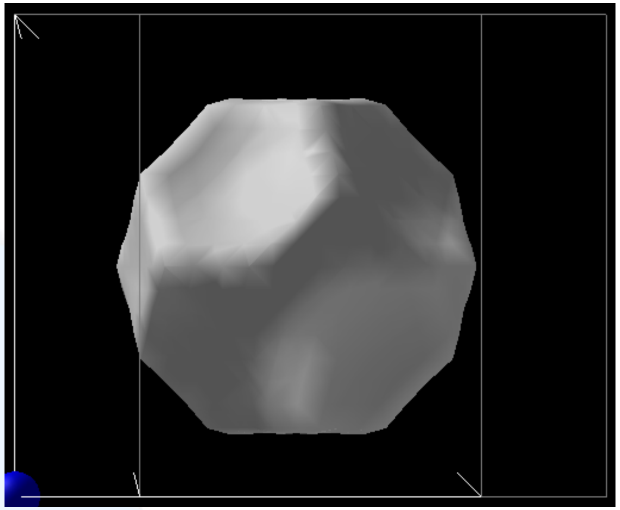
$Fe_{sd}$ is much softer

[Olsson MRL 2016]

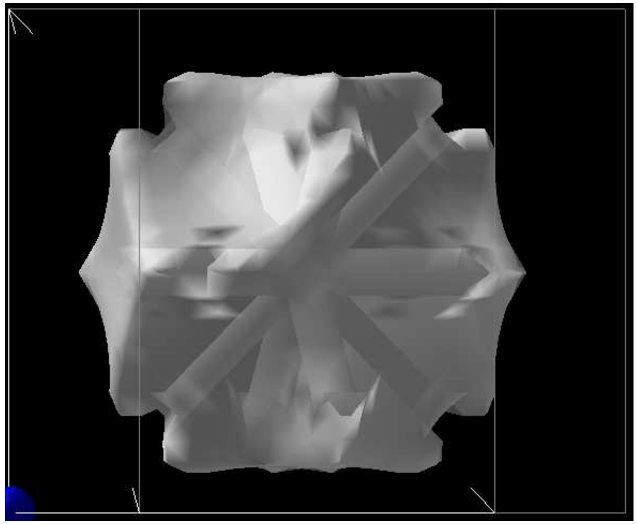
# Drag atoms: isosurface

Isosurface
18 eV

$Fe_{psd}$

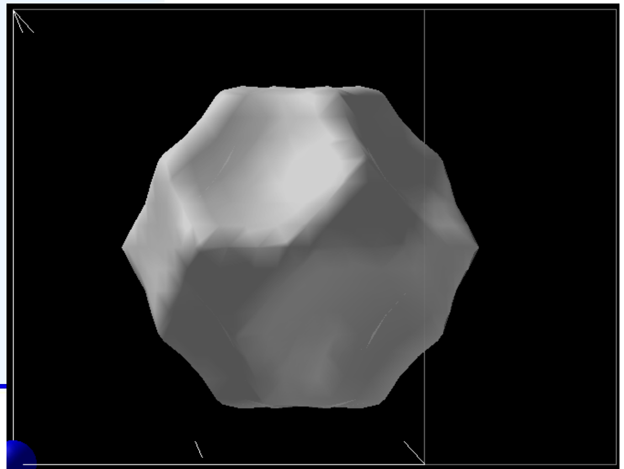


$Fe_{sd}$

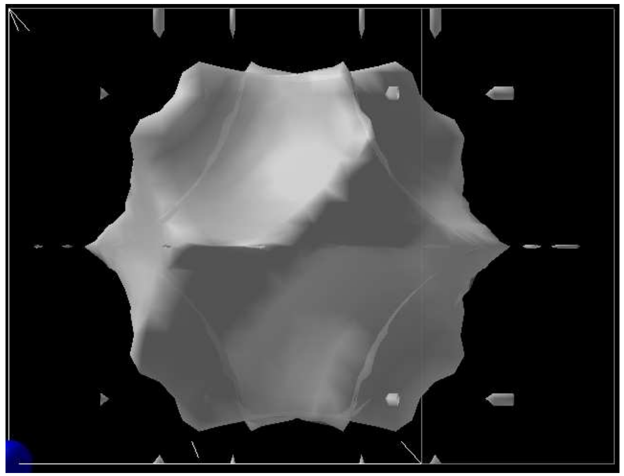


Isosurface
25 eV

$Fe_{psd}$

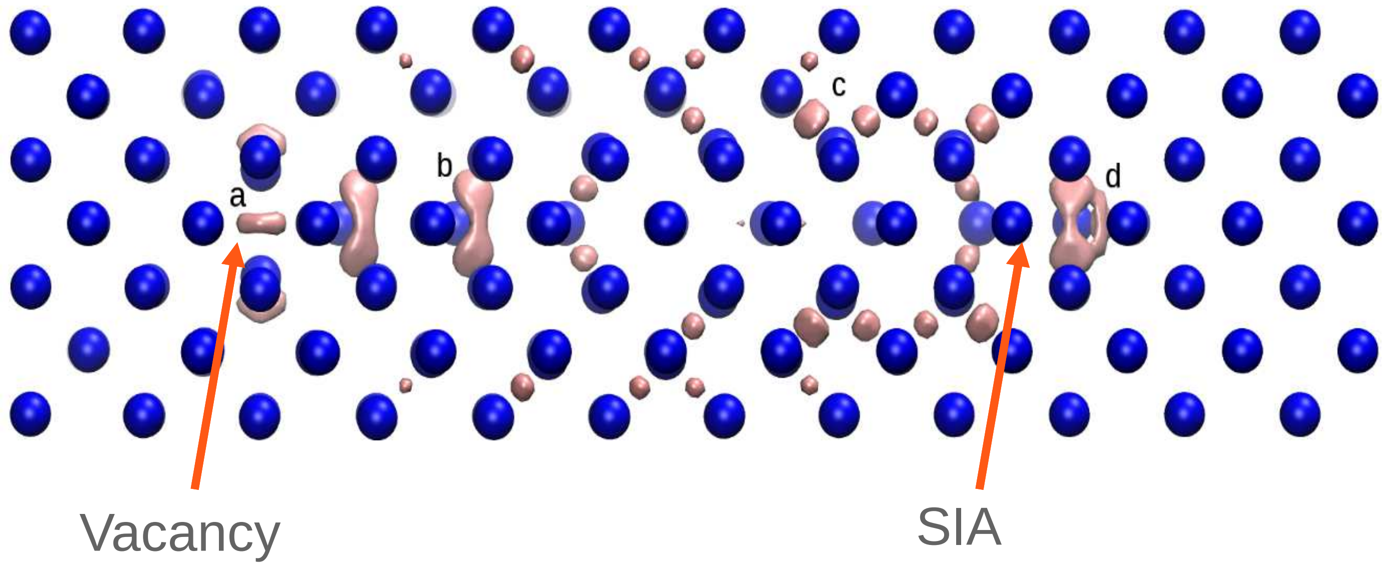


