2137-31

Joint ICTP-IAEA Advanced Workshop on Multi-Scale Modelling for Characterization and Basic Understanding of Radiation Damage Mechanisms in Materials

12 - 23 April 2010

Atomistic Simulations of irradiation in nanocrystalline materials

M. Samaras

Paul Scherrer Institut
Villigen
Switzerland

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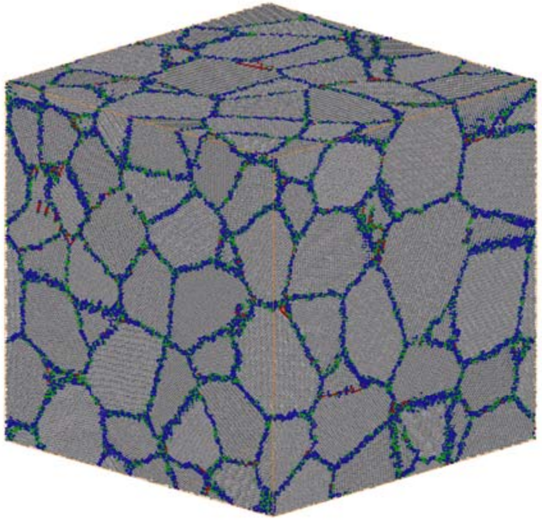
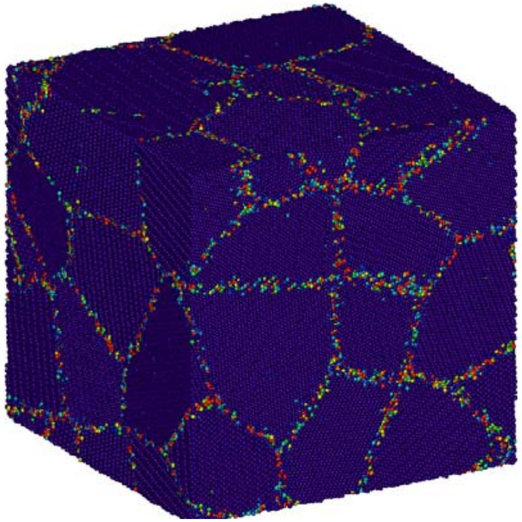


IAEA- ICTP Workshop
Trieste, 16th April 2010



Collaborators

PSI

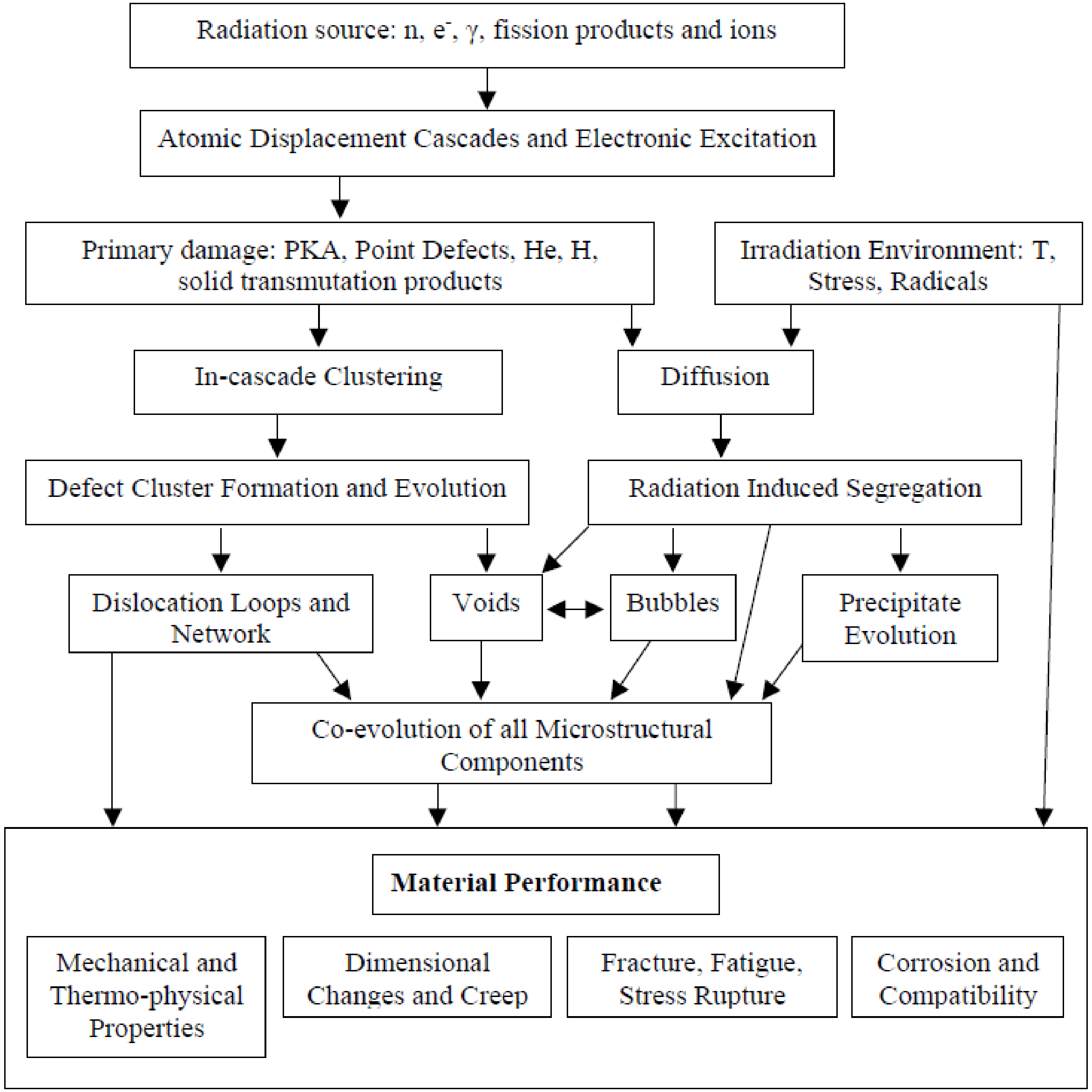
P. M. Derlet (NUM)

W. Hoffelner (NES)

H. Van Swygenhoven (NUM)

UPM

M. Victoria



Radiation source: n, e^-, γ, fission products and ions

Atomic Displacement Cascades and Electronic Excitation

Primary damage: PKA, Point Defects, He, H, solid transmutation products

Irradiation Environment: T, Stress, Radicals

In-cascade Clustering

Diffusion

Defect Cluster Formation and Evolution

Radiation Induced Segregation

Dislocation Loops and Network

Voids

Bubbles

Precipitate Evolution

Co-evolution of all Microstructural Components

Material Performance

Mechanical and Thermo-physical Properties

Dimensional Changes and Creep

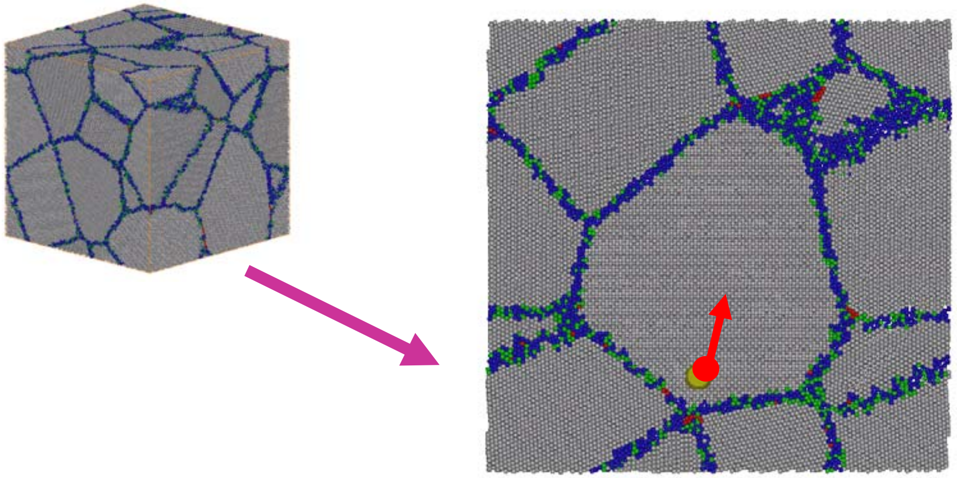
Fracture, Fatigue, Stress Rupture

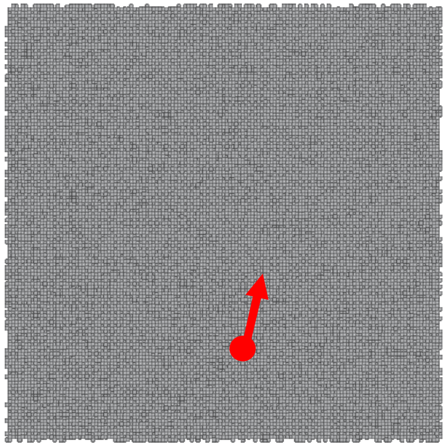
Corrosion and Compatibility

Stoller

Simulation Data

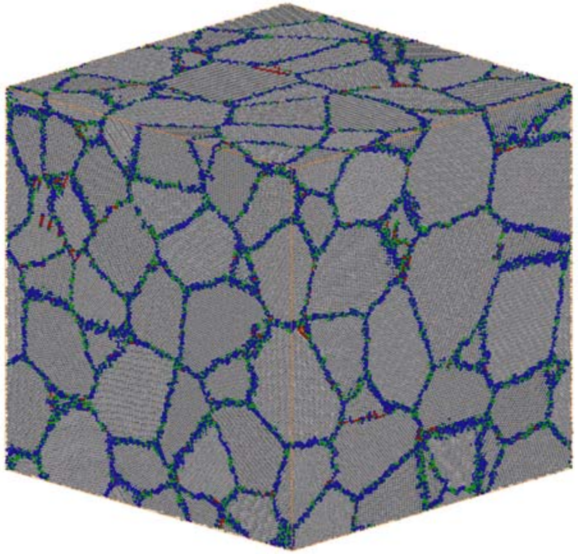
- **300K**
- **Periodic Boundary Conditions**
- **Modified 2nd moment TB potential (Cleri-Rosato PRB 1993), including high-energy corrections (Ziegler *et al.* 1987)** **fcc nc Ni**
- **Ackland potential, Calder and Bacon corrections (non-magnetic)** **bcc nc Fe**





Local crystalline order

Topological short range analysis (Honeycutt and Andersen, 1987).



