Damage distribution in f.c.c. and b.c.c. metals from molecular dynamics and its influence on microstructure evolution

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Technical Meeting on
A Database of Atomic Configurations Formed in Collision Cascades, IAEA, Vienna, Nov. 2017

Collaborators and co-authors

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- Naoki Soneda, CRIEPI, Japan
- C. Björkas, A. Sand, K. Nordlund, University of Helsinki
- M. J. Aliaga, UA
- Anna Prokhodtseva, R. Schaeublin, ETH-Zurich
- M. Hernández-Mayoral, CIEMAT

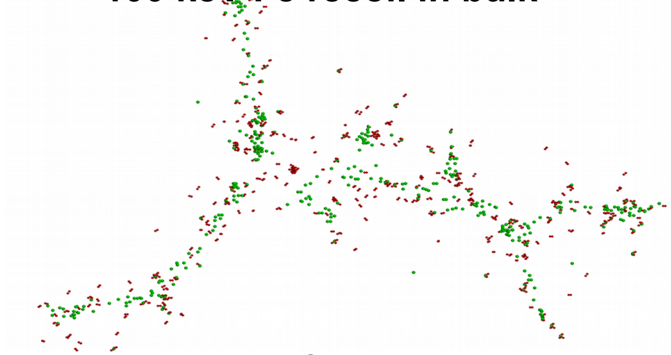
Outline

- Effect of crystal structures: collision cascades in f.c.c. vs. b.c.c. materials - Cu vs. Fe and microstructure evolution
- Bulk and surface effects: collision cascades in Fe and microstructure evolution
- Outlook: modeling MeV damage distribution

MD database + DFT data → OKMC → Experiments

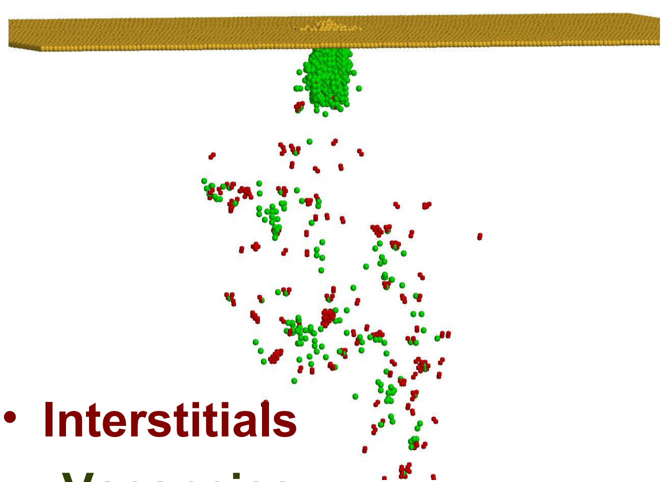
MD + DFT → OKMC → Exp

100 keV Fe recoil in bulk



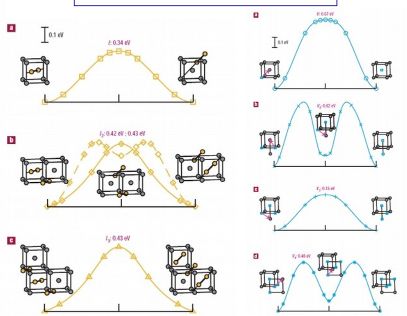
70 nm

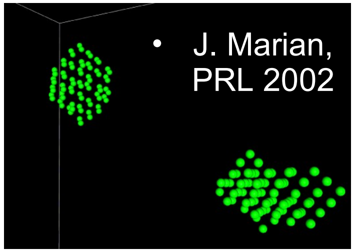
100 keV Fe recoil in thin film

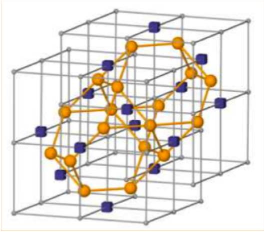


- **Interstitials**
- **Vacancies**

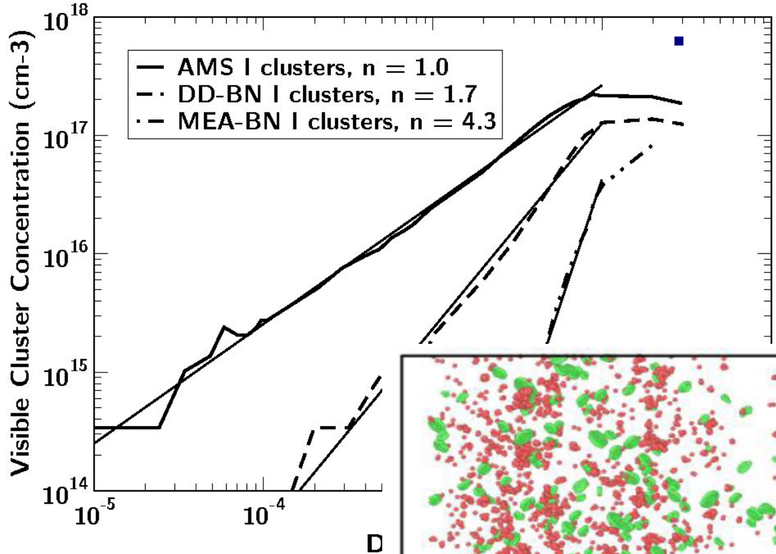
C. C. Fu et al.
Nature Mat. (2004)

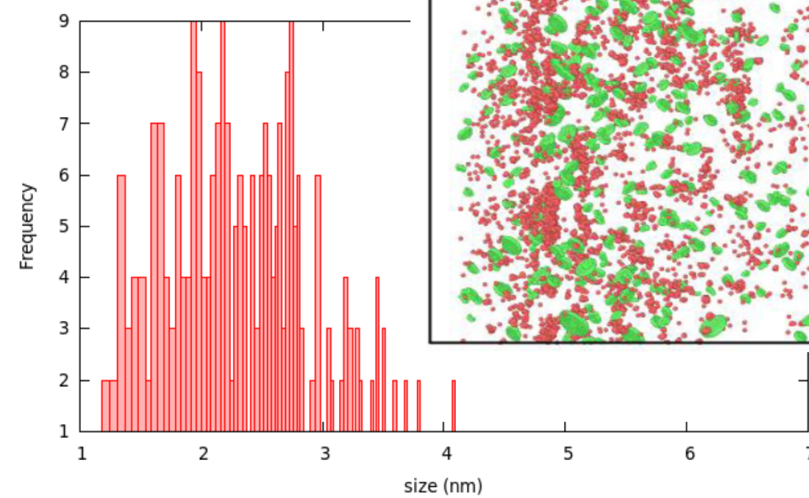


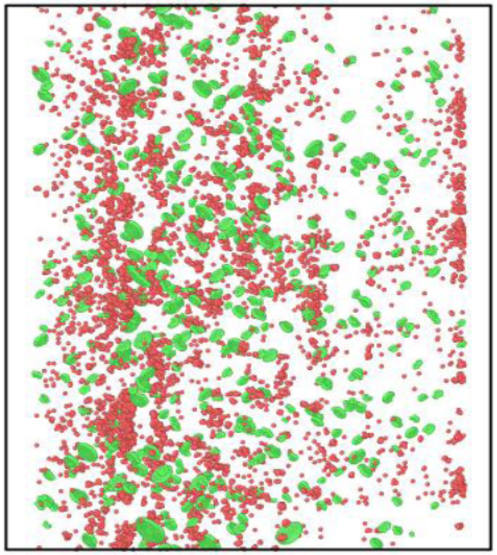




Marinica PRL (2012)

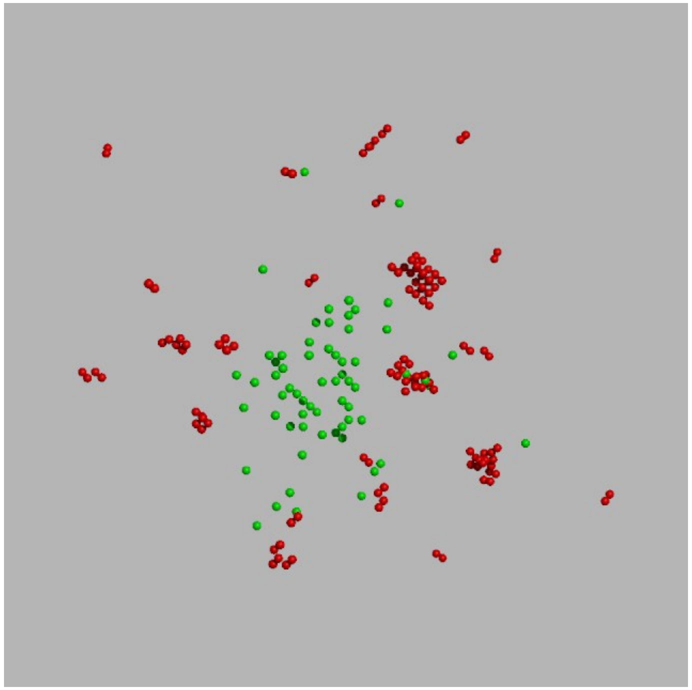






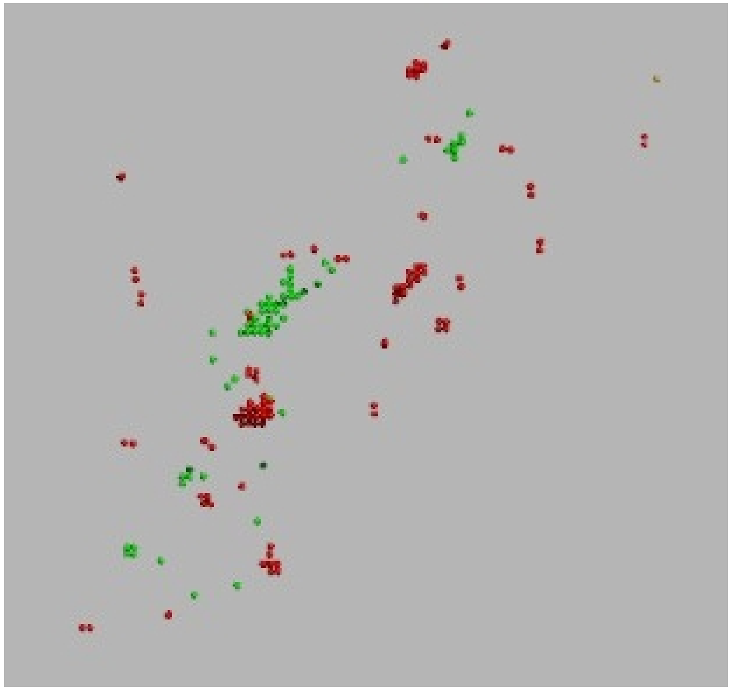
Primary damage: influence on microstructure evolution

b.c.c. Fe



Fe 30keV, 66 defects

f.c.c. Cu



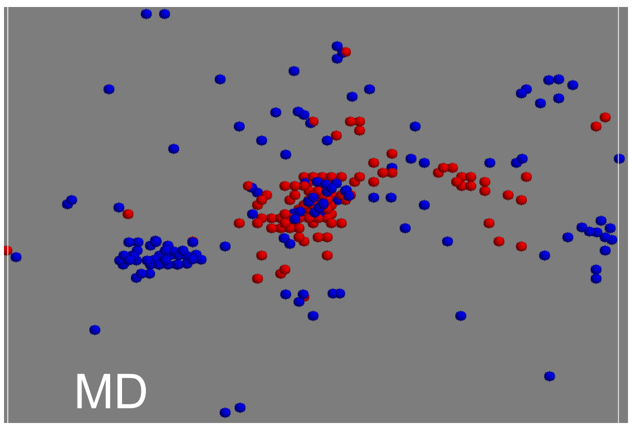
Cu 30keV, 69 defects

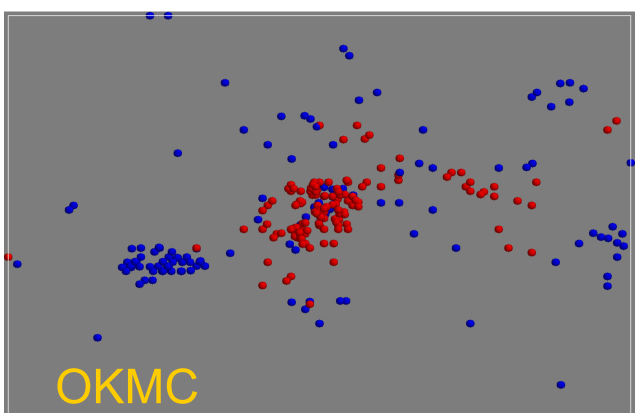
Similar number of defects but more vacancy clustering in Cu than in Fe
This has important consequences in the subsequent damage evolution