EAM (AM04)



# Density Functional Theory: Dynamic simulation of defect creation

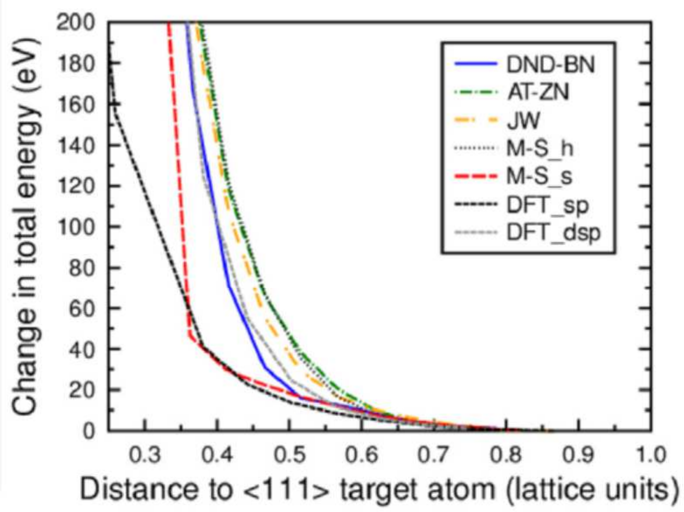
- DFT simulation of 40 eV knock-on in <100> direction
- BO-DFT



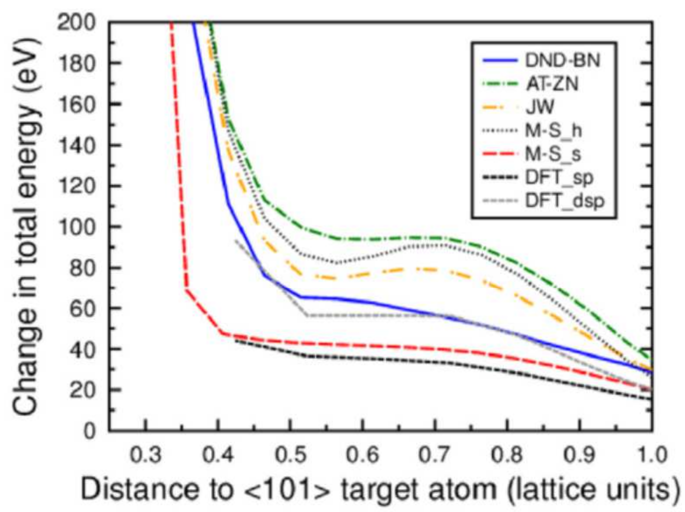

Static Calculations:

W

[JNM 470 (2016) 116]




(a) Displacement in the ⟨111⟩ direction.