● BCC

● FCC

● HCP

● Other 12

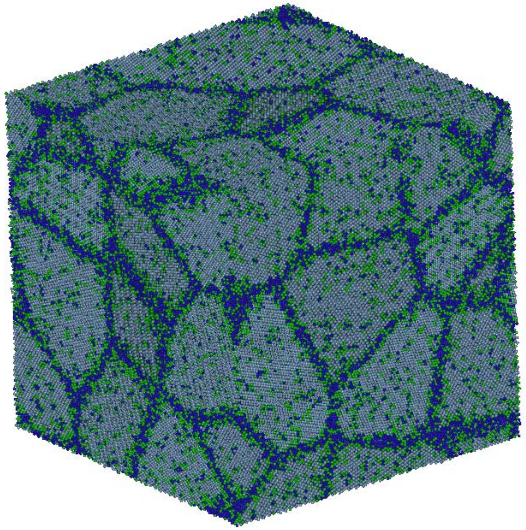
● Non-12

fcc nc Ni

● Other 8

● Non-8

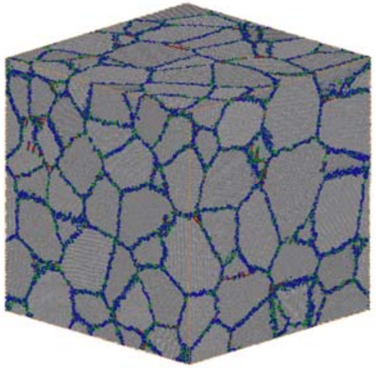
bcc nc Fe



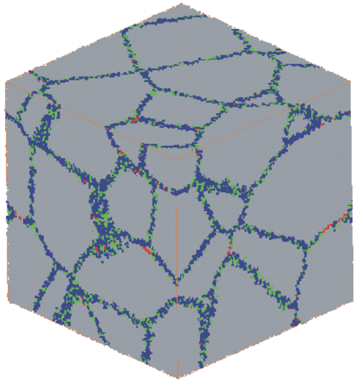
Sample Sizes

fcc nc Ni

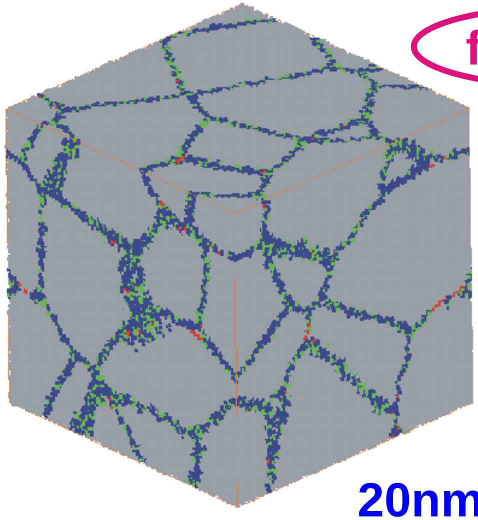
1.2 million atoms



6nm grain size
125 grains



12nm grain size
15 grains

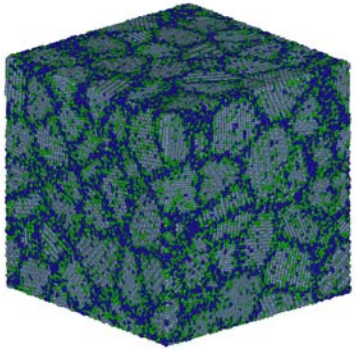


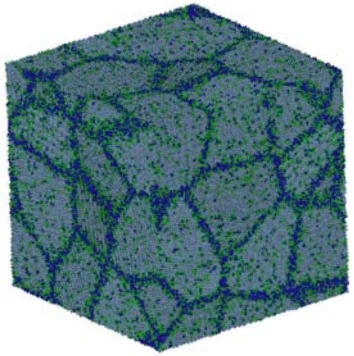
15 grains

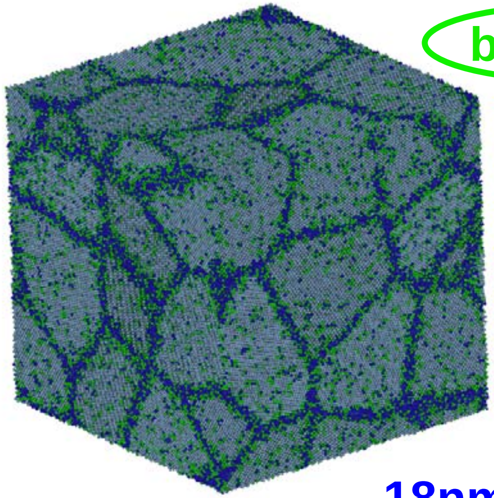
20nm grain size
5.8 million atoms

bcc nc Fe

1.4 million atoms