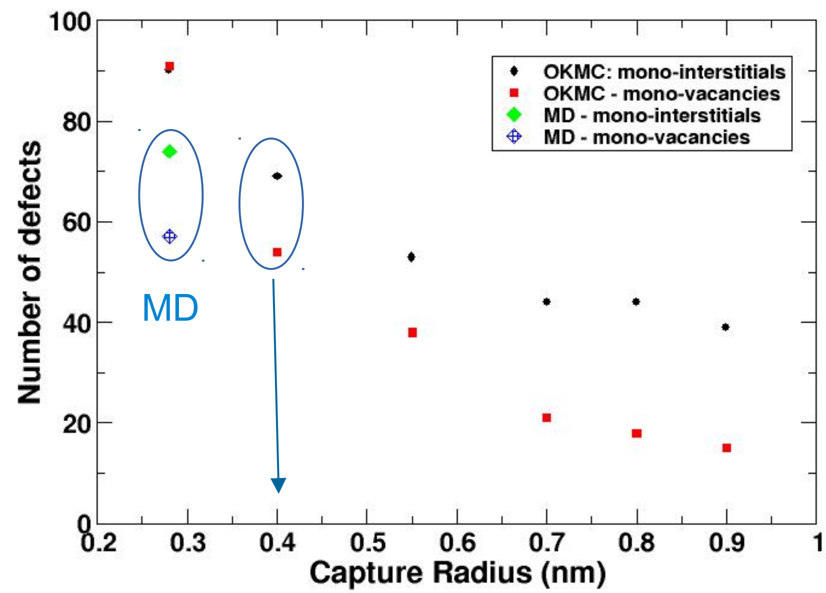
Transfer of data from MD to OKMC

Modular Monte Carlo MMonCa

Capture radius for individual defects selected to reproduce the isolated number of defects obtained in MD





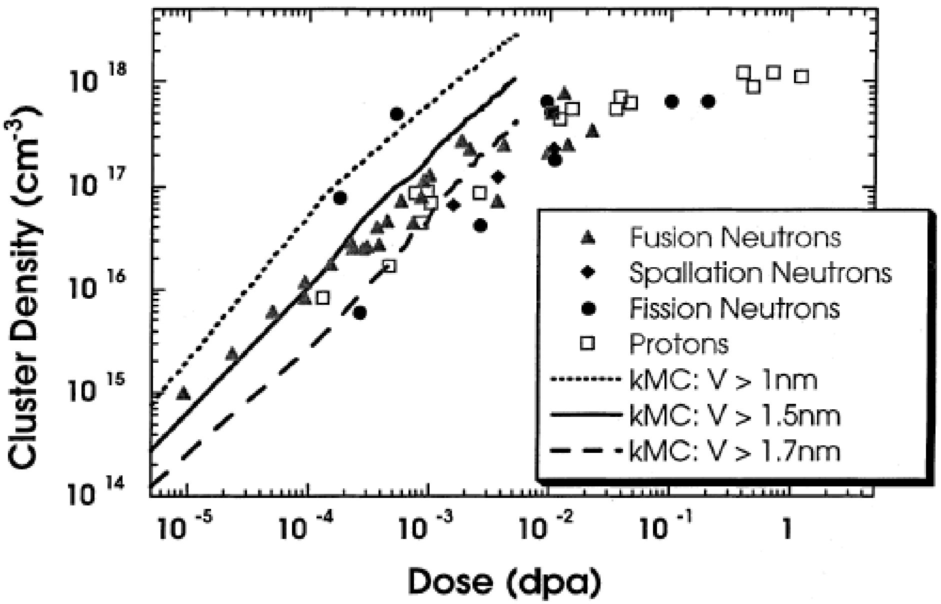


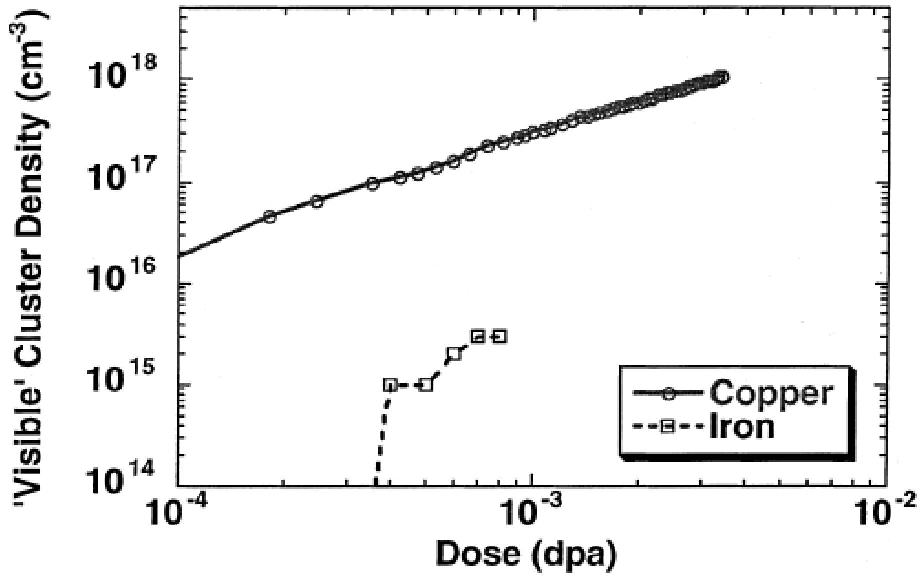
Capture radius: 0.4 nm

Damage accumulation in Cu and Fe

Damage accumulation in Cu and Fe compared to experiments

Fe calculations – N. Soneda

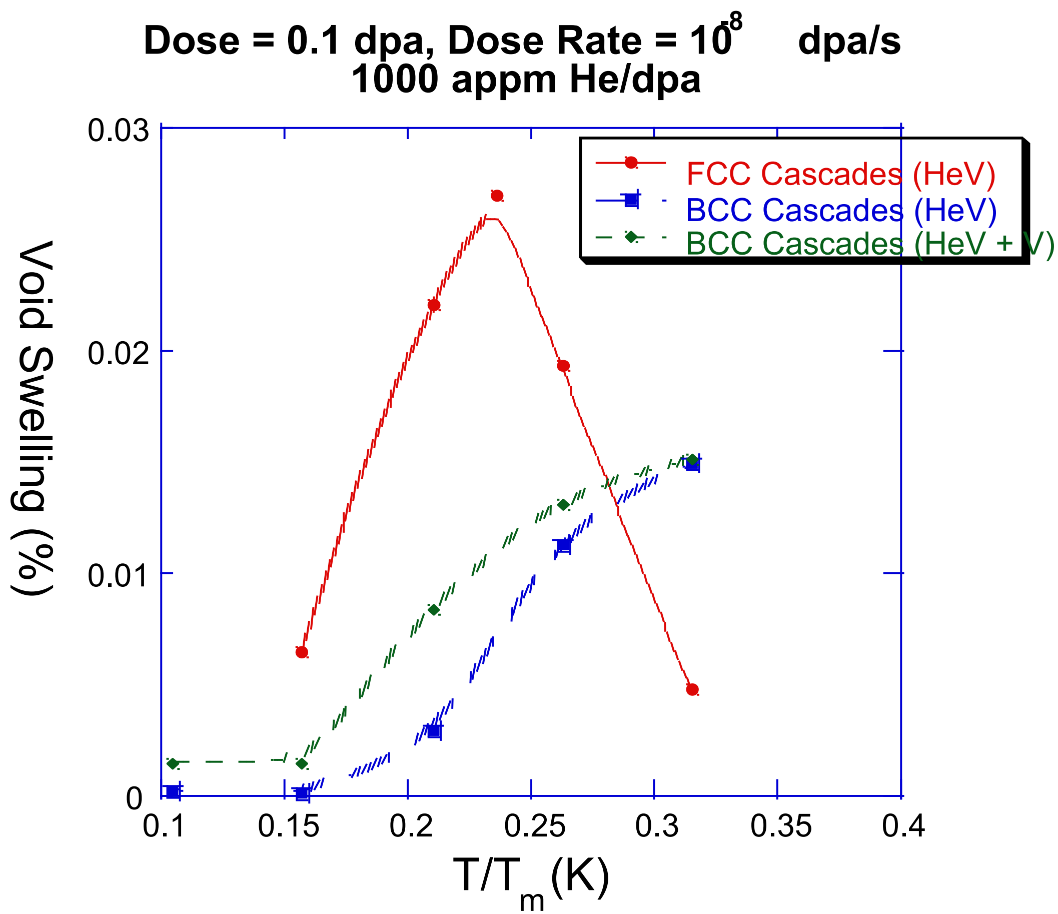




Simulations explain the basic differences observed experimentally in Cu and Fe: nucleation of vacancy clusters in Cu together with fast migration of self-interstitials, the presence of traps in Fe and the visibility under TEM

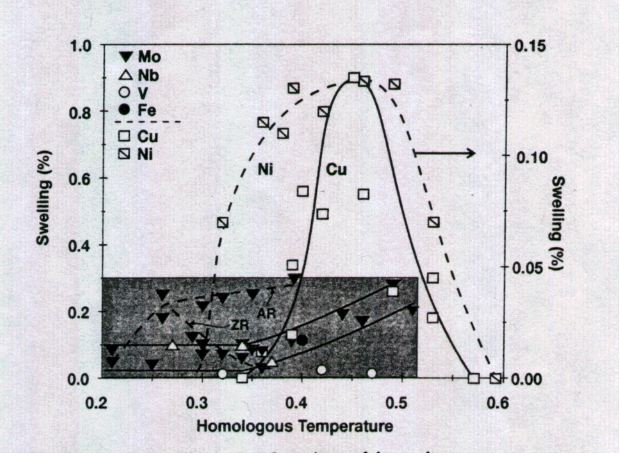
M. J. Caturla, N. Soneda, et. al, JNM 276, 12 (2000)

Long term evolution of He-V clusters depends on initial damage state



M. J. Caturla, N. Soneda, T. Diaz de la Rubia, M. Fluss, J. Nucl. Mat. 2006, 351, 78

KMCO reproduce qualitatively the experimental swelling dependence with temperature for fcc and bcc

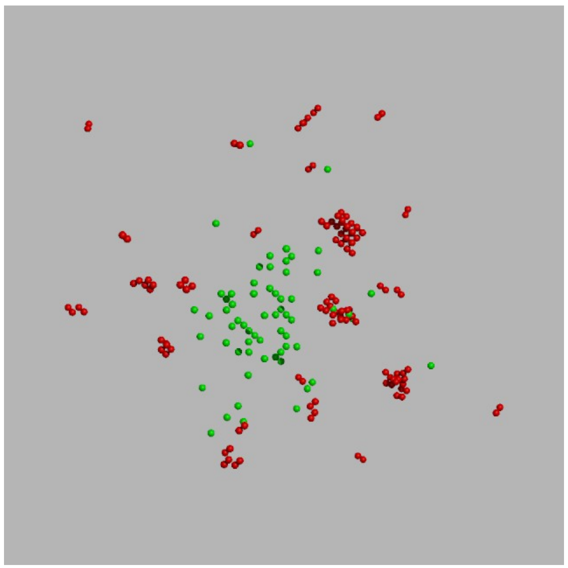


Void swelling in FCC and BCC metals irradiated with fission neutrons
B. N. Singh, J. H. Evans, JNM 226 (1995) 277-285

Influence of initial cascade damage distribution on damage accumulation (Carolina Björkas, Univ. Helsinki)

Question addressed: Is the long term evolution of defects affected by the picosecond cascade damage distribution or does it only depend on migration and binding energies?