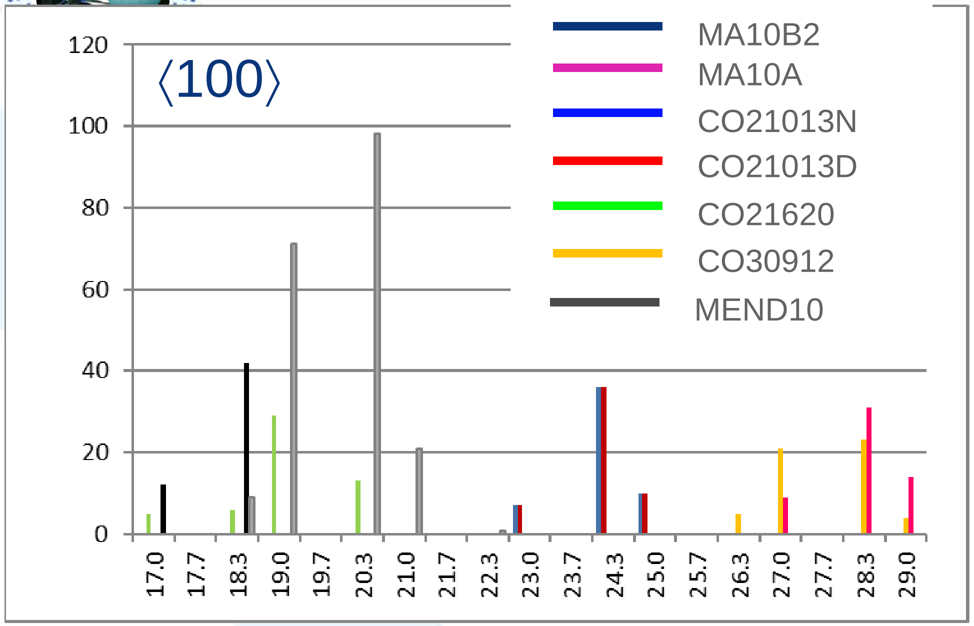


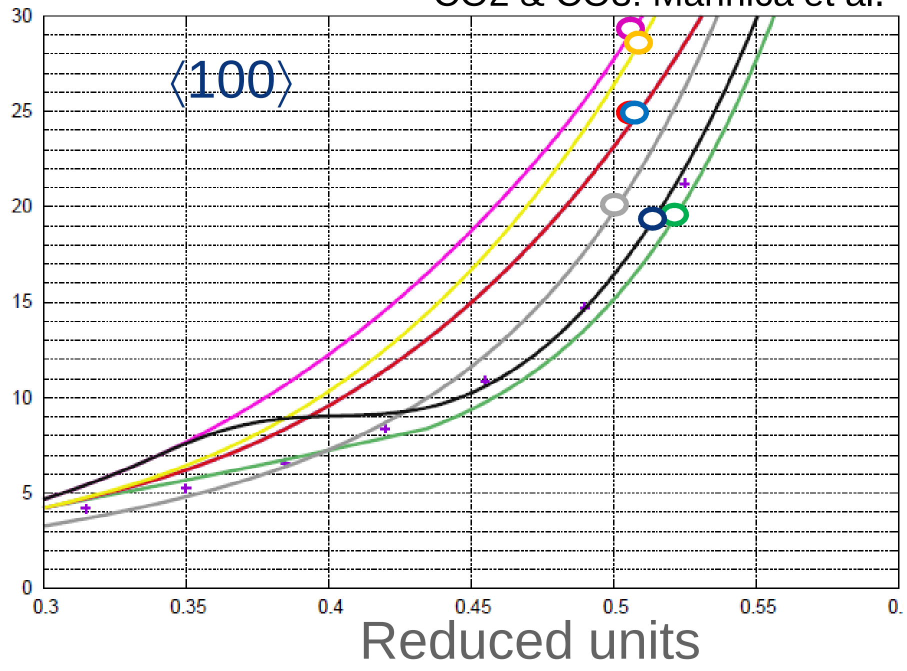

(b) Displacement in the ⟨101⟩ direction.

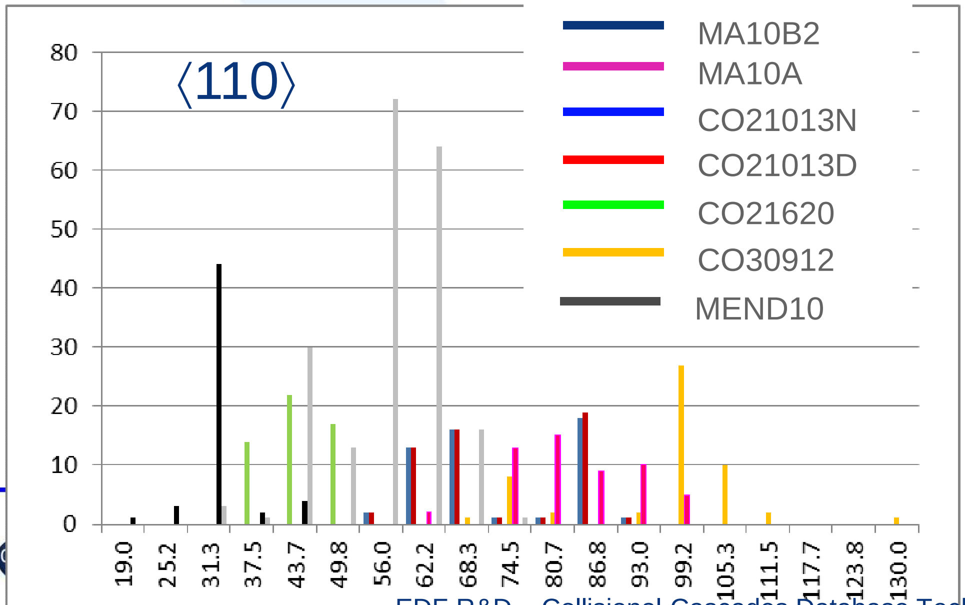
[Sand JNM2016]

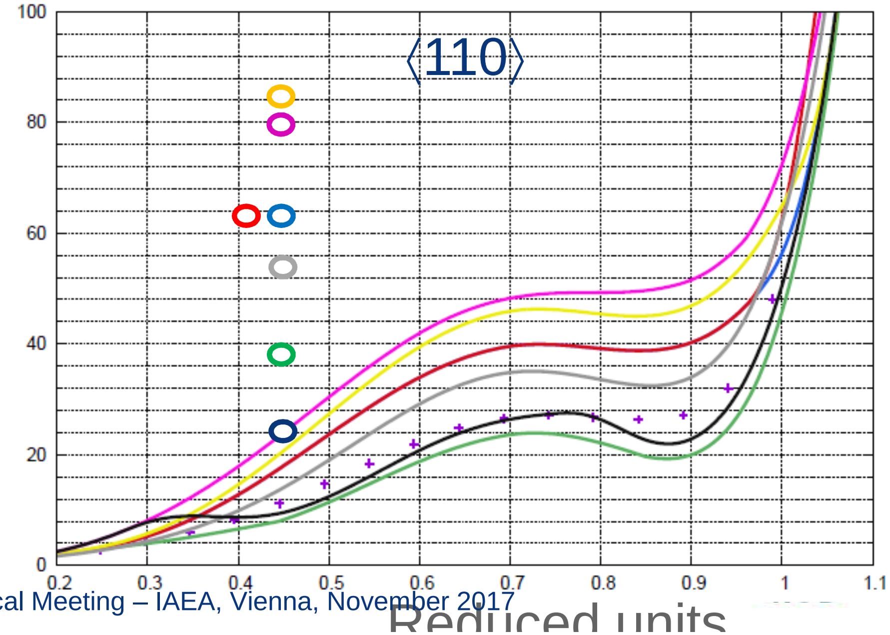
# TDE & Quasi Static Drag (QSD) correlation