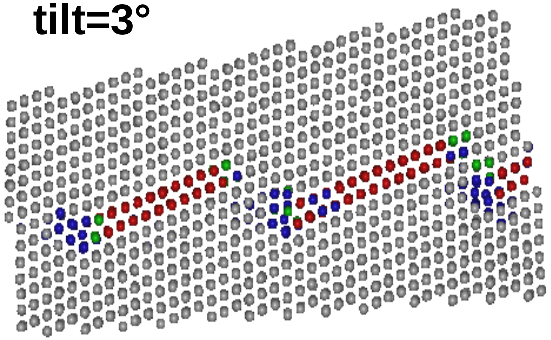




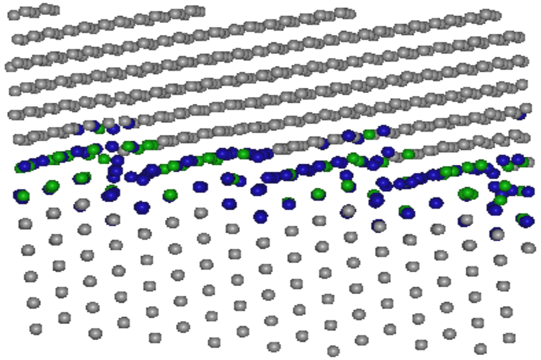
18nm grain size
7.3 million atoms

Grain Boundaries

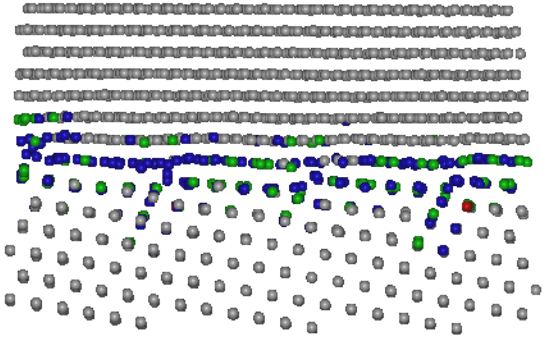
tilt=3°



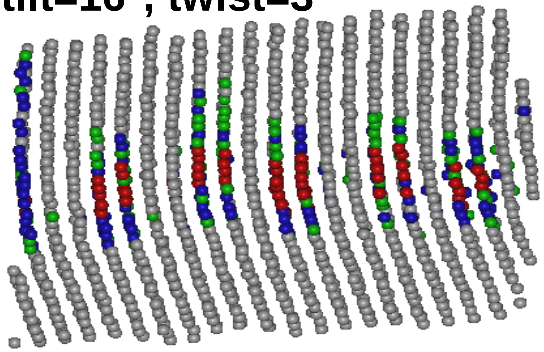
tilt=14°, twist=19°



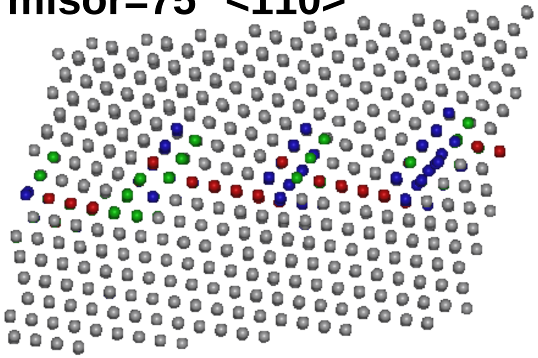
tilt=47°, misor=59.5°



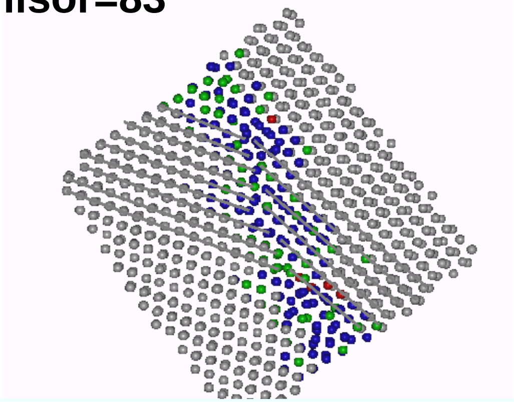
tilt=16°, twist=3°



misor=75° <110>



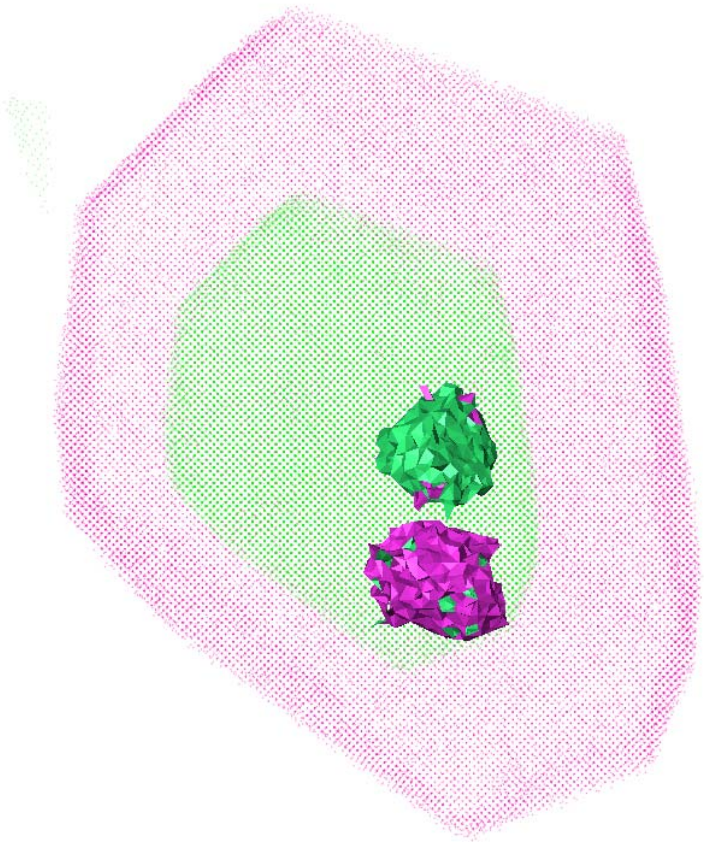
misor=83°



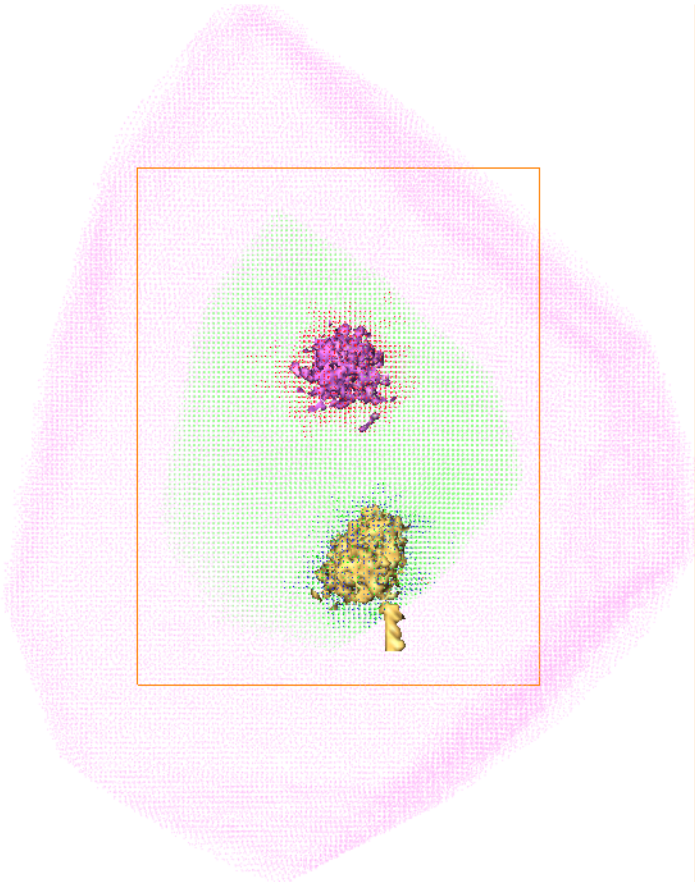
Structurally ordered units and misfit areas with less order