30keV Fe in bcc Fe



OKMC calculations using cascade damage distributions from 3 different interatomic potentials, AMS [1], DD-BN [2,3] and MEA-BN [3, 4]

[1] G. J. Ackland, M. I. Mendelev, et al. J. Physics: Condens. Matter, 16 (2004) [2] S. L. Dudarev and P. M. Derlet. J. Phys.: Condens. Matter, 17 (2005) [3] C. Bjorkas and K. Nordlund, Nucl. Instrum. & Meth. B 259 (2007) [4] M. Muller, P. Erhart, and K. Albe, J. Phys.: Condens. Matter, 19 (2007)

NO EXPERIMENTAL VALIDATION OF MD RESULTS ON SINGLE CASCADE DAMAGE

C. Björkas, et. al. Phys. Rev. B 85, 024105 (2012)

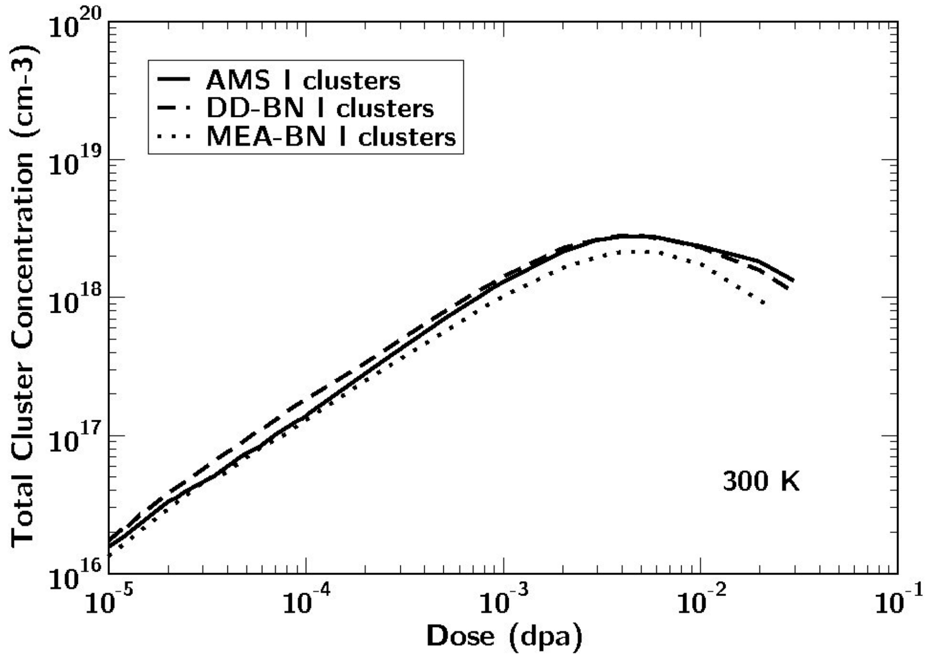
Influence of initial cascade damage distribution on damage accumulation (Carolina Björkas, Univ. Helsinki)

OKMC simulations

TOTAL DEFECT CONCENTRATION:

no significant difference between the three potentials

I > 5 mobile <111> + traps (0.9 eV)



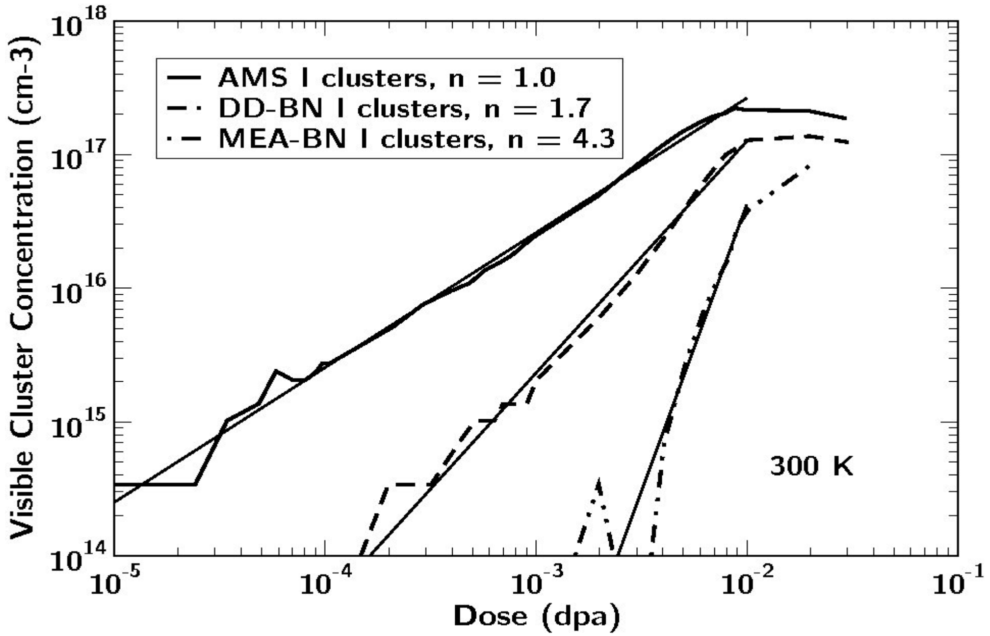
Influence of initial cascade damage distribution on damage accumulation (Carolina Björkas, Univ. Helsinki)

VISIBLE DEFECT CONCENTRATION:

only those clusters of interstitials > 55 (loop of 1nm radius)

only those clusters of vacancies > 350 (void of 1nm radius)

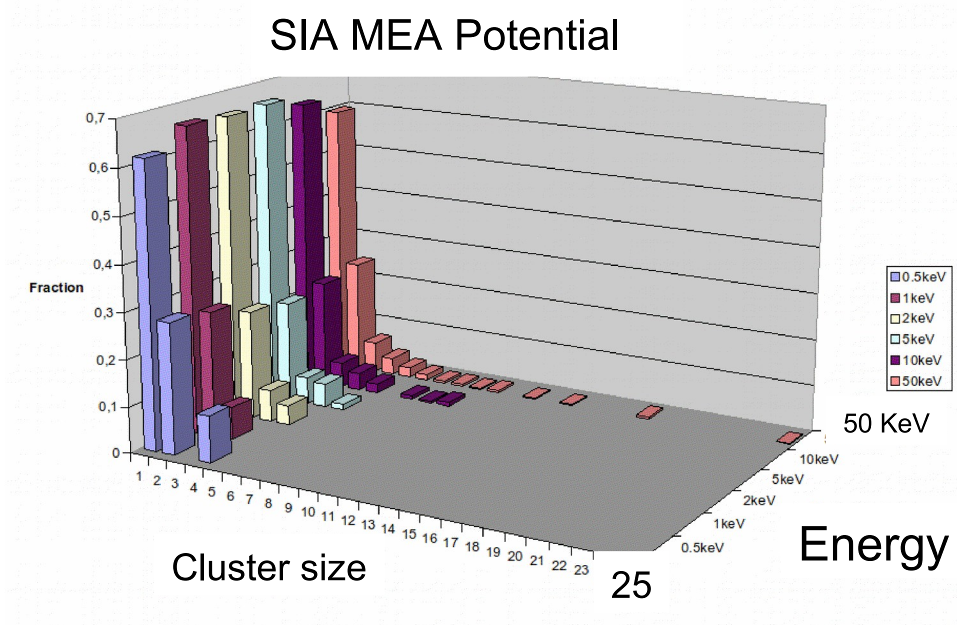
I > 5 mobile <111>
+ traps (0.9 eV)

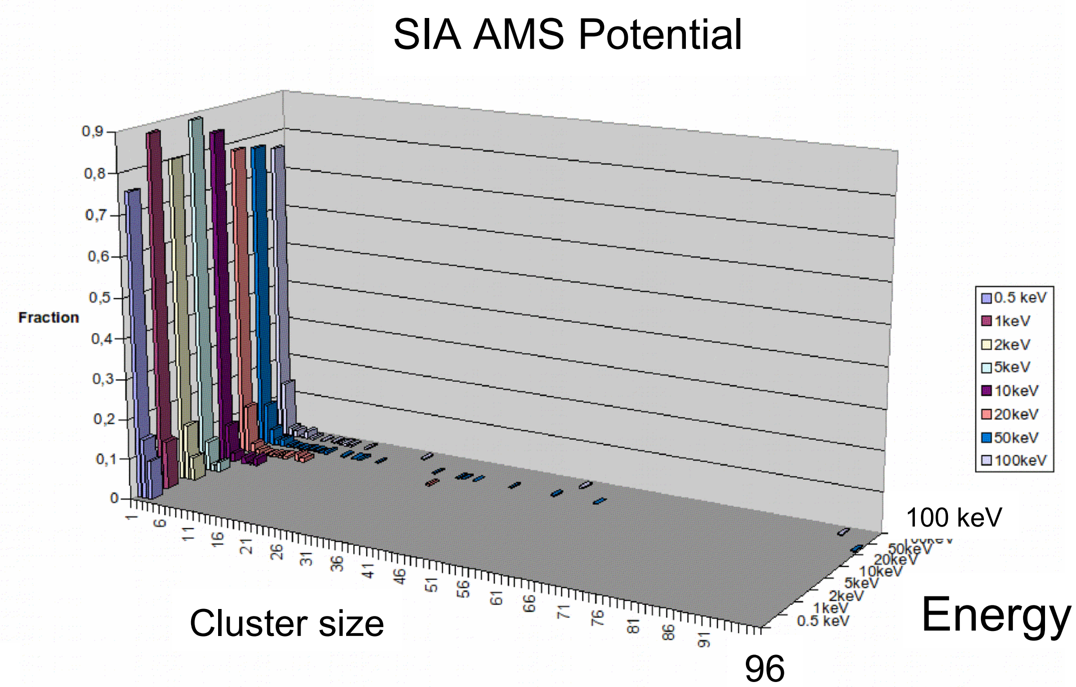


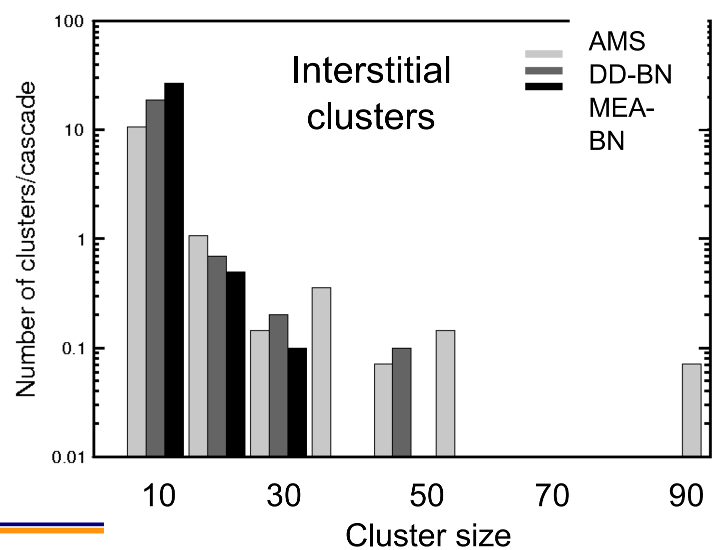
Large differences are now observed between the three potentials

Universitat d'Alacant
Universidad de Alicante

Differences in cluster size distribution with int. potential (Carolina Björkas, Univ. Helsinki)





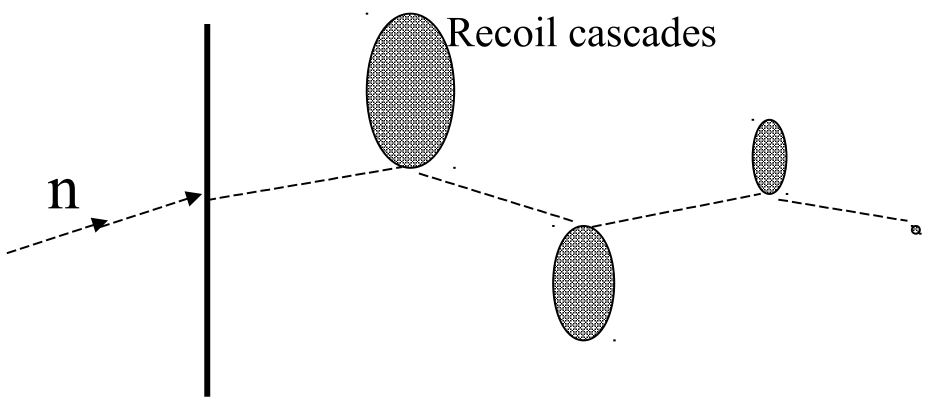


AMS potential predicts significantly larger self-interstitial clusters at 50keV cascades

Experimental validation of models

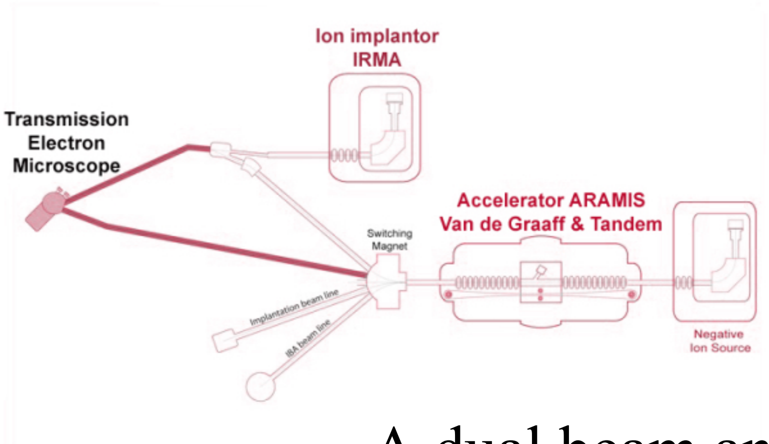
Multiscale modeling can only work with the proper experimental validation

Need to understand neutron damage up to 14 MeV
⇩
recoil production of 10s of keVs