MEND10: Ackland 2004
MA10: Marinica 2010
CO2 & CO3: Marinica et al.

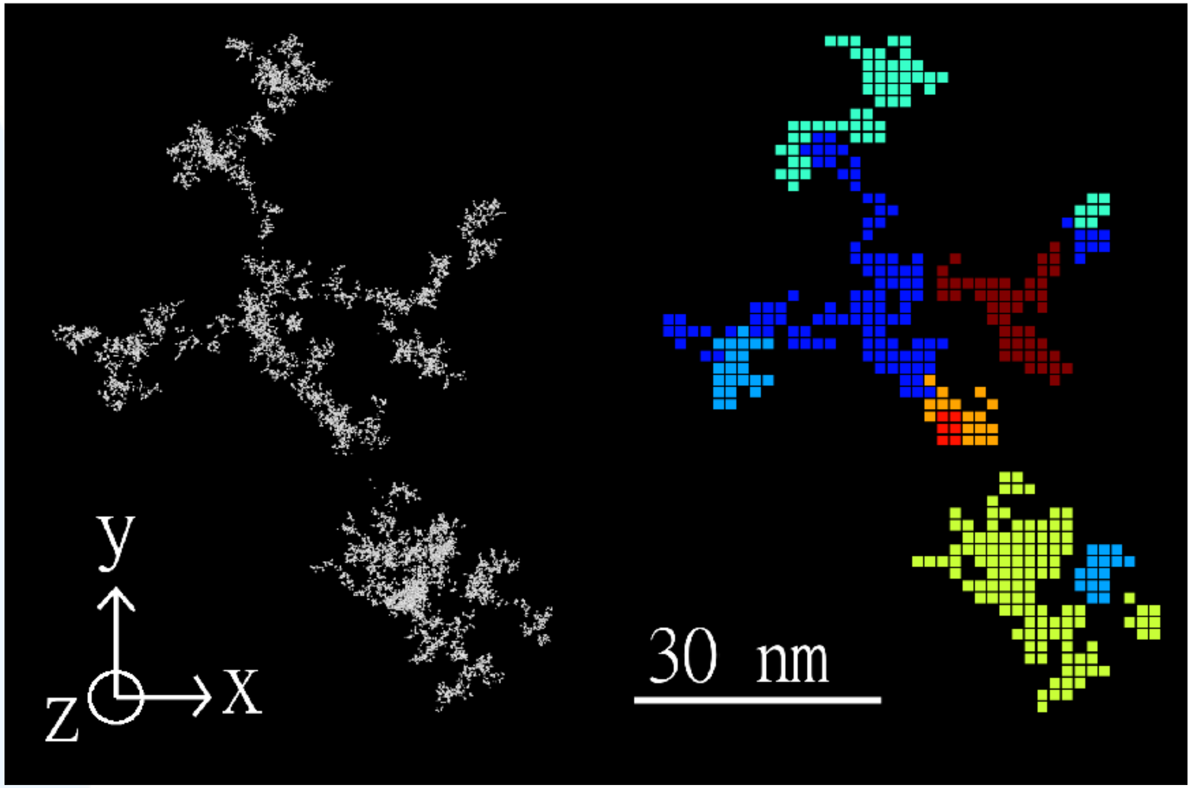


# BCA (SDTrimSP) – MD cross comparison Sub-cascades analysis

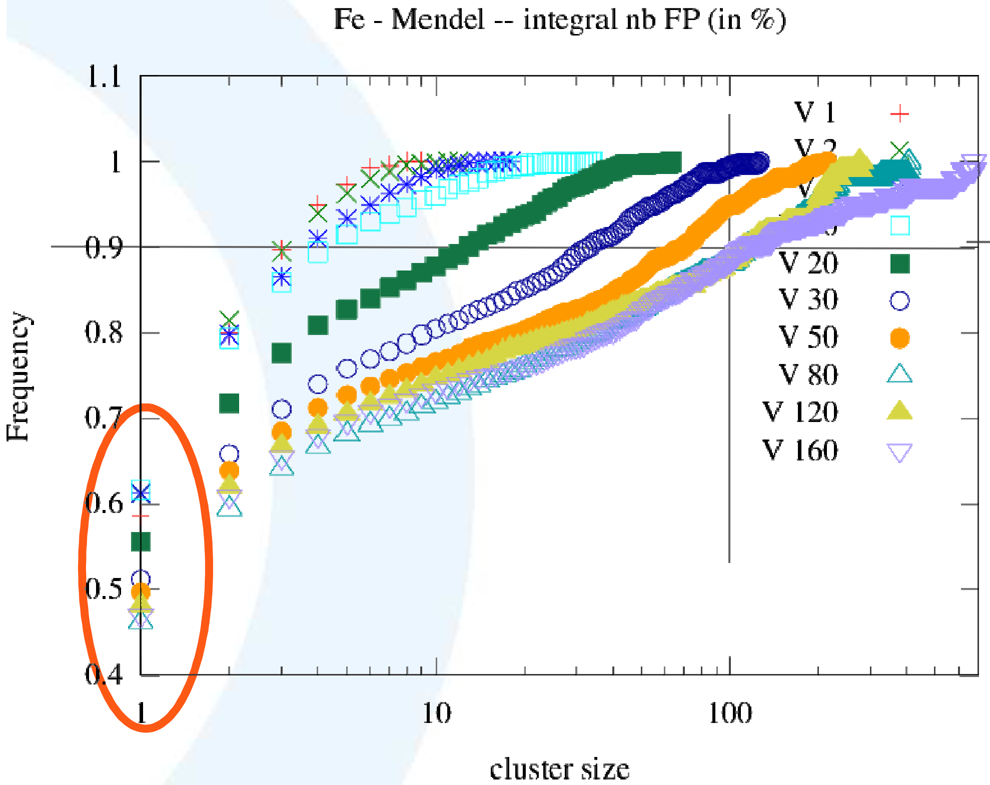


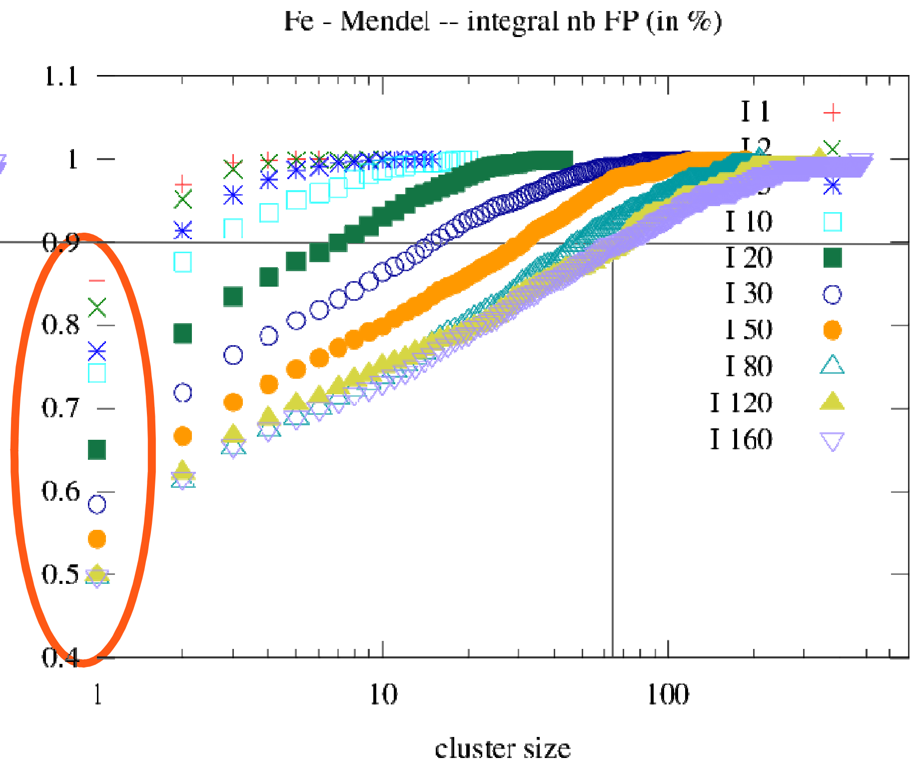

1 MeV PKA in W

[De Backer EPL2016]

# Defect size distribution

MD cascades – DYMOKA code – <135> & random PKA
PBC – constant volume
Very large statistics
Around 500 – 1000 cascades / PKA energy / potential / T
PKA energy: 1 keV to 160 keV (@ 100K)