Cascade Size

bcc nc Fe



fcc nc Ni



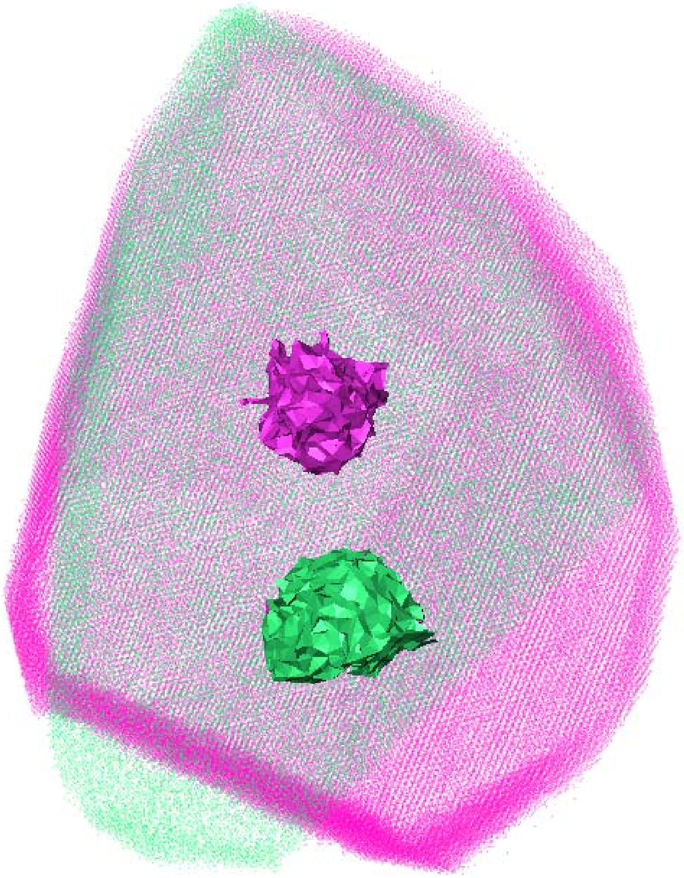
5keV

20nm grain

12nm grain

Bcc vs fcc: cascade size comparison

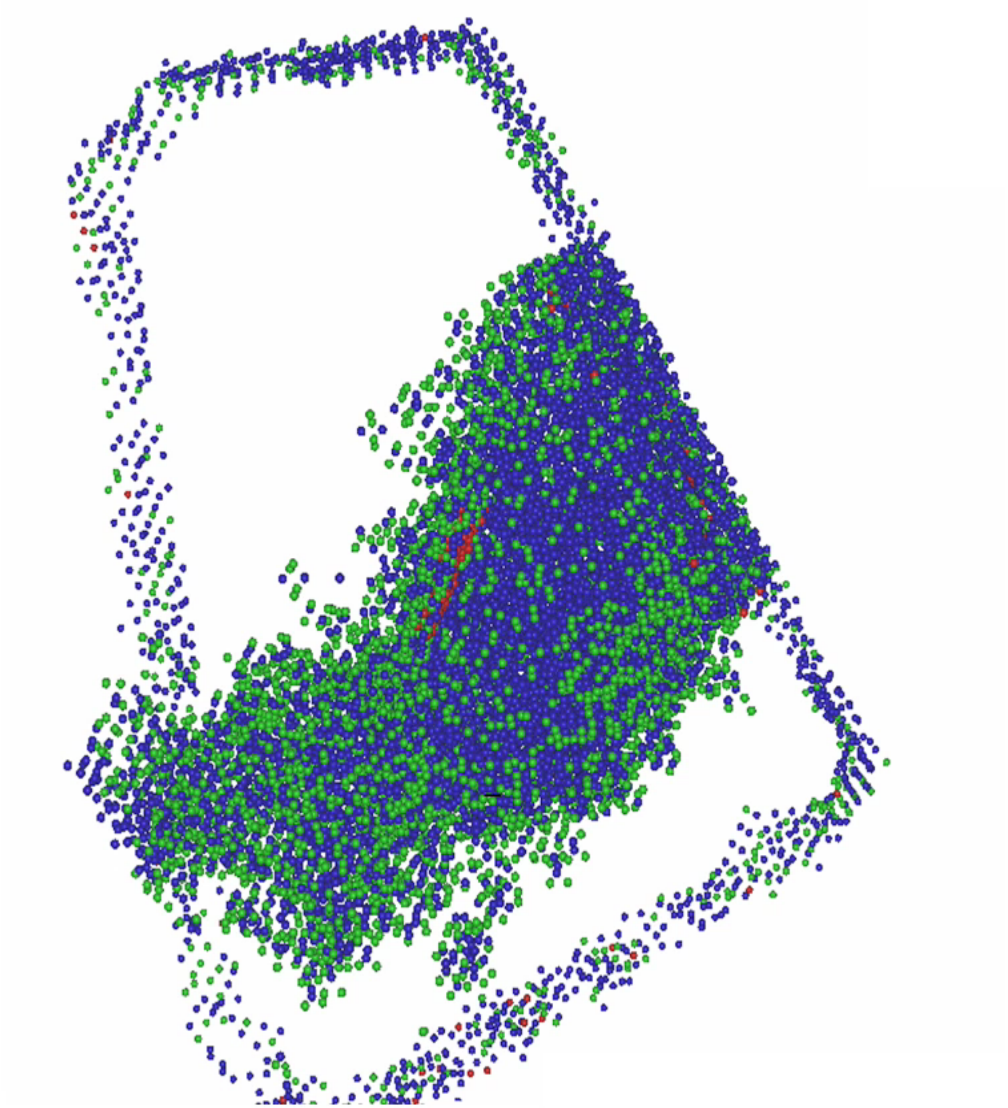
5keV



20nm grain fcc Ni
18nm grain bcc Fe

Displacement cascade

20 keV

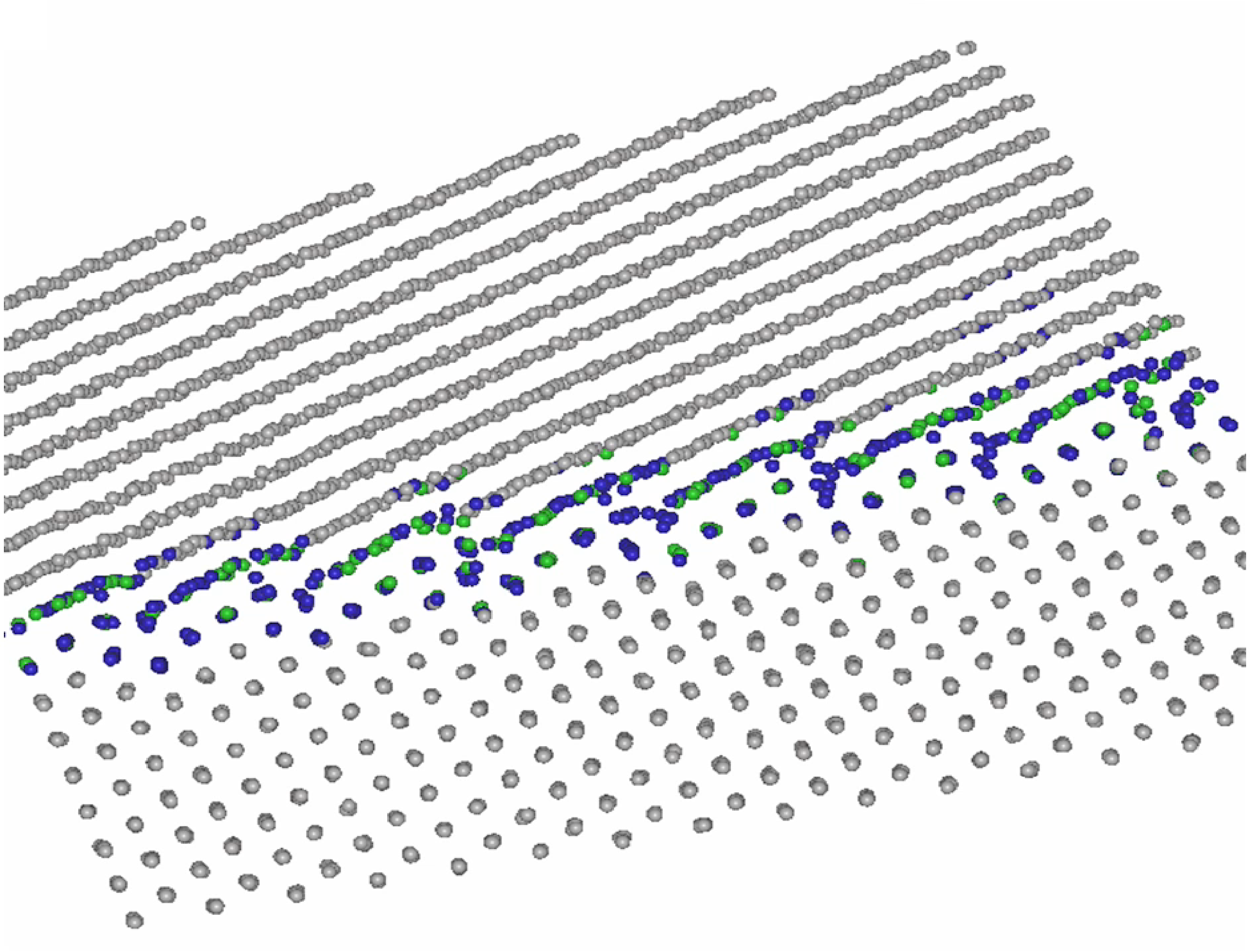


fcc nc Ni

movie

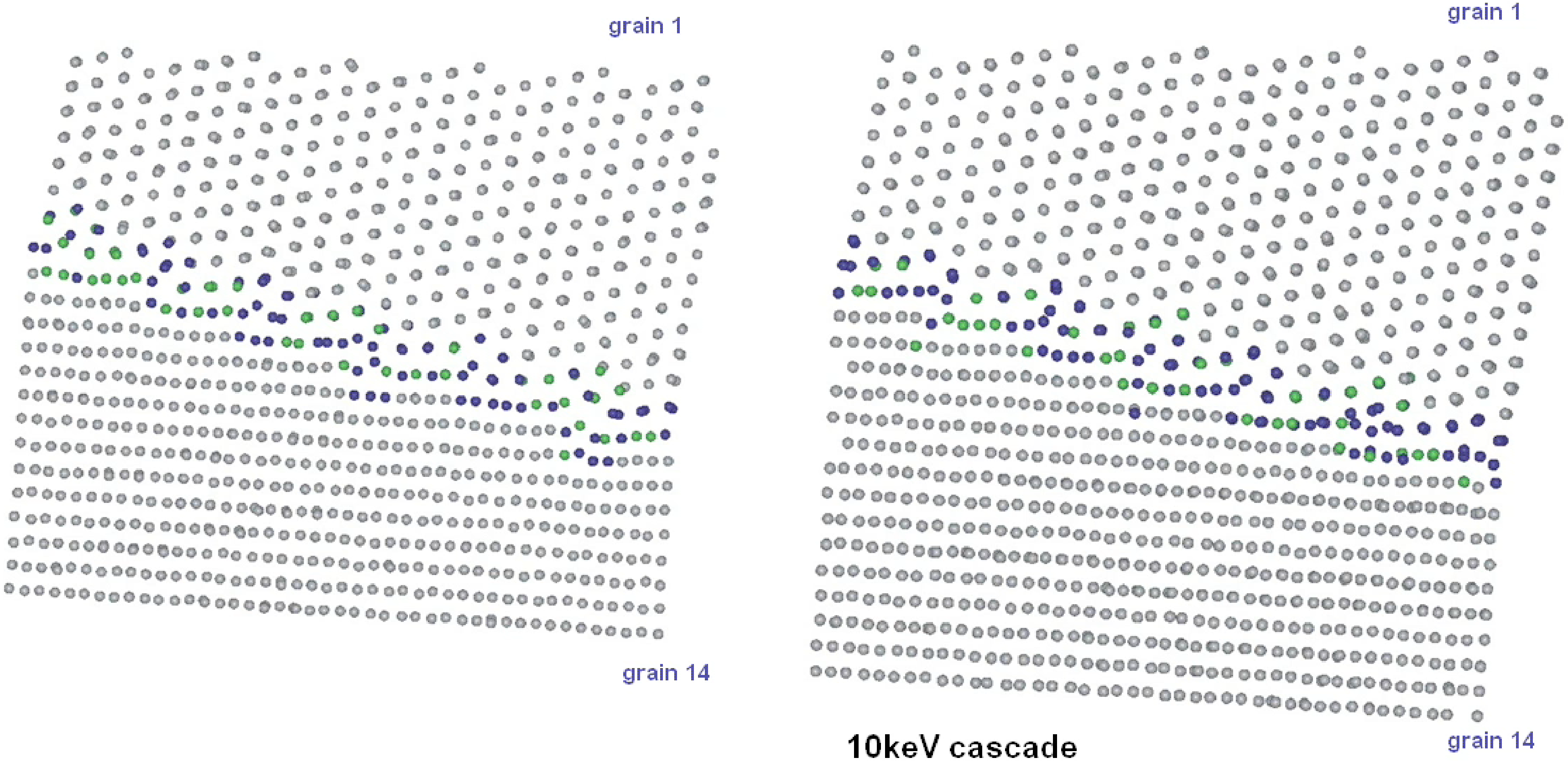