Lack of neutron sources for fusion conditions

Use of ion irradiation to understand defect production and evolution



JANNUS

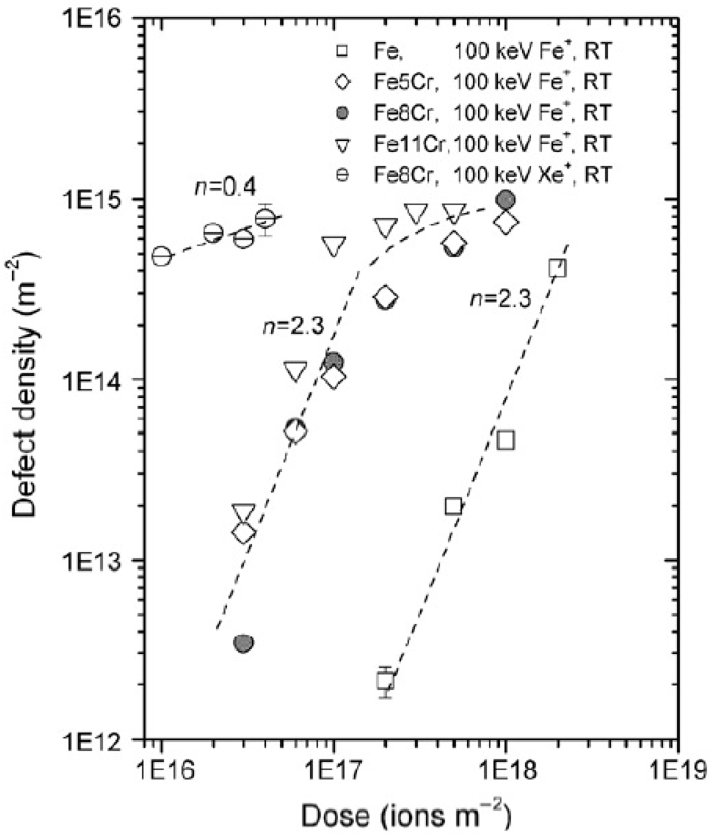
A dual beam and triple beam facility at CEA, France

http://jannus.in2p3.fr/

Model validation with ion sources – extrapolation to neutron irradiation conditions

Damage near the surface in pure Fe: experimental evidence

Z. Yao, et al., Phil. Mag. 88, 2851 (2008)

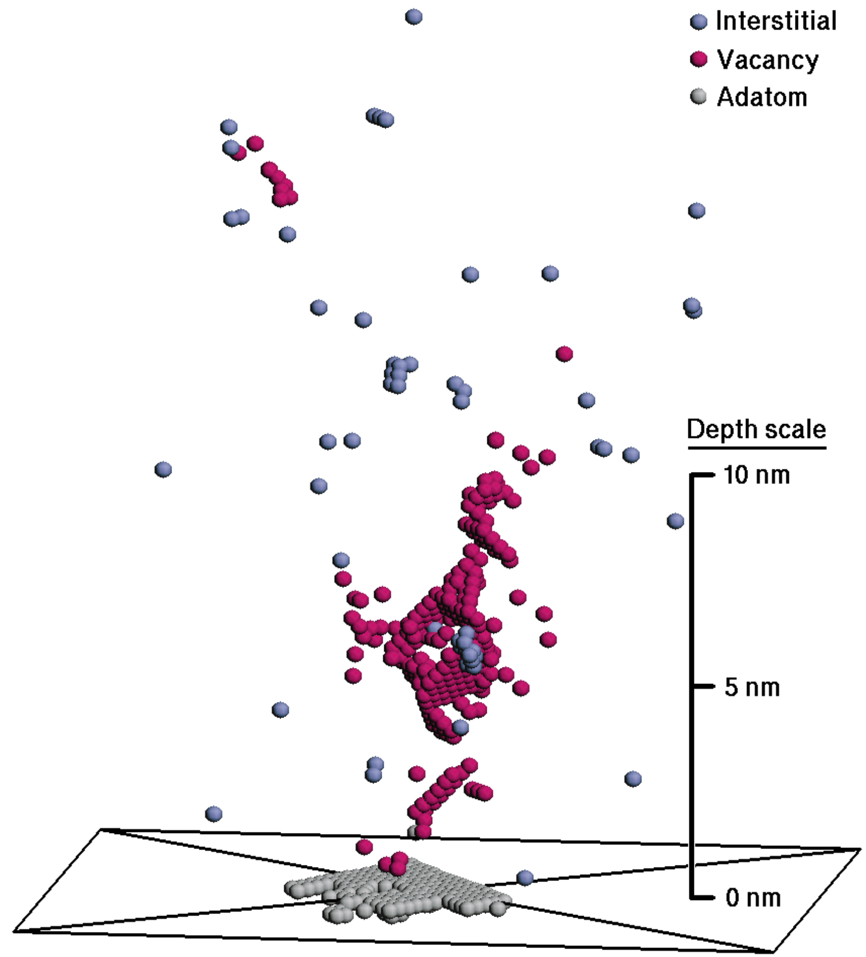


- Many of these experiments are performed using **thin foils** (less than 100nm)
- In pure and UHP Fe at **low doses** most of the loops are of type <100>
- **Loops near the surface** have been identified as of **<100> vacancy type** (for irradiation with Ga+)

Effect of free surfaces on cascade damage formation in Au
M. Ghaly, R. S. Averback & K. Nordlund

Dislocation structure

M. Ghaly and R. S. Averback,
"Effect of Viscous Flow on Ion Damage near Solid Surfaces," Phys. Rev. Let. 72, 1994.

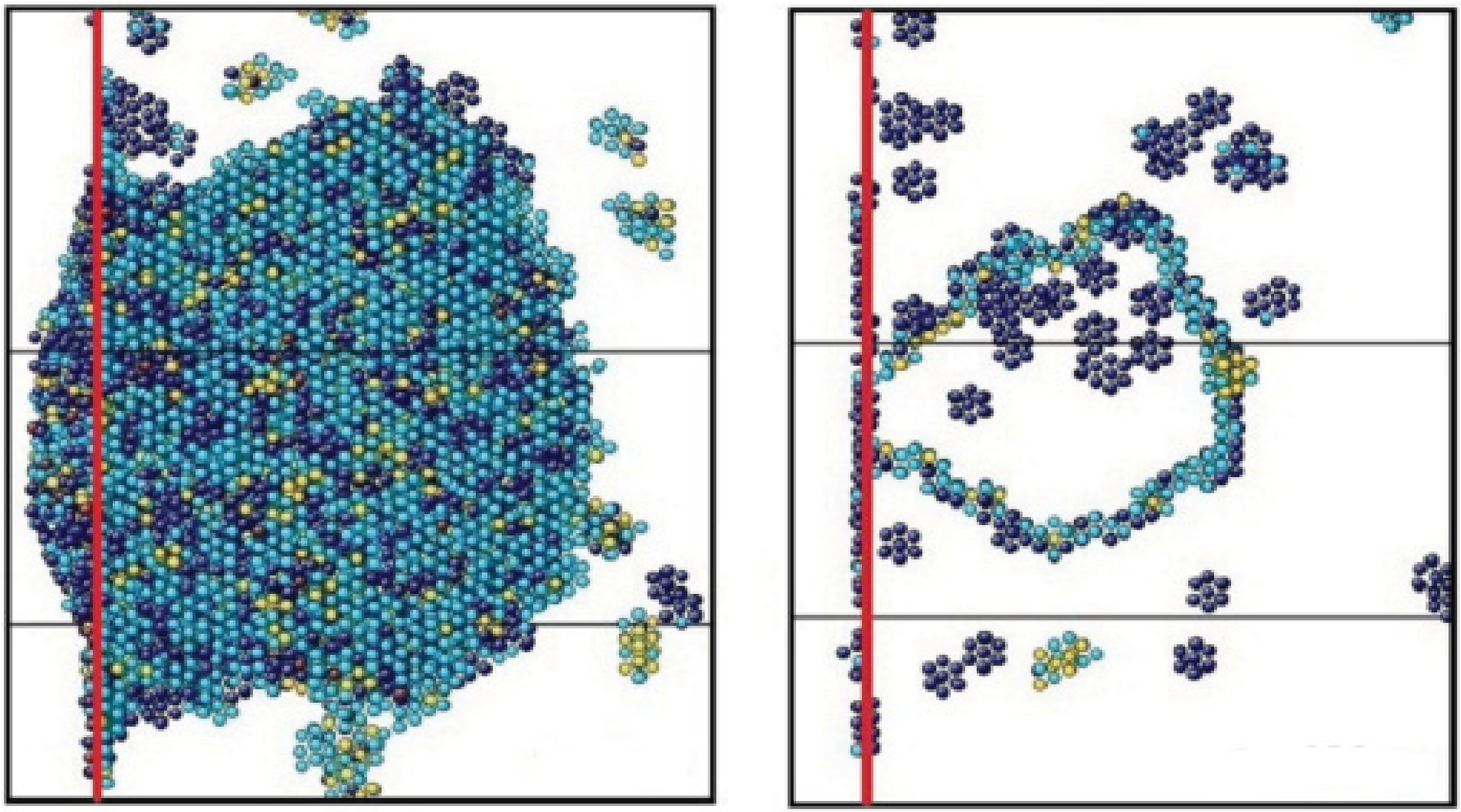


Coherent displacement

K. Nordlund et al., "Coherent displacement of atoms during ion irradiation", Nature 398, 1999

Effect of free surfaces on cascade damage formation in Mo
Sergey V. Starikov et al.

Vacancy loop formation

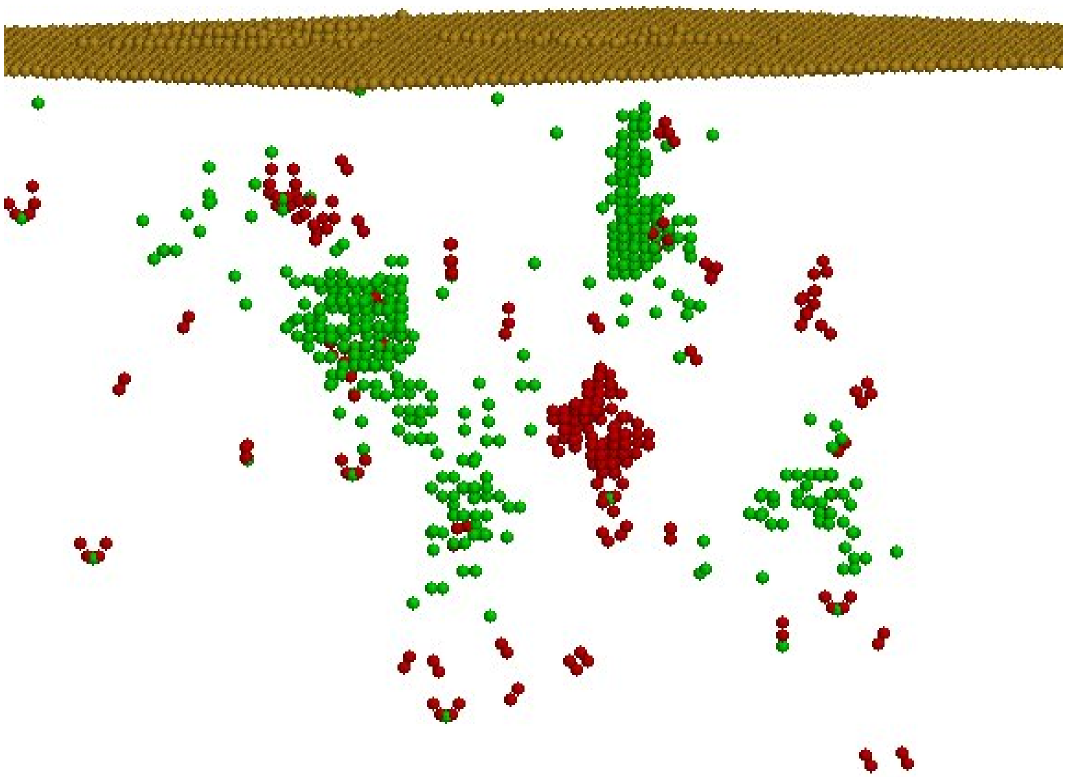


5.5 ps 89.3 ps

Sergey V. Starikov et al.,
“Radiation-induced damage and evolution of defects in Mo,” Phys. Rev. B 84, 2011.