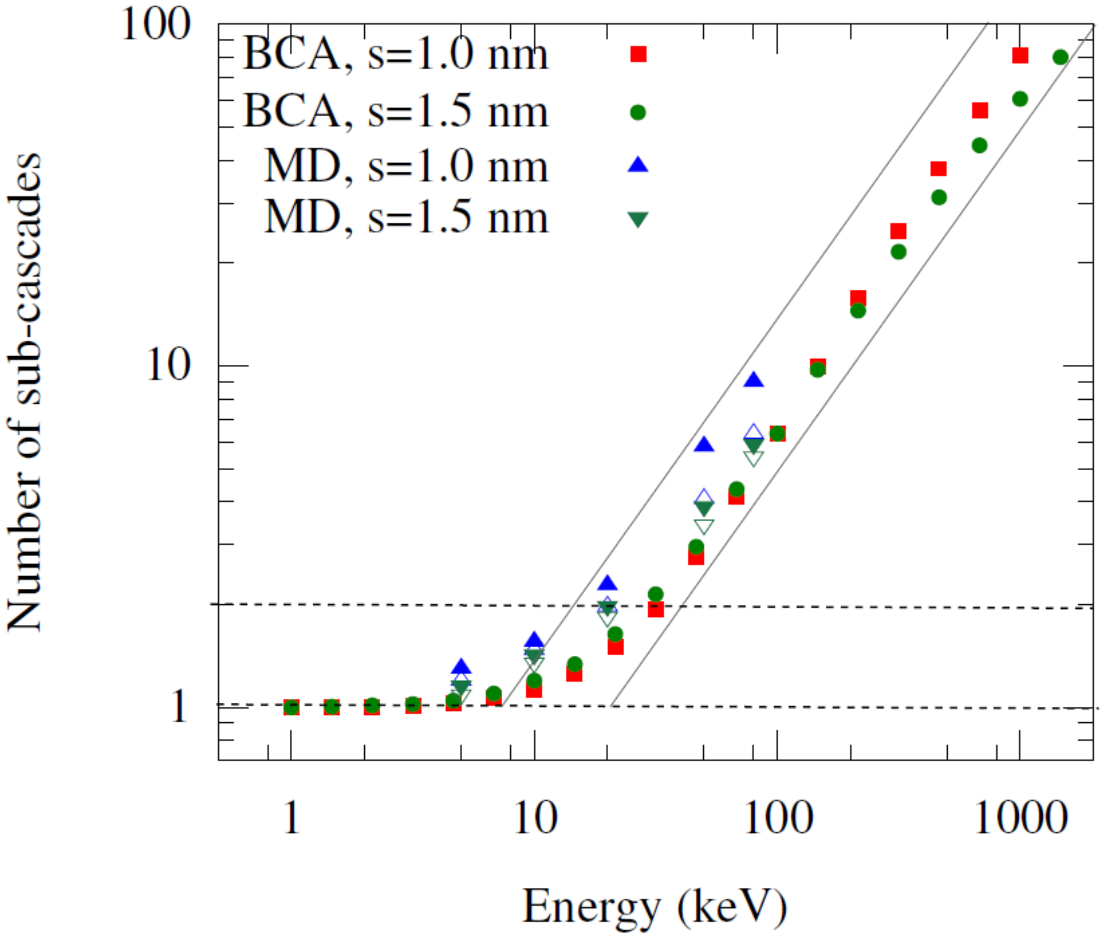

For PKA >=80 keV

- 50% mono defects
- 10% SIA clusters > 100

Pot Fe: EAM Ackland 2004

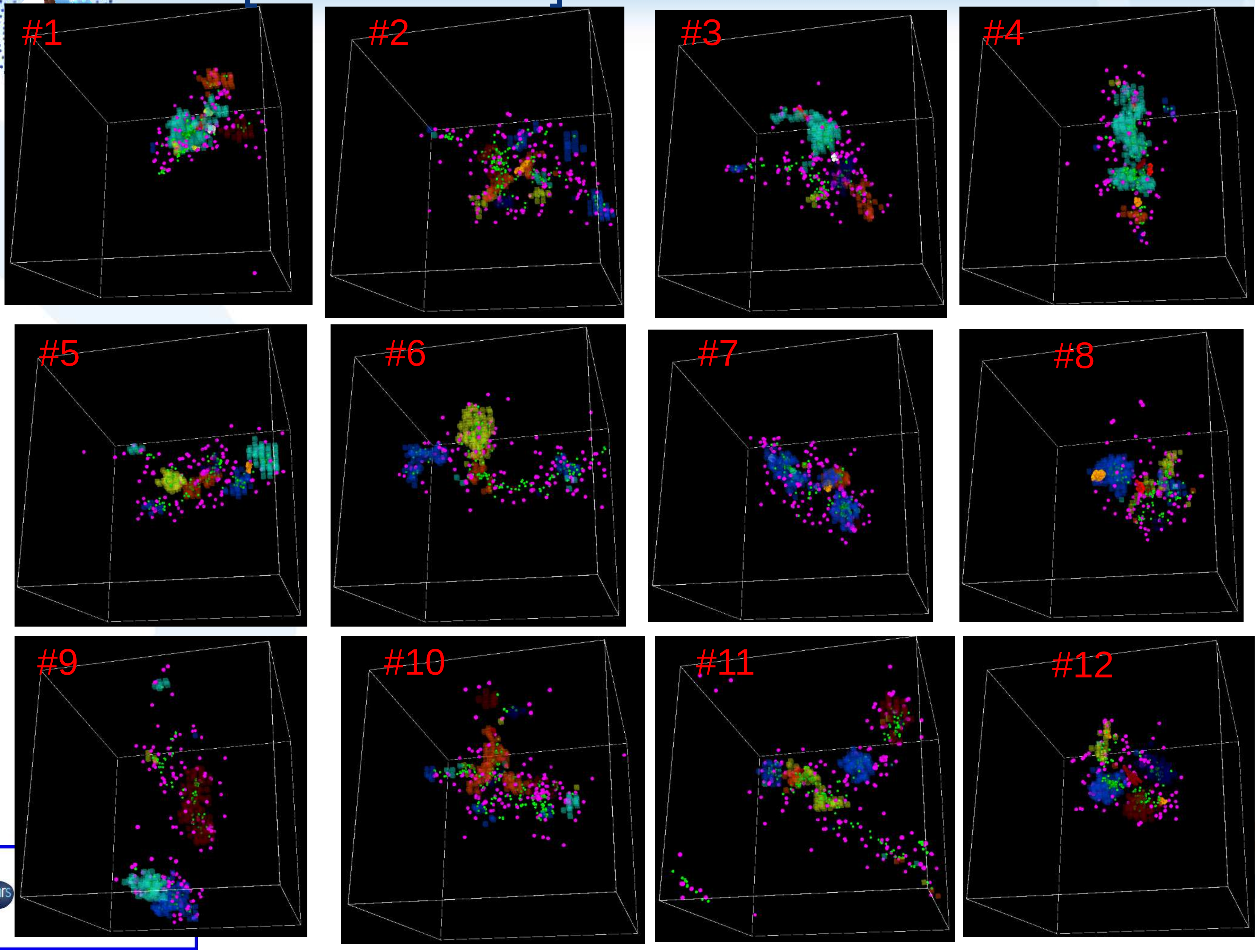
[Domain to be published]