movie

Densification of the GB



fcc nc Ni

GB Flexibility- movement of GB towards cascade direction



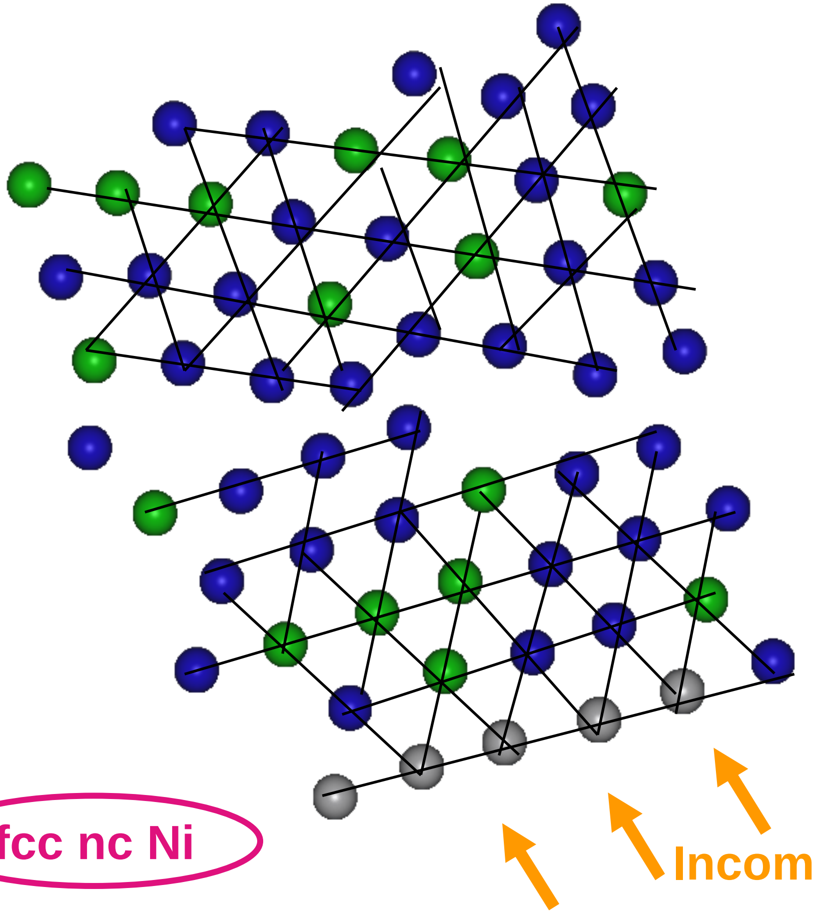
10keV cascade

fcc nc Ni

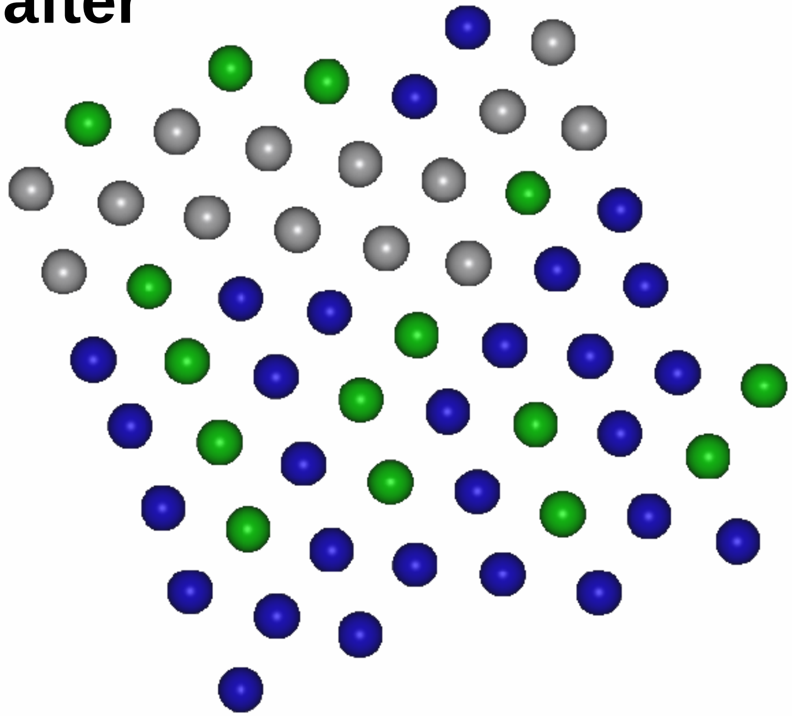
movie

Close up of atoms in the GB plane

before



after



fcc nc Ni

Incoming SIAs

GBD at line d

↓

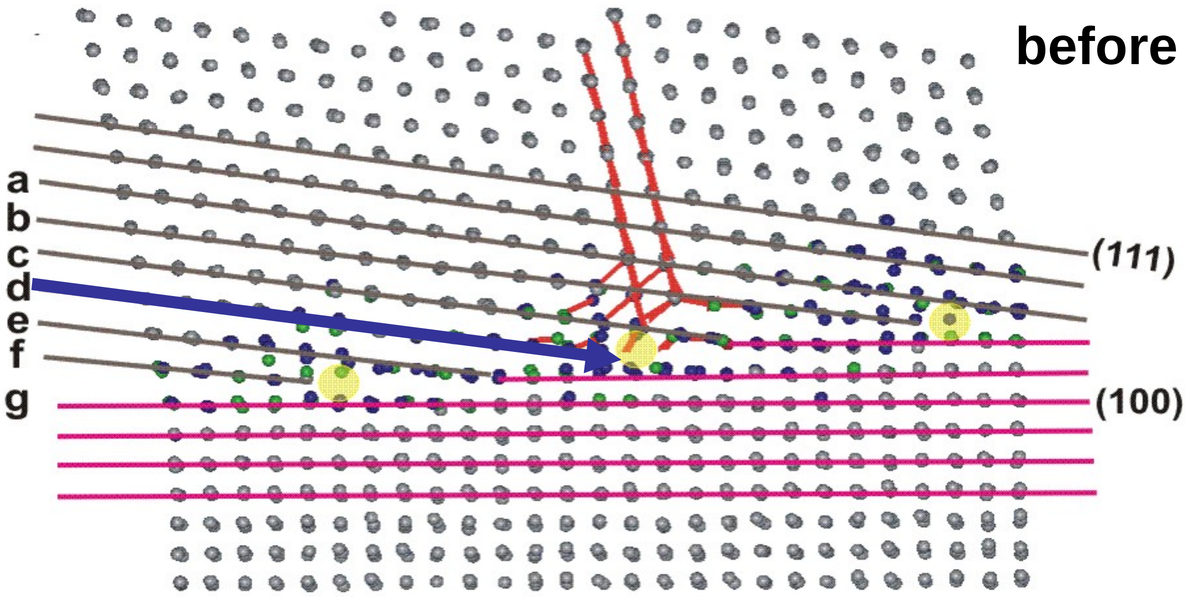