Ion implantation in thin films for in situ TEM
Cascade damage for **50keV Fe in Fe** with AMS potential

50nm thickness



- Interstitials
- Vacancies

79% of all vacancies are in clusters
57% are in large clusters (>55 defects = 1nm loop)

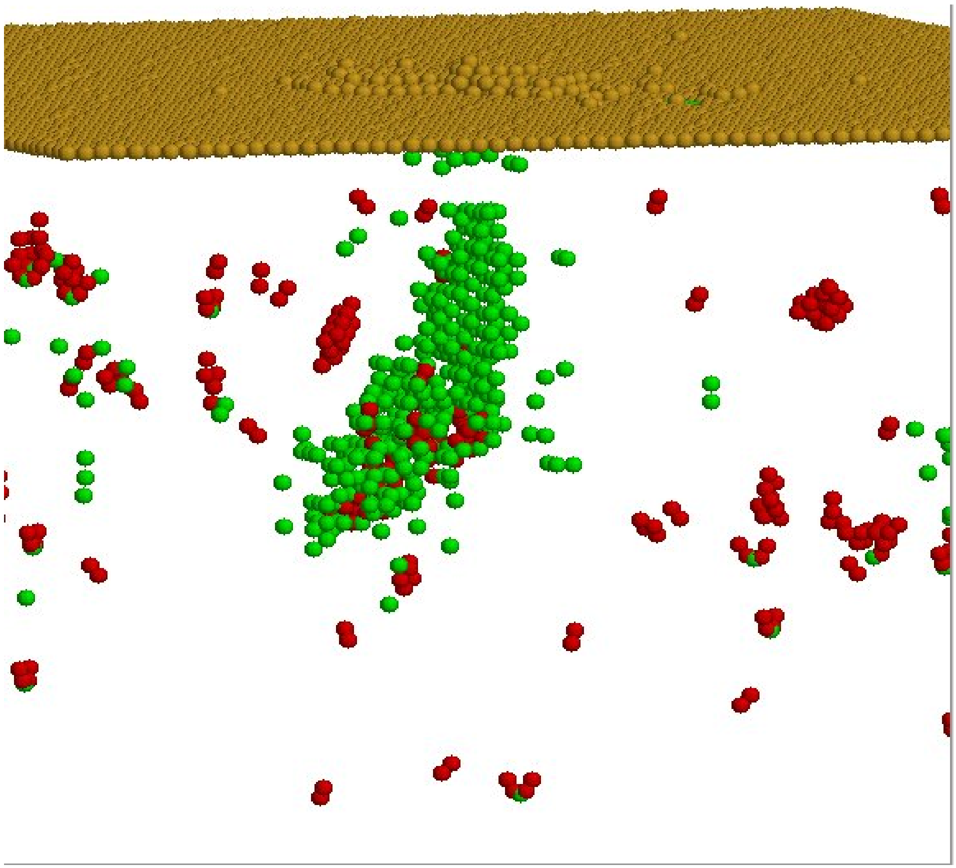
98% of all interstitials in clusters
21% in large clusters

296 ad-atoms

Larger clustering of vacancies compared to bulk cascades

Ion implantation in thin films for in situ TEM
Cascade damage for **50keV Fe in Fe** with AMS potential

50nm thickness



- Interstitials
- Vacancies

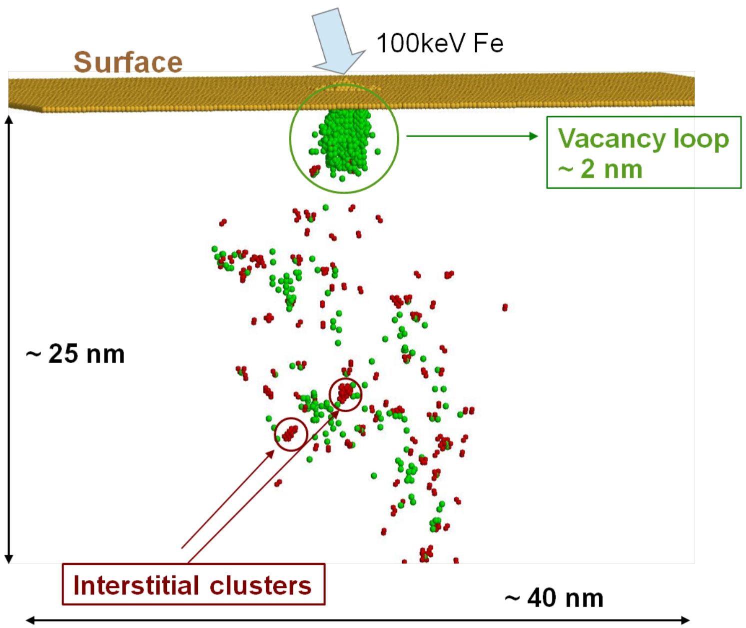
83% of all vacancies are in clusters
67% are in large clusters

100% of all interstitials in clusters
0 in large clusters

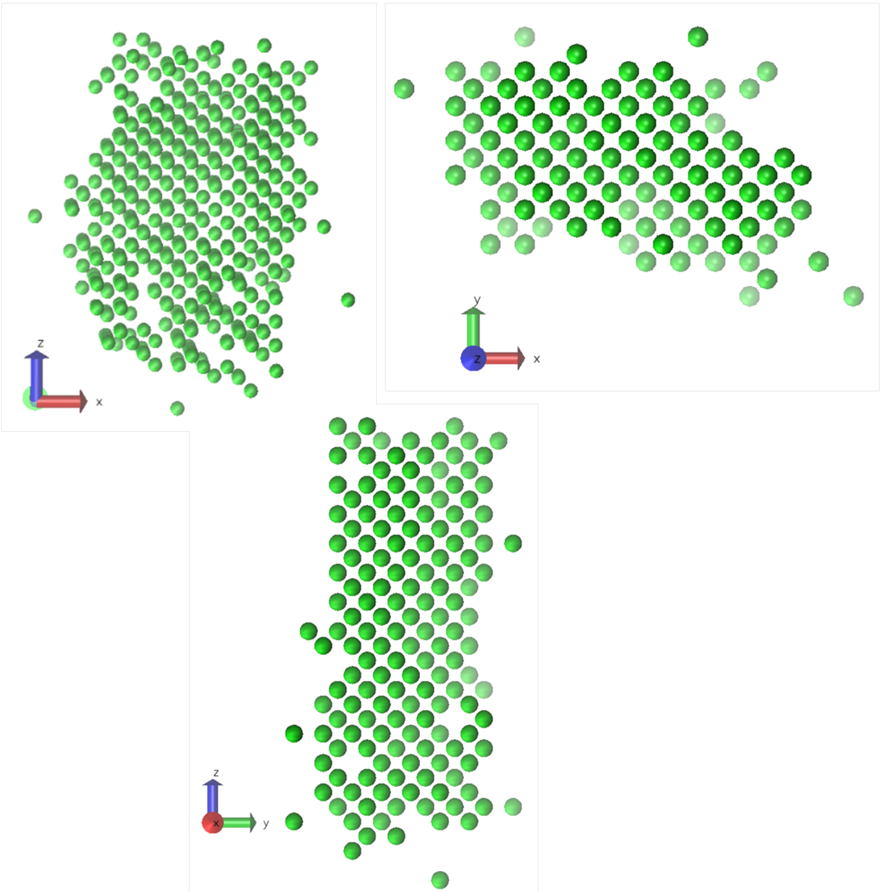
312 ad-atoms

Larger clustering of vacancies compared to bulk cascades

MD simulations of irradiation in Fe thin films
Enhanced production of vacancy loops, mostly <100>



(a)



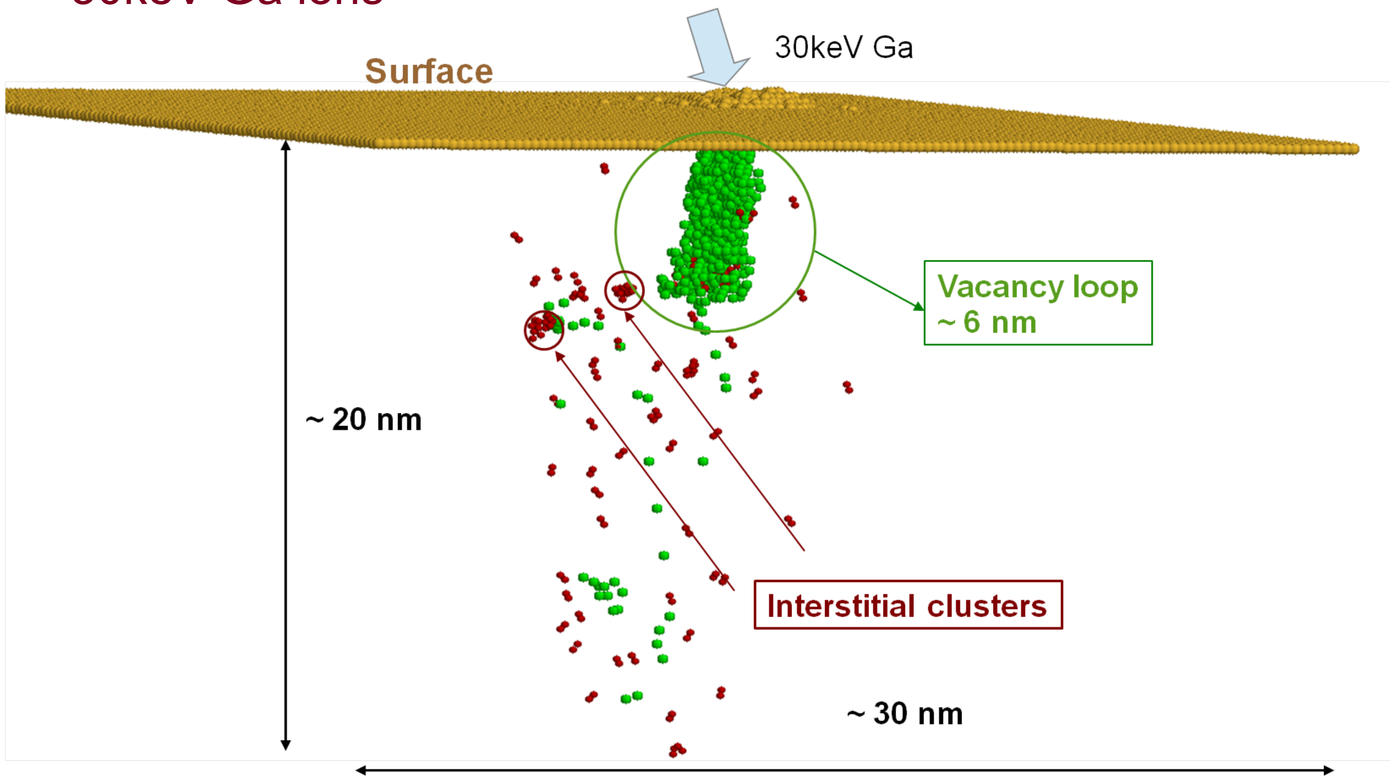
(b)

Irradiation of thin films at low energies (50-150keV) show the formation of large (~1nm radius) <100> vacancy loops. Mostly square loops as expected from energy considerations (Gilbert et al J.Phys:Cond.Mat. 2008)

M. J. Aliaga, et. al, Acta Mat. (2015)

Damage produced by Ga ions in Fe at low energies (30keV)

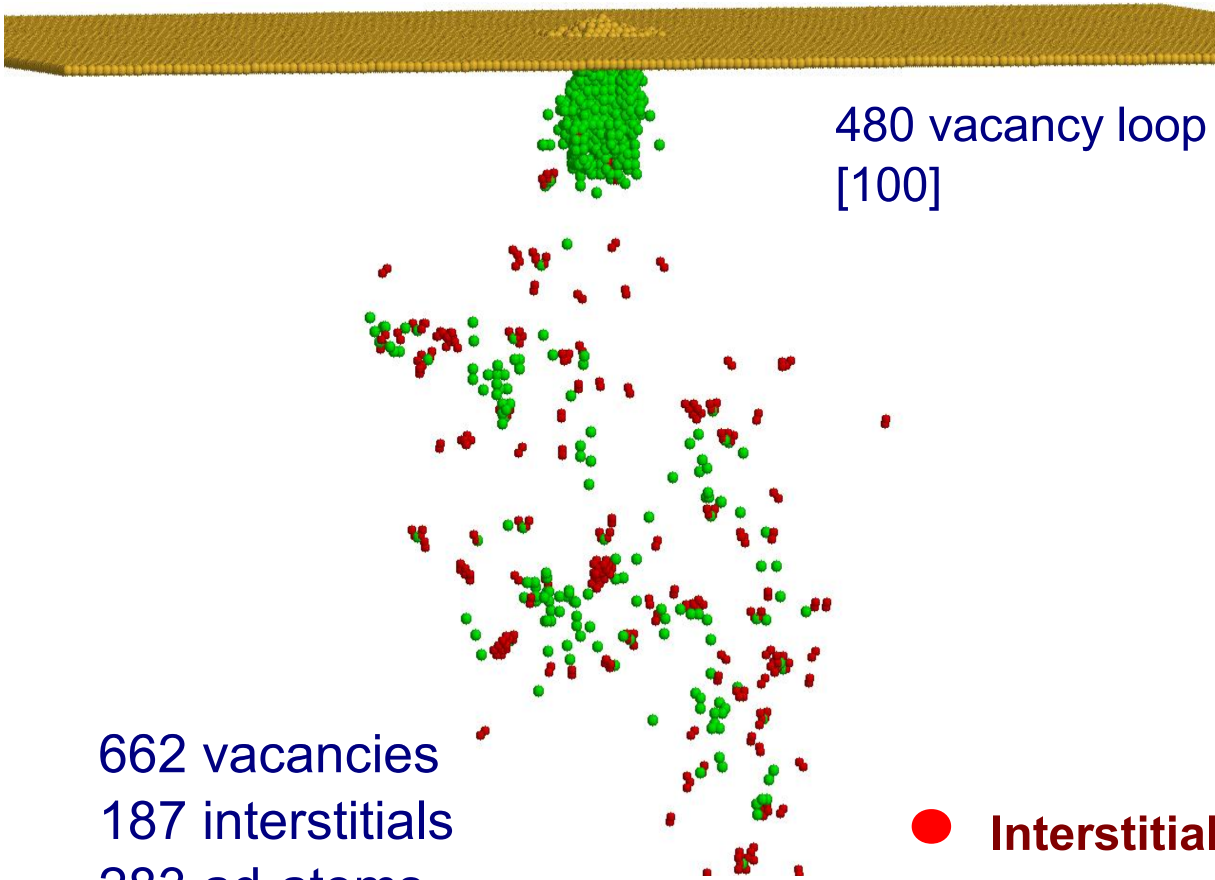
Thin film irradiation with
30keV Ga ions