# Sub cascades
# BCA (SDTrimSP) – MD cross comparison

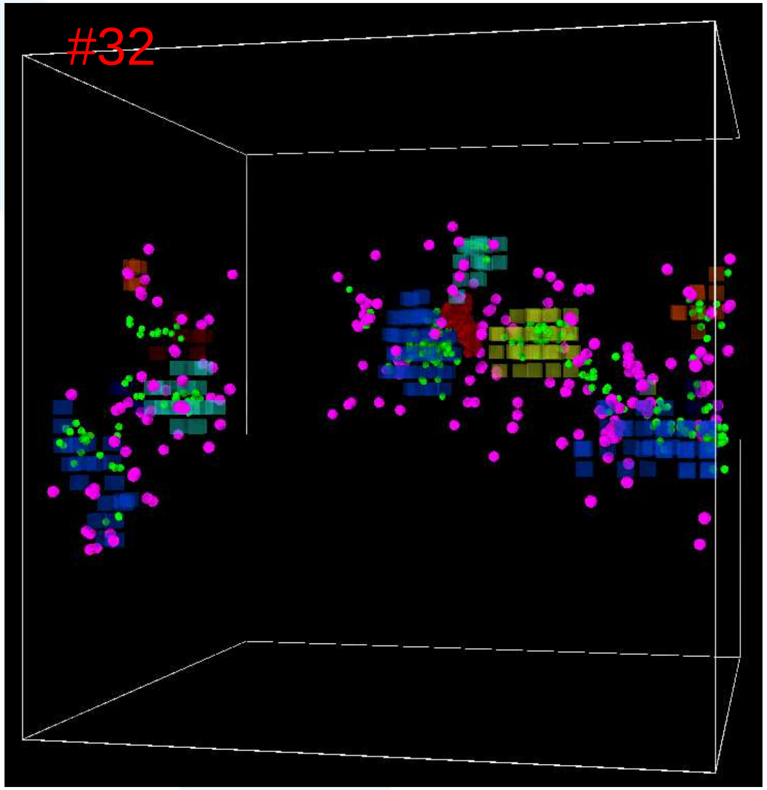


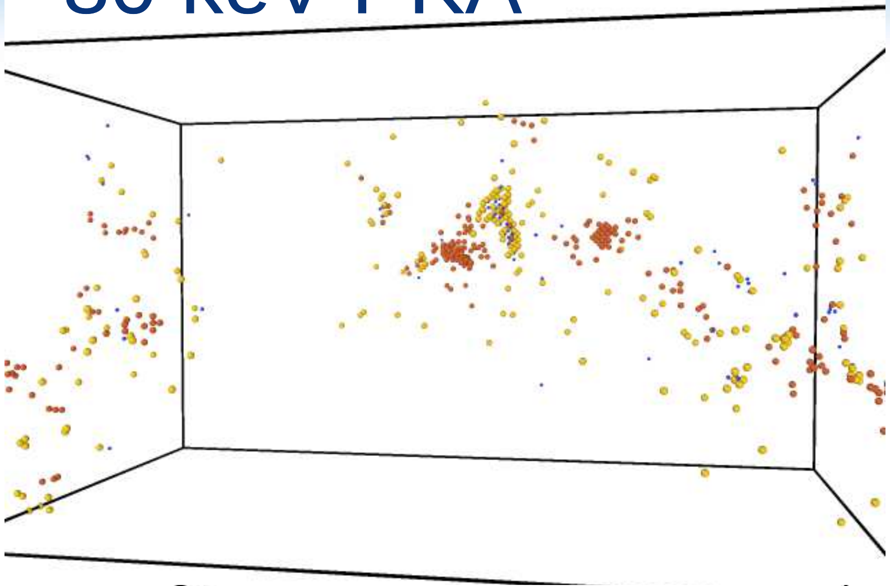

[De Backer to be published]