6 SIA cluster enters

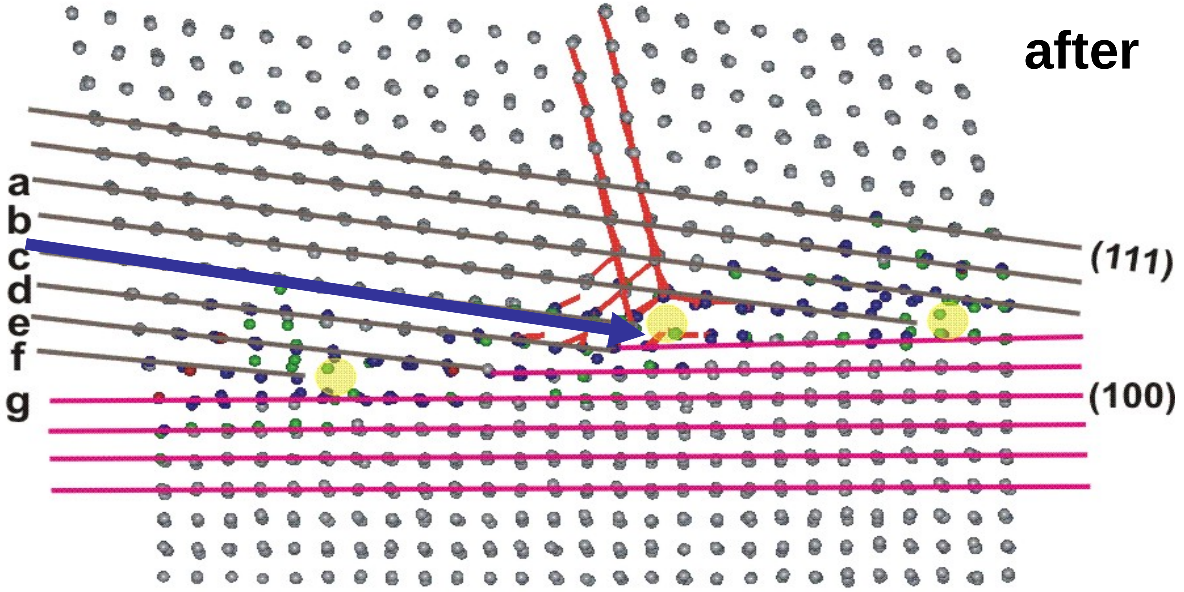
↓

local climb

↓

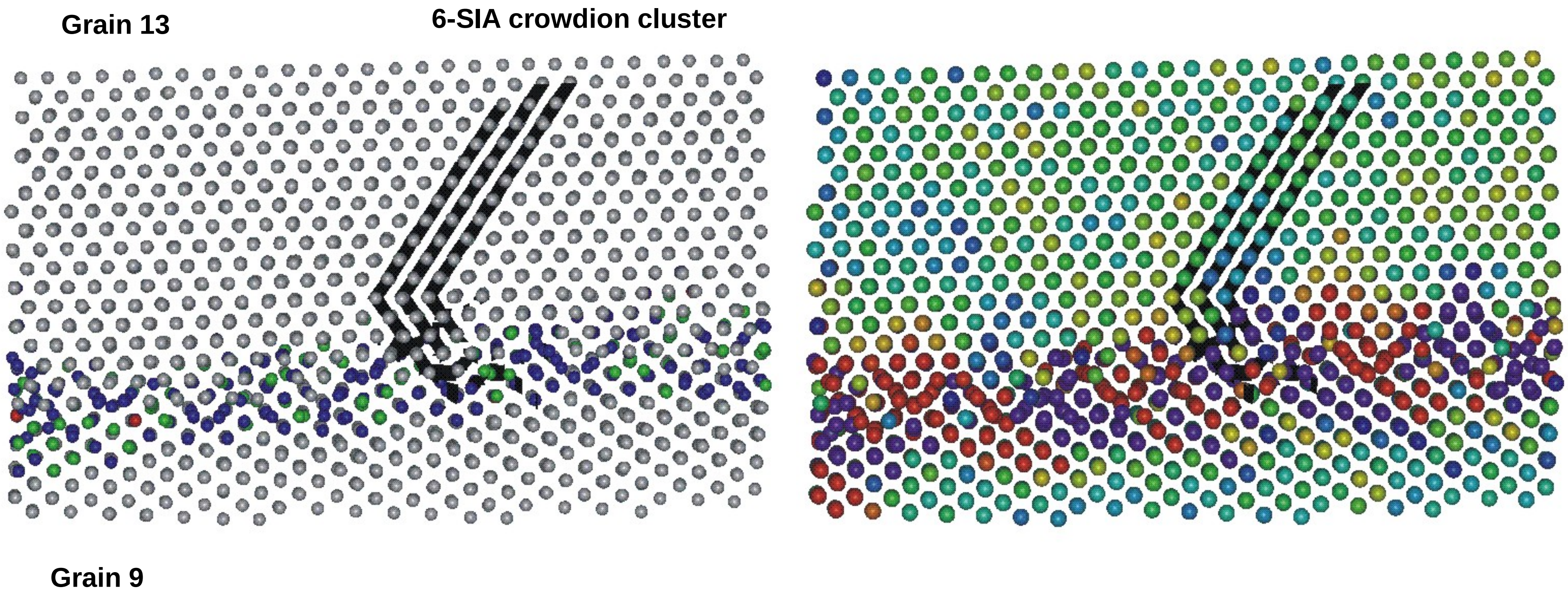
GBD at line c





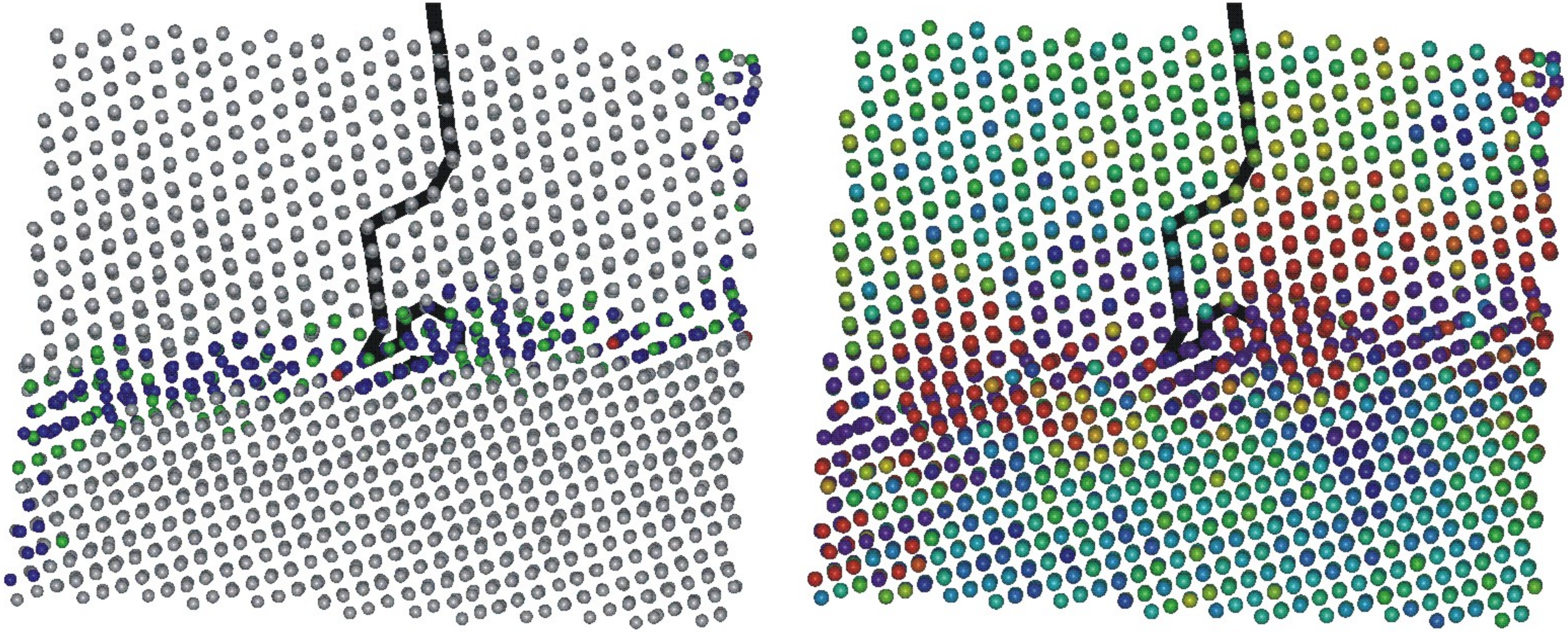
5keV PKA

Atomic Pressure in a 5keV PKA 12nm grain size Sample



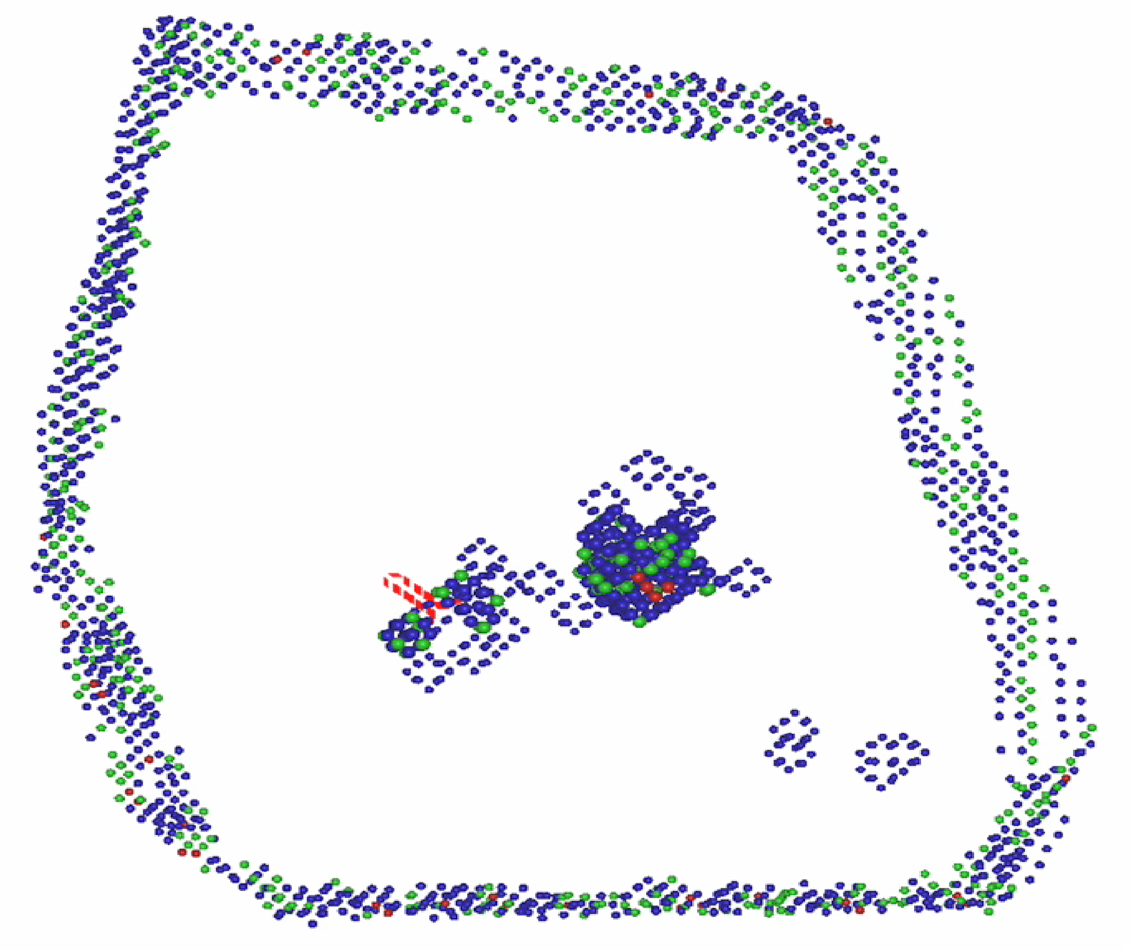
fcc nc Ni

Atomic Pressure in a 5keV PKA 12nm grain size Sample



fcc nc Ni