Heavier ion (Ga) produces much larger vacancy clusters also of <100> type even at lower energies (30 keV), in agreement with experiments, M. L. Jenkins Nature (1976) & Z. Yao Phil. Mag. 2008

Ion implantation in thin films for in situ TEM
Cascade damage for **100keV Fe in Fe** with the AMS potential

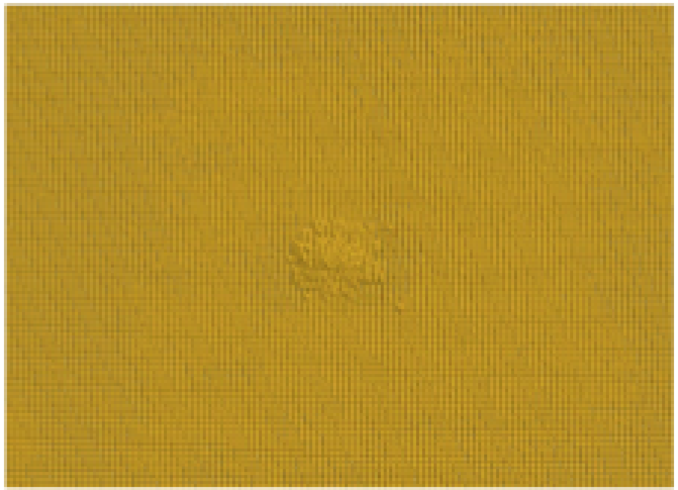
50nm thickness

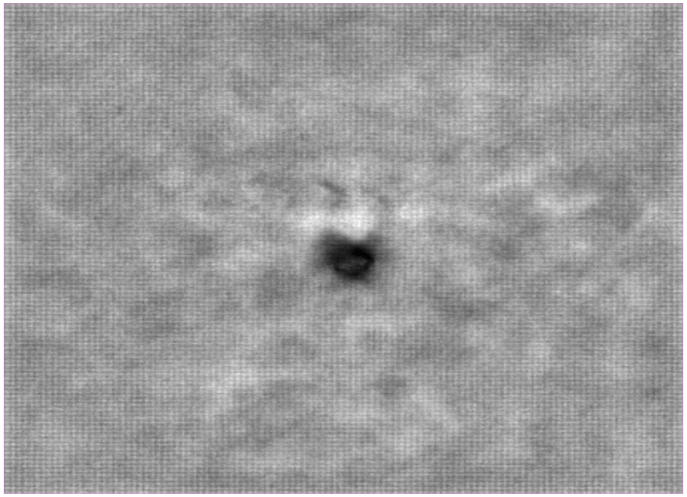


480 vacancy loop
[100]

662 vacancies
187 interstitials
283 ad-atoms

Interstitials
Vacancies

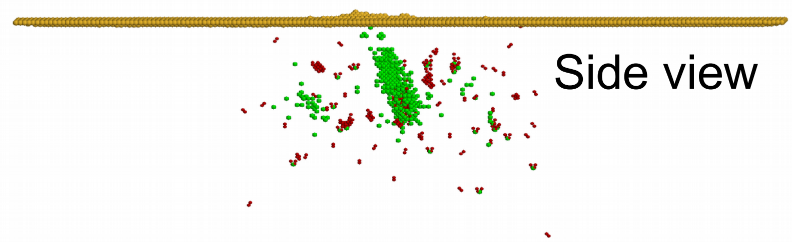




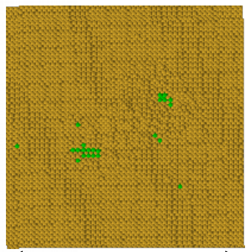
Simulated HRTEM image to compare to experiments – Robin Schaeublin

TEM image simulations: 50 keV cascade in Fe

R. Schäublin
M. J. Aliaga



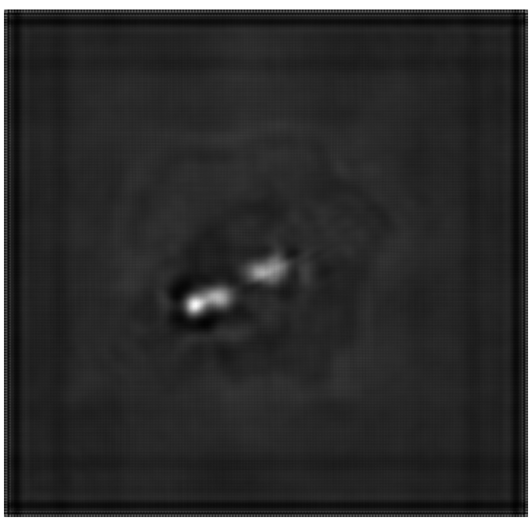
Side view



Top view

~ 13 nm

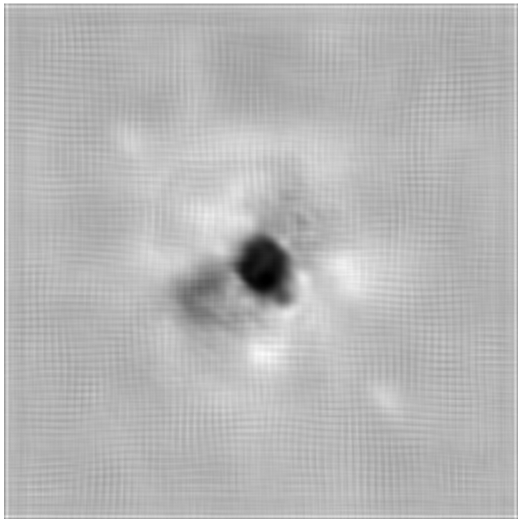
TEM image simulation
(depth 7 nm)



~ 50 nm

~ 50 nm

TEM image simulation
(depth 40 nm)

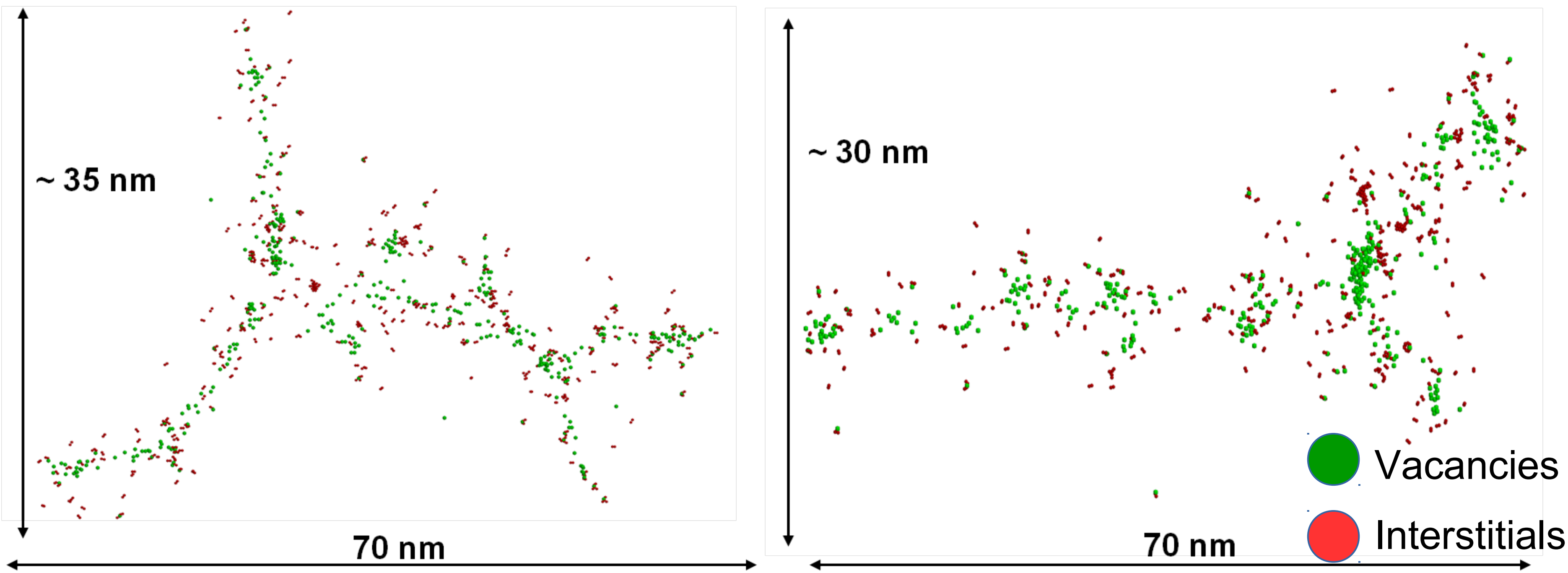


Contrast of large vacancy clusters overshadow smaller defects

Vacancy cluster sizes close to surface clearly visible under TEM resolution

Simulating damage in metals: surface vs. bulk irradiation

Bulk irradiation with 100keV PKA in Fe



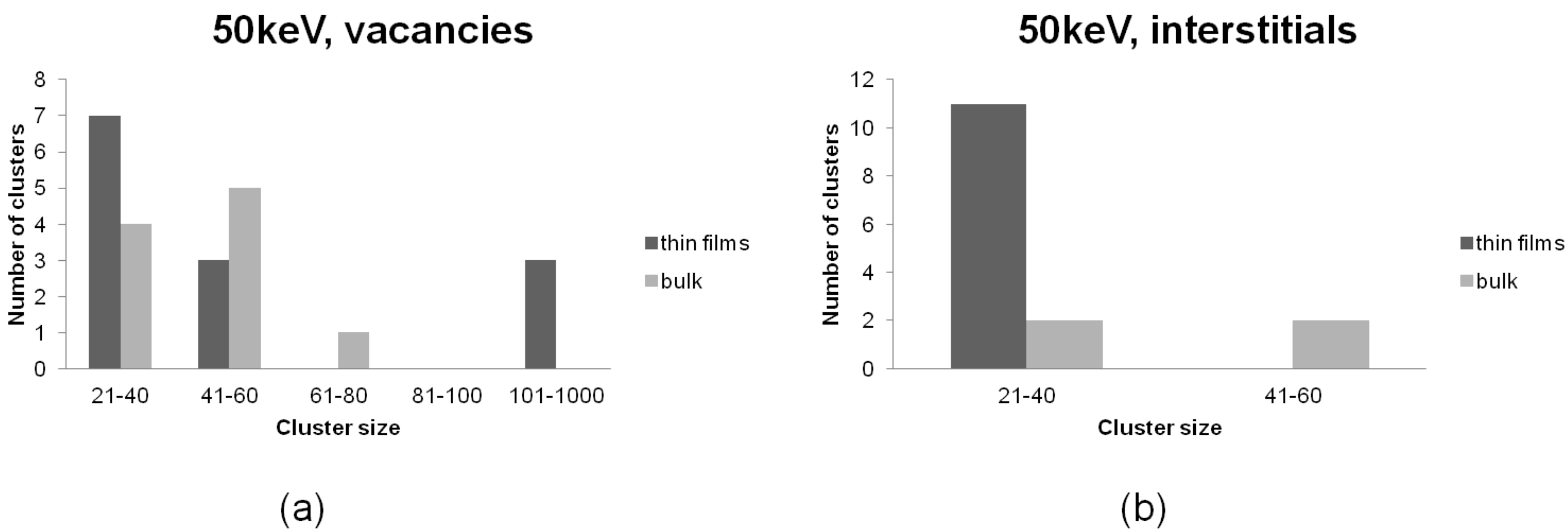
(a) (b)

- Bulk irradiation shows the formation of self-interstitial loops
- Some large vacancy loops are also observed.
- Note the sub-cascade formation

M. J. Aliaga, et. al, Acta Mat. (2015)

Statistical analysis of MD cascades

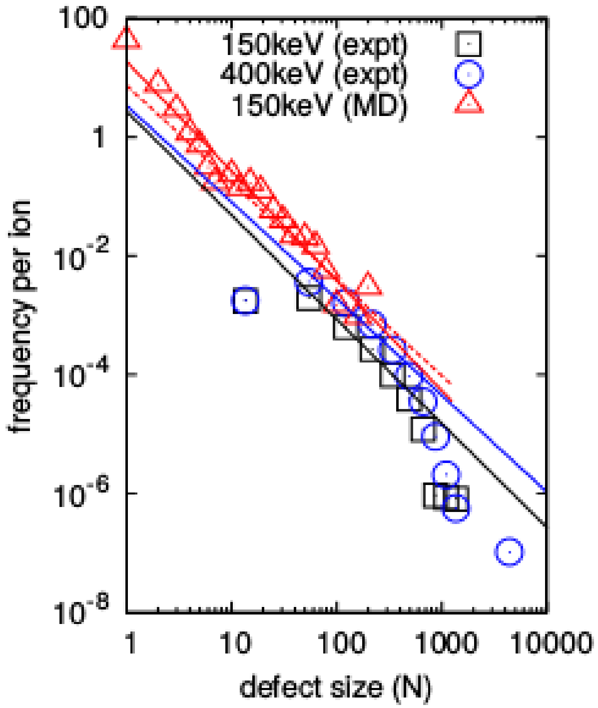
Cluster size differences between bulk and thin films