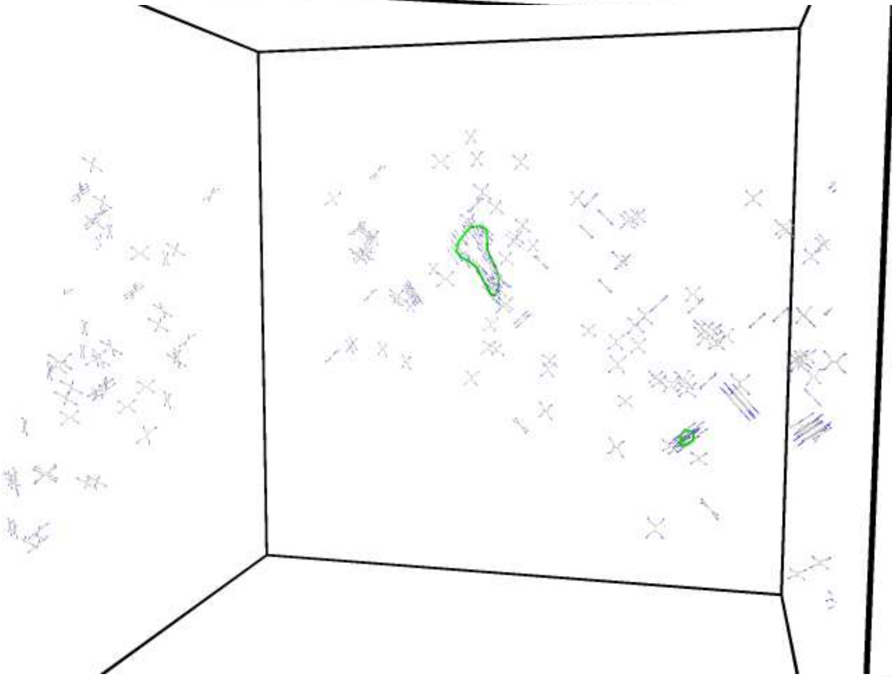
# Fe [Ackland 04] – 80 keV PKA



# Fe [Ackland 04] – 80 keV PKA

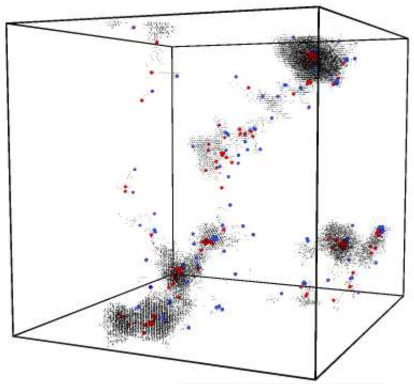


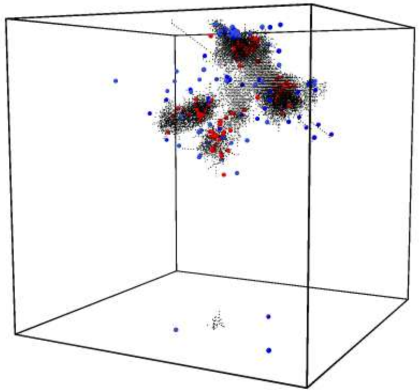


# Transition metals comparison (Zr, Fe, Ni, W)

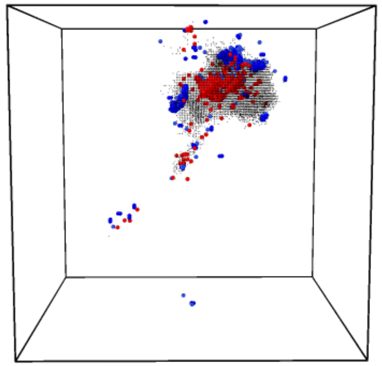
E_PKA = 50 keV



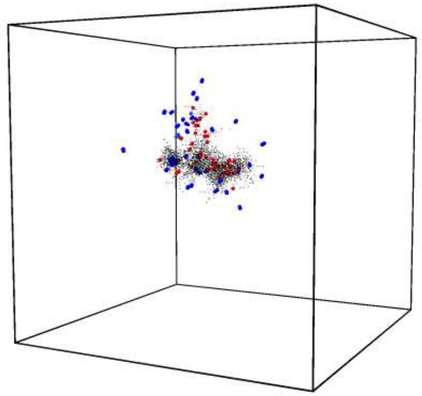
Zr



Fe

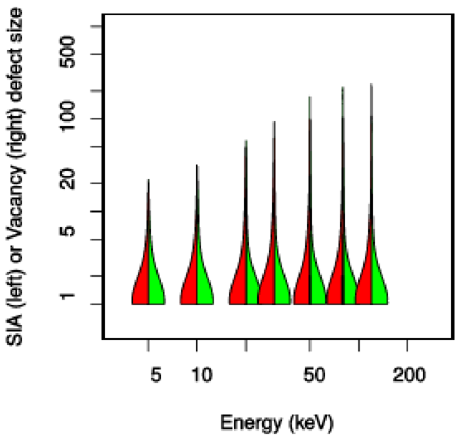


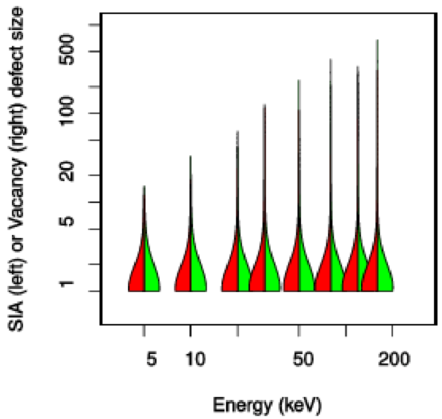
Ni



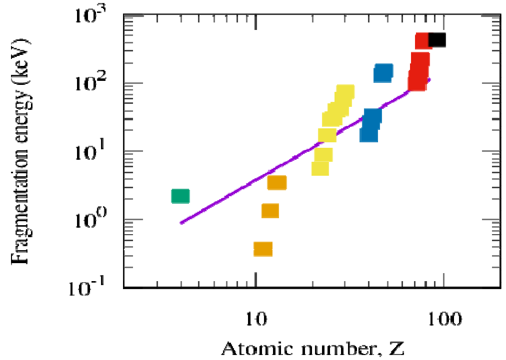
W (MSh)

Defect size distribution

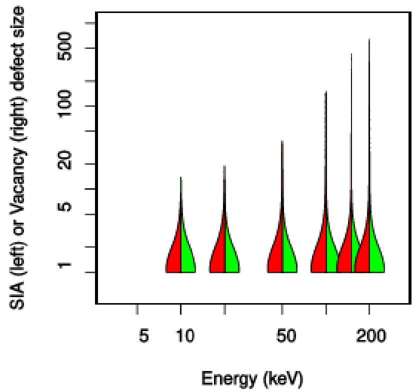



[Domain to be published]




[De Backer to be published]



# Conclusions

- Large cascade database
  - **Defect size distribution(PKA energy, potentials)**
  - **Good comparison and complementarity with BCA**
- Effect of potentials: equilibrium & hardening
  - **Assessment / hardening of potentials based on DFT**
  - **Some Similarities for other metals (e.g. Zr, Ni, W, Mo)**
- Impact on microstructure modelling
  - **Different class of objects formed (e.g. loops)**
- Database
  - **Potential: tabulated (no functions)**
  - **All atomic positions (XYZ format)**
- Experimental validation
  - **TEM invisible defects: HDS, …**
  - **Low temperature controlled irradiation, isochronal annealing**
  - **Modelling of experiments (e.g. TEM, HDS, PA)**