1D/3D motion



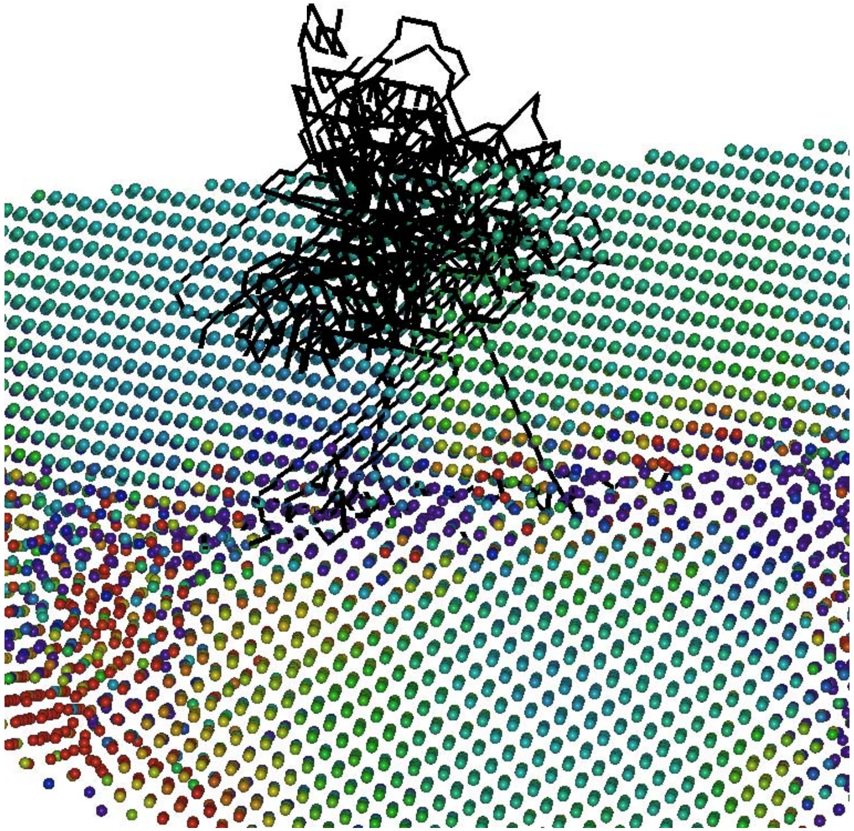
Cooling of 20keV cascade

fcc nc Ni

movie

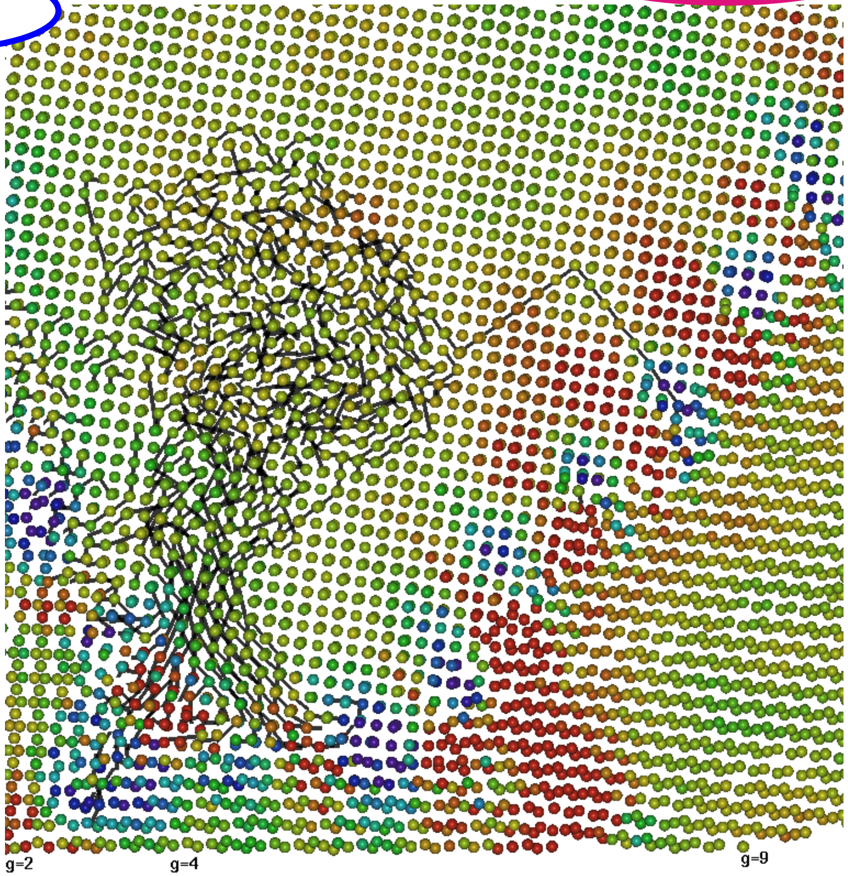
Influence of GB on SIA movement

bcc nc Fe



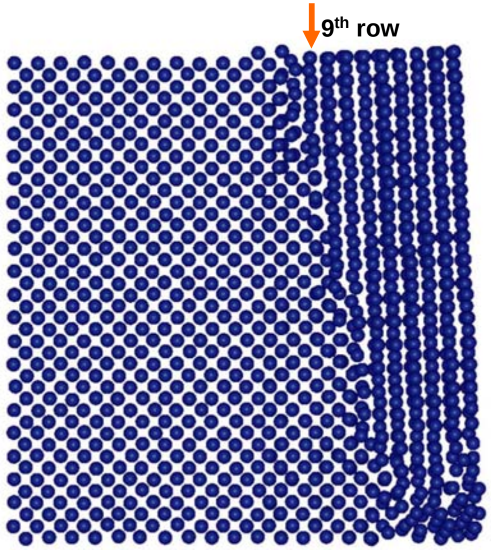
12nm

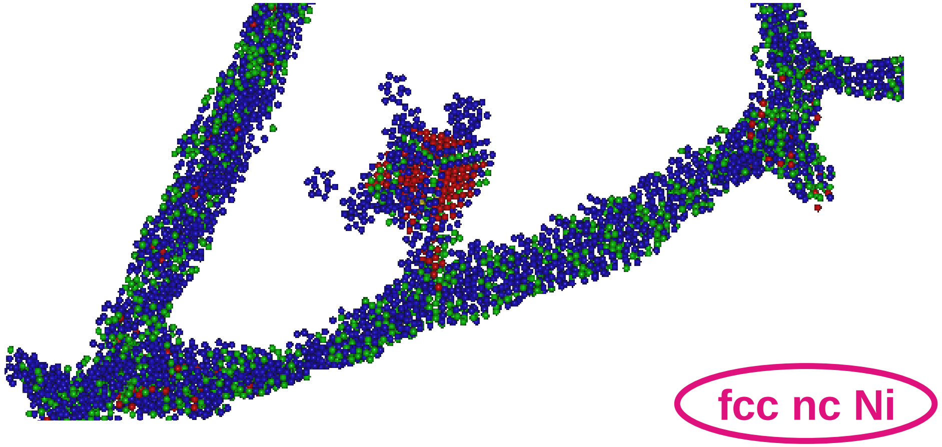
fcc nc Ni



Experiment: GBs work as effective sinks (Rose *et al.* 1991, Chimi *et al*. 2001).

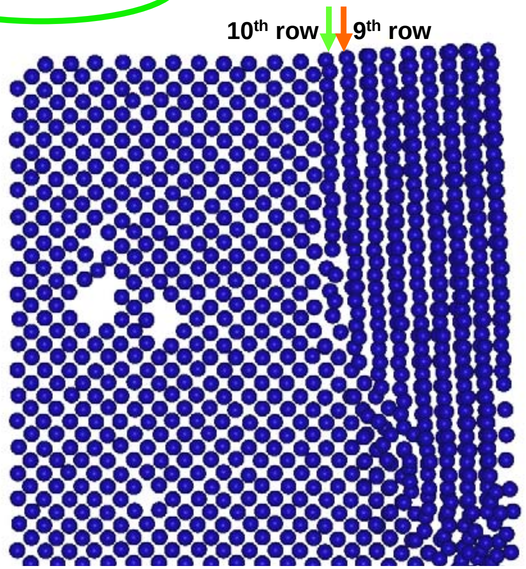
Influence of GB on vacancies



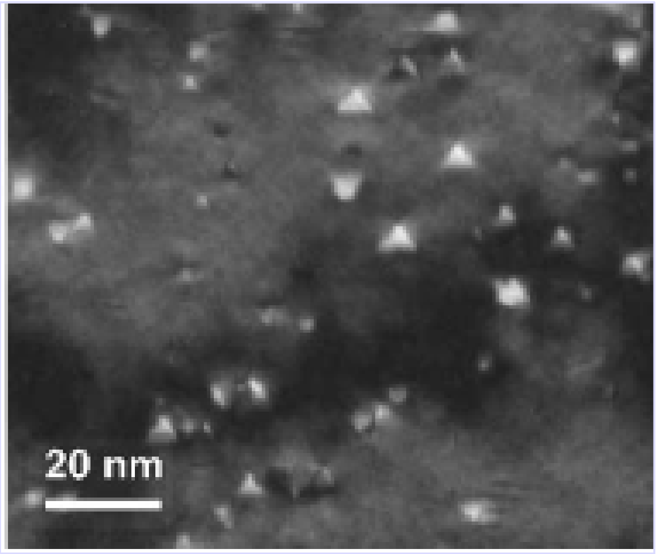


fcc nc Ni

bcc nc Fe



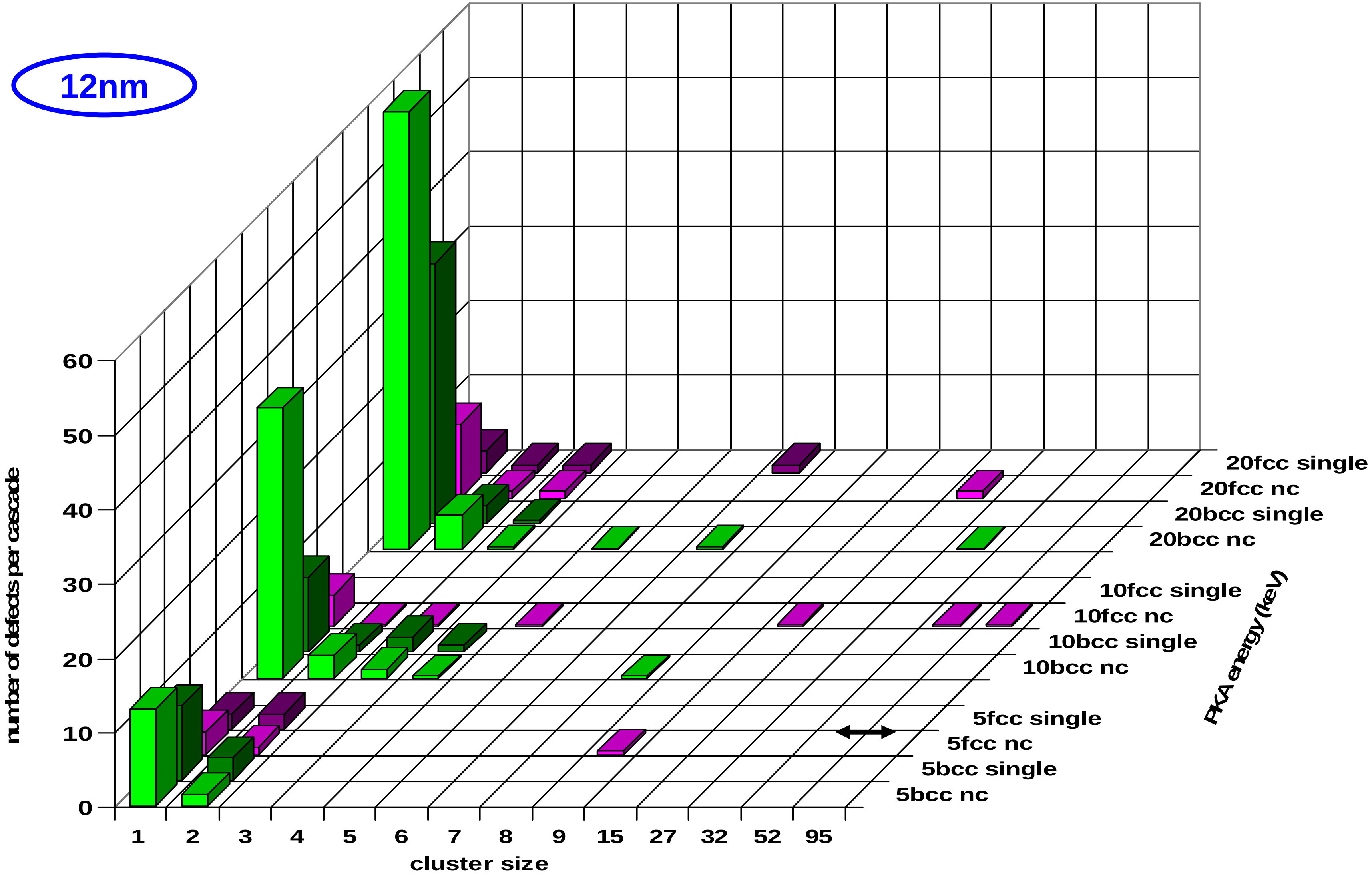
12nm



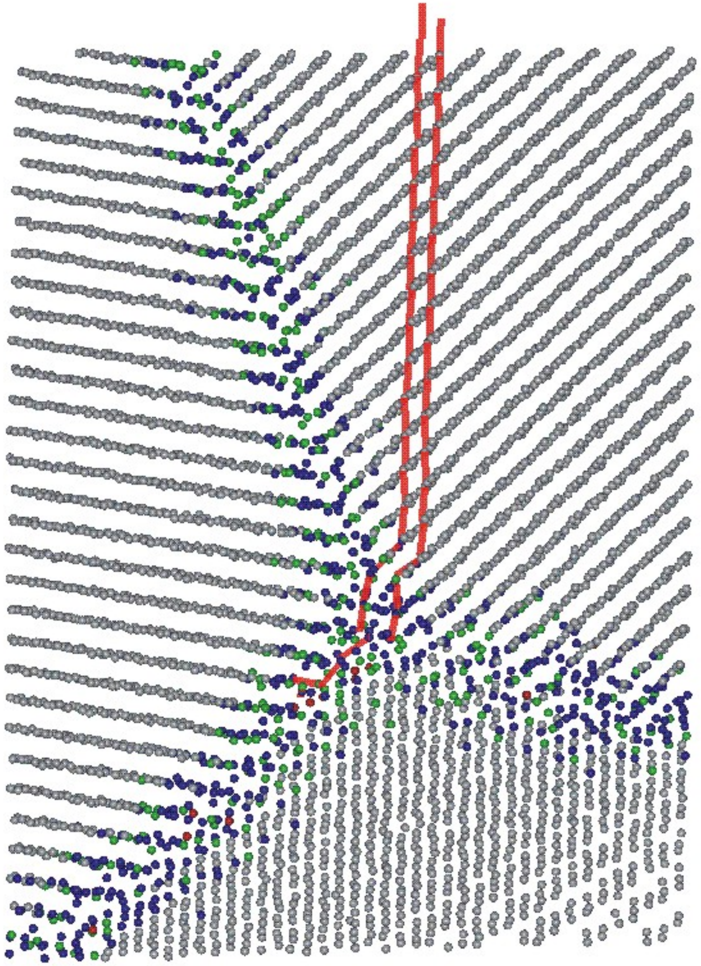
Schäublin *et al.* 2001

Defect distribution: single + nano crystal, fcc vs bcc

12nm

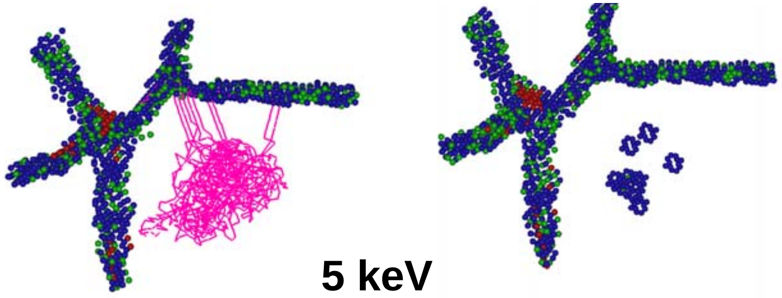


Movement of interstitials



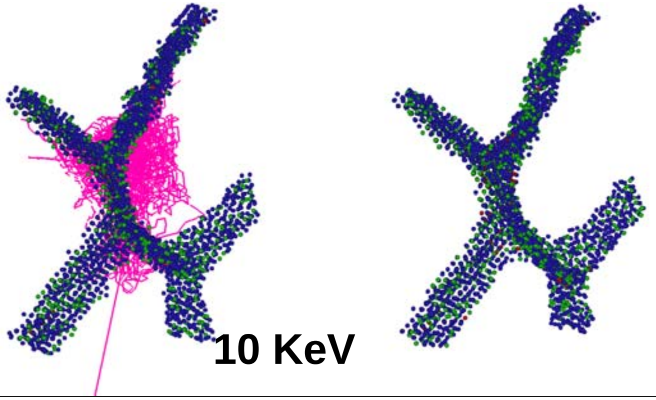
fcc nc Ni

RCS to GB: vacancy dominated damage



5 keV

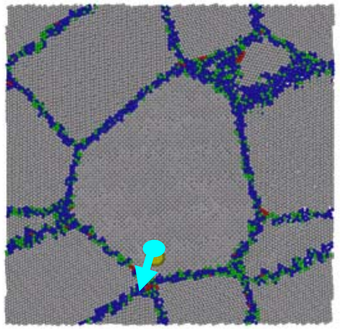
Cascade on TJ: no damage left



10 KeV