- Significant difference between the size of the clusters in bulk and thin films for the same energy
- Vacancy clusters much larger in thin films (> 100 defects)
- Self-interstitial clusters significantly larger in bulk irradiation

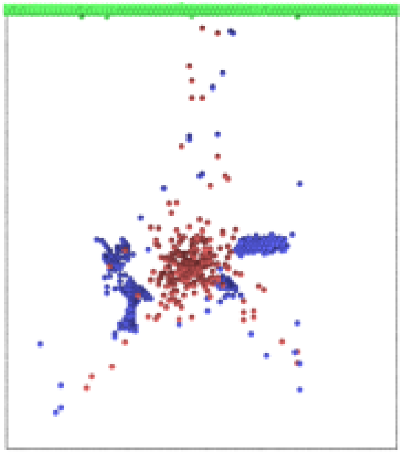
M. J. Aliaga, et. al, Acta Mat. (2015)

Correlation between experiments and simulations: Tungsten (Yi et al)



X. Yi , A.E. Sand, D.R. Mason, M.A. Kirk, G. Roberts, K. Nordlund, S.L. Dudarev

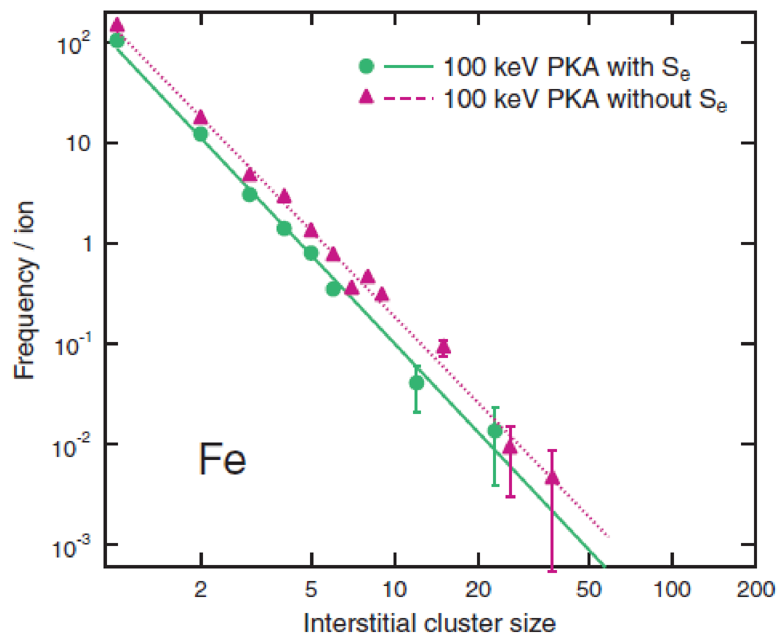
EPL (2015)



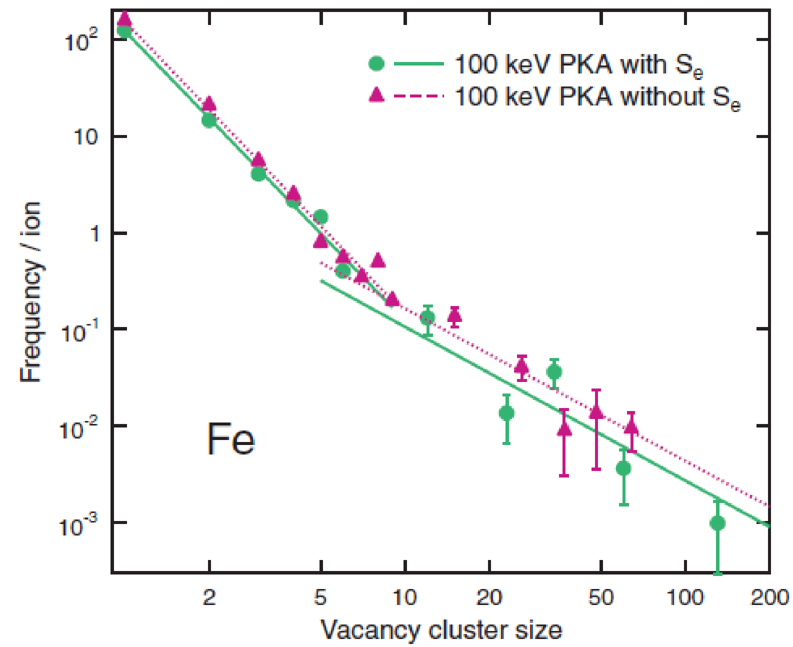
Very good correlation between cluster sizes from MD simulations and experimental measurements with TEM

Correlation between experiments and simulations: W vs. Fe

The case of W: A. E. Sand, et al., EPL (2016)



The case of Fe



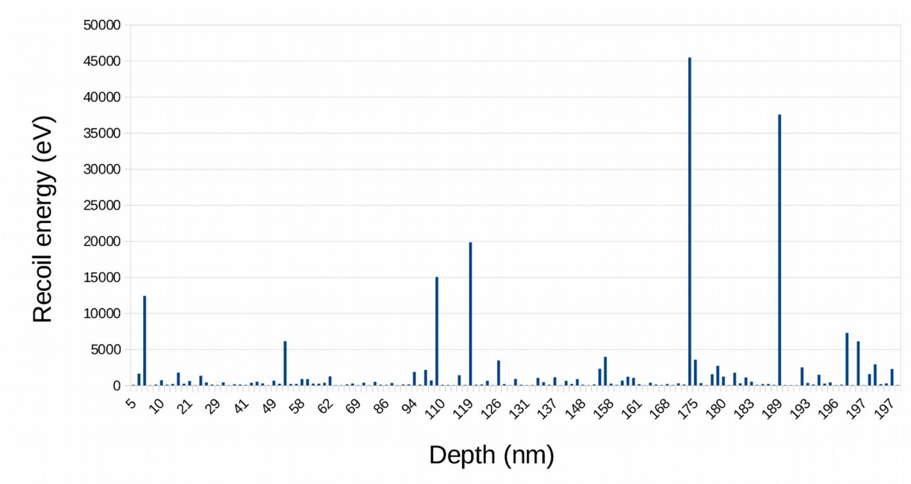
Interstitial cluster sizes obtained In cascades in Fe are very small (not visible under TEM)

Building MeV recoils from SRIM/MDRANGE + MD database

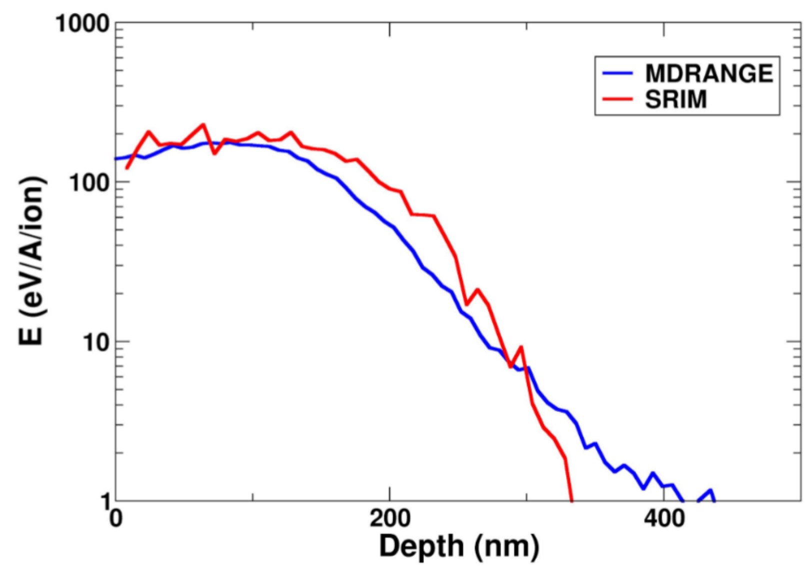
Two approaches

Individual cascades

Recoil spectra as a function of depth



0.5 MeV Fe in Fe, 22°

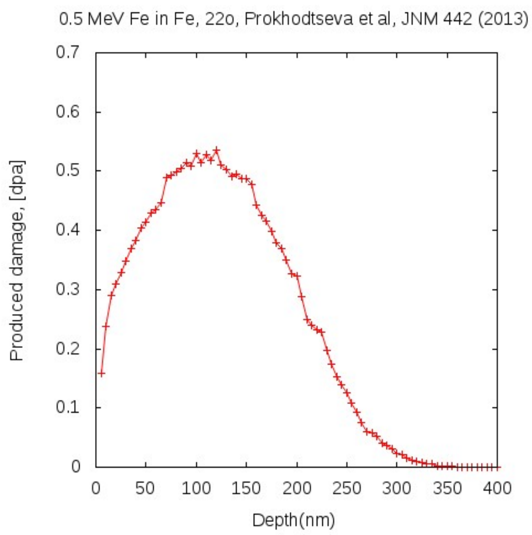


Reference experiments for MeV ion implantation

Prokhodtseva, Schäublin,
Acta Mat (2013)

- 500 keV Fe in Fe, 22°, **RT**
- Thickness ~ 50nm - 180nm
- In-situ experiments
- UHP Fe:

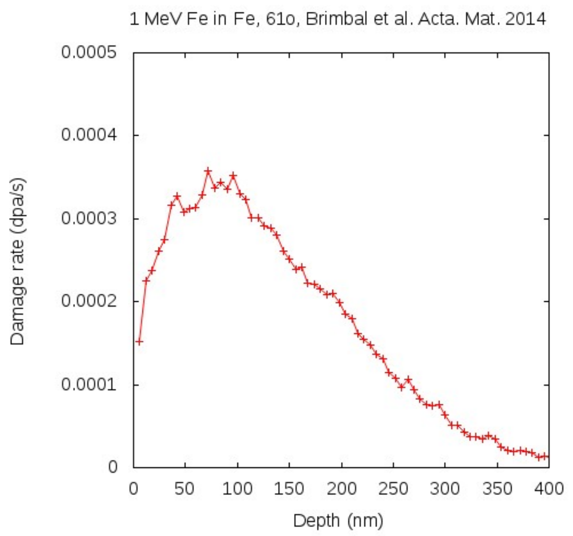
At very low dose: $3x10^{15}$ m^{-2} ~ 0.0015 dpa
only 1/2<111> loops
At higher doses: $2x10^{18}$ m^{-2} ~ 1 dpa mostly <100> loops



Brimbal et al. (2014)

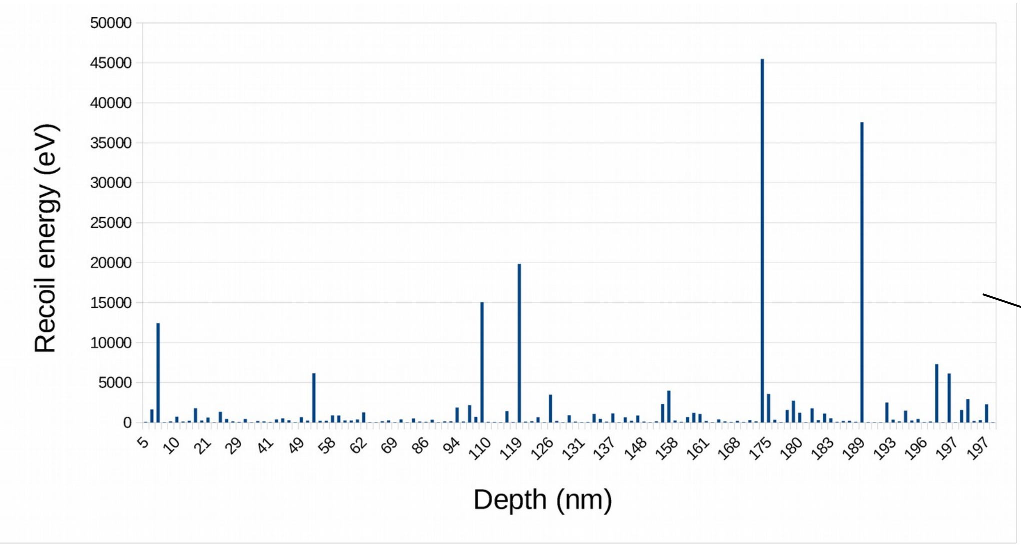
- 1 MeV Fe in Fe, 61°, **500°C**
- Thickness ~ 150nm
- In-situ experiments
- Pure Fe:

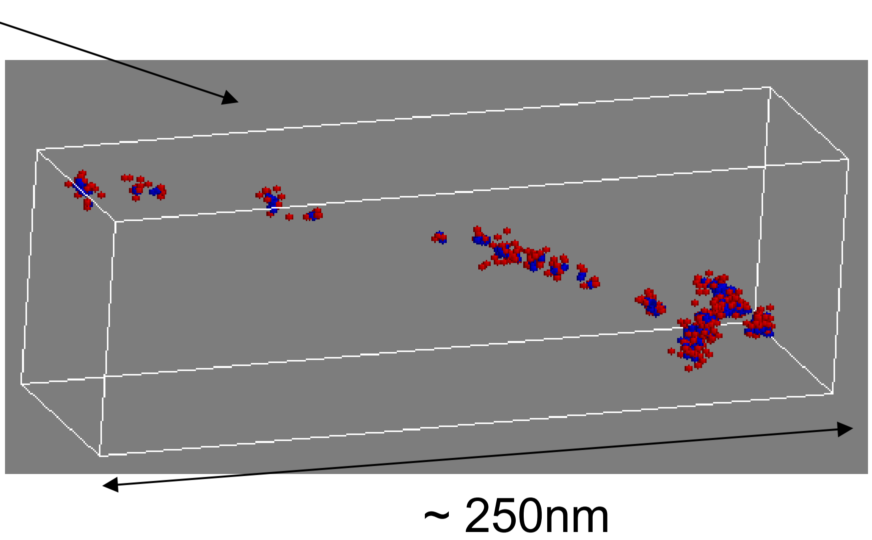
~ 0.8 dpa only <100> loops



Building MeV recoils from SRIM/MDRANGE + MD database

Individual cascades



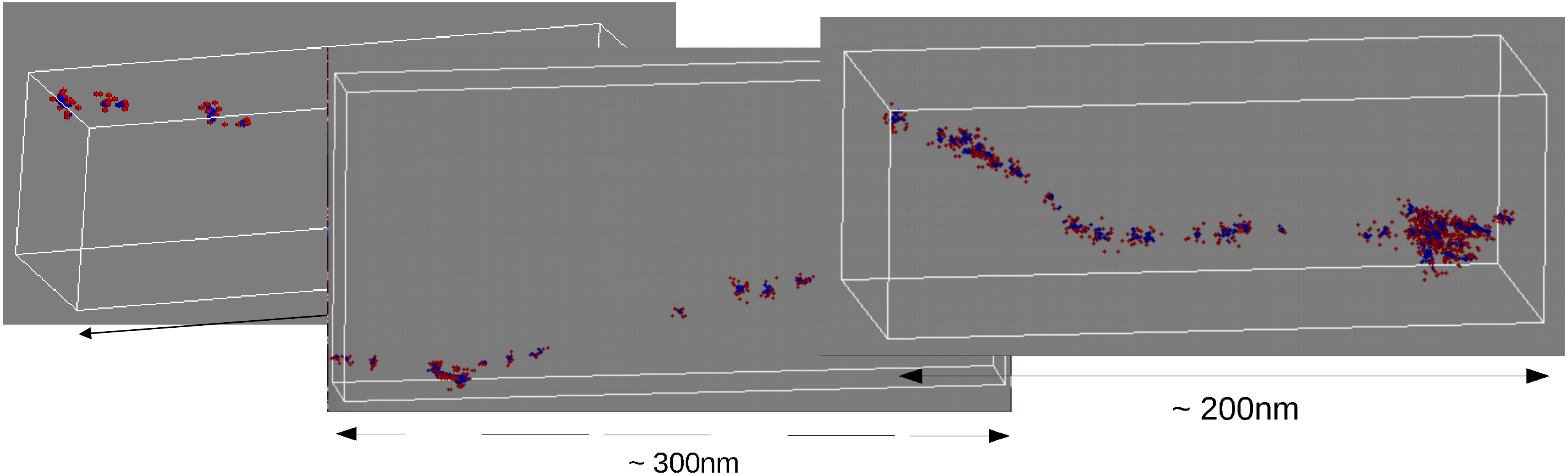


Building MeV recoils from SRIM/MDRANGE + MD database

Two approaches

Individual cascades

Recoil spectra as a function of depth



Comparison to full MD / MD + BCA (C. Ortiz) / A. DeBacker

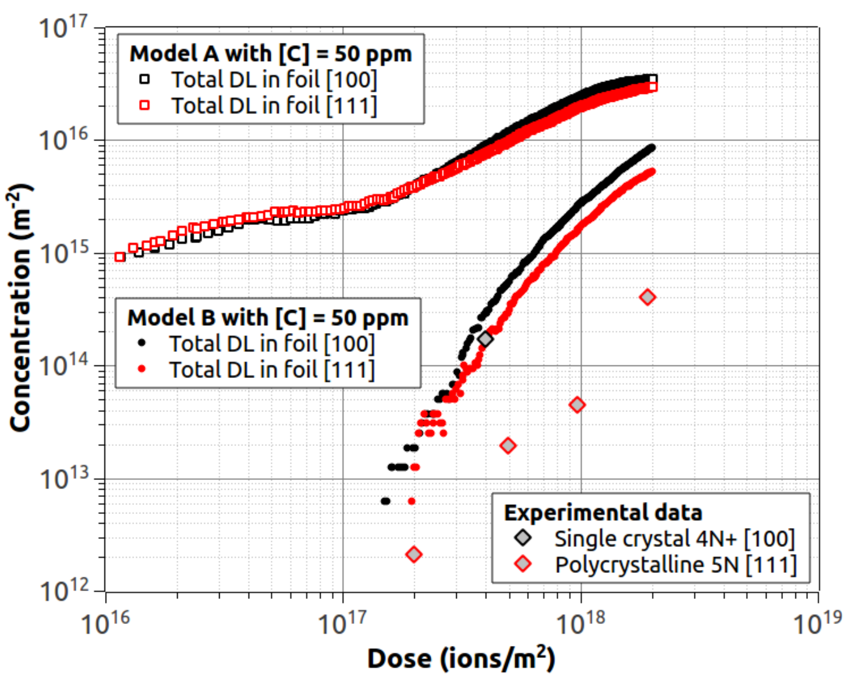
Model applied to low energy ion implantation (100 keV)

Including Carbon impurities

► Concentration of DL increases in **Model A & B**

► Large increase of both <100> and ½ <111> concentrations and size in **Model A** from low doses

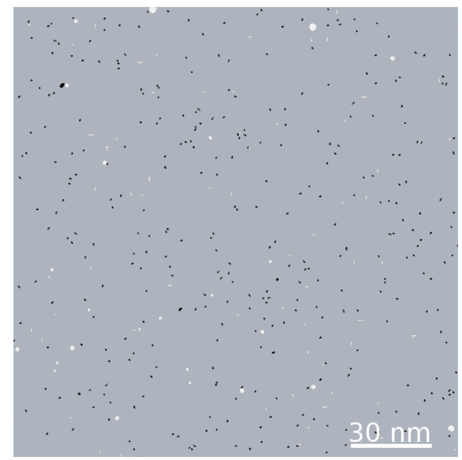
► **Model B**: **better** agreement with experimental data



[Exp: Z. Yao, M. Hernández-Mayoral, M.L. Jenkins and M.A. Kirk. 2008]

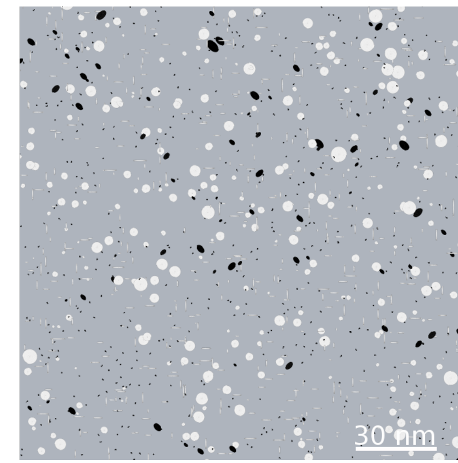
Model B

Dose: $3.2\cdot10^{17}$ ions/m^2



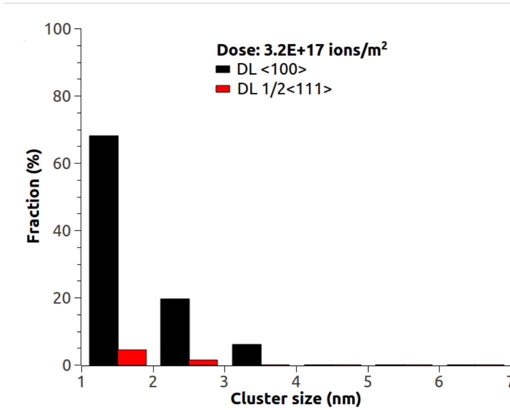
Model B

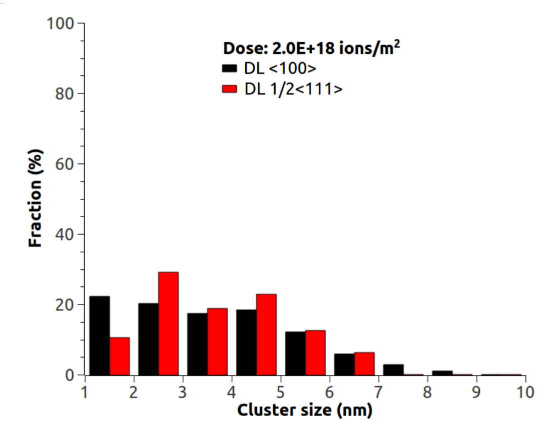
Dose: $2\cdot10^{18}$ ions/m^2



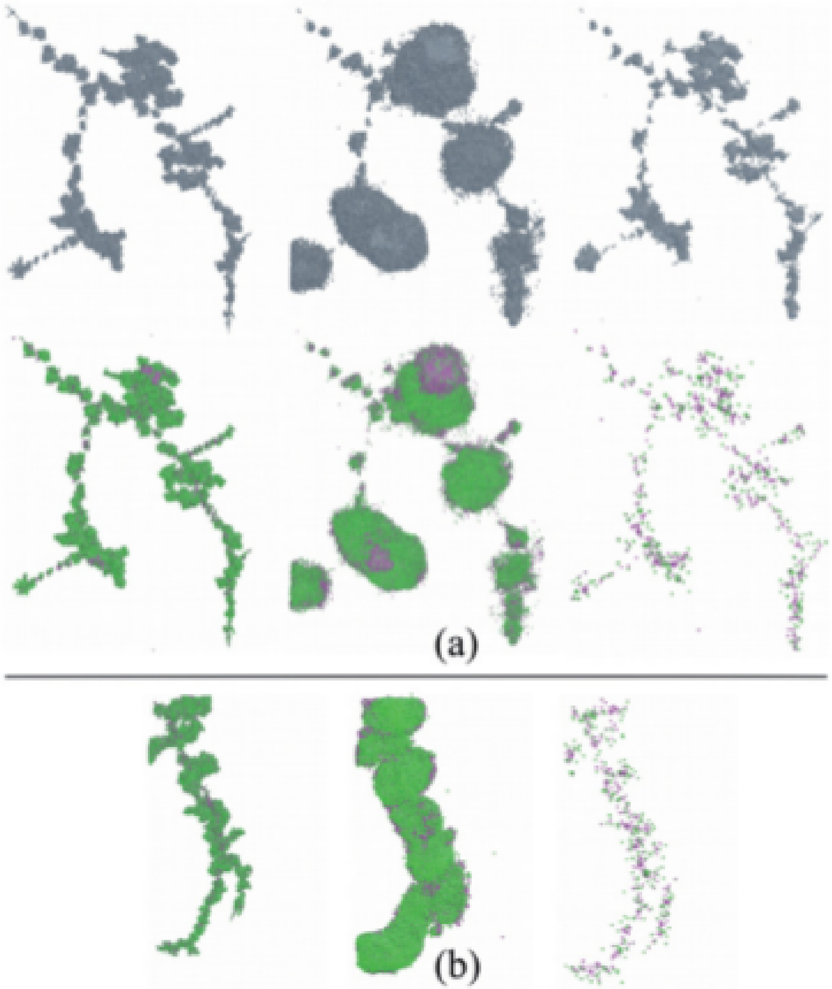
All DL loops are displayed in these images (> 0.6 nm)

●<100> clusters ●½ <111> clusters





Do all these mechanisms just add up?
1 + 1 = 2 ?



500 kev cascade in Fe

E. Zarkadoula et al,
J. Phys. Condense. Matter 25 (2013) 125402

Conclusions

- Initial defect distribution affects significantly microstructure evolution

- Cascade damage database for Fe irradiation at 50 keV, 100 keV and 150 keV irradiation of Fe thin films and 50 keV and 100 keV for bulk Fe.

- Quantified damage in terms of cluster size and type and total number of defects.

Open questions

- Can we validate further the results from the first few picoseconds of the collision cascade with experiments?
- Is it enough with a cascade database below subcascade splitting to build the whole energy spectrum?
- Is there a need for higher energy cascades?
- Is there a need for cascade damage in alloys?
- How do we share this information? (Gigabytes of data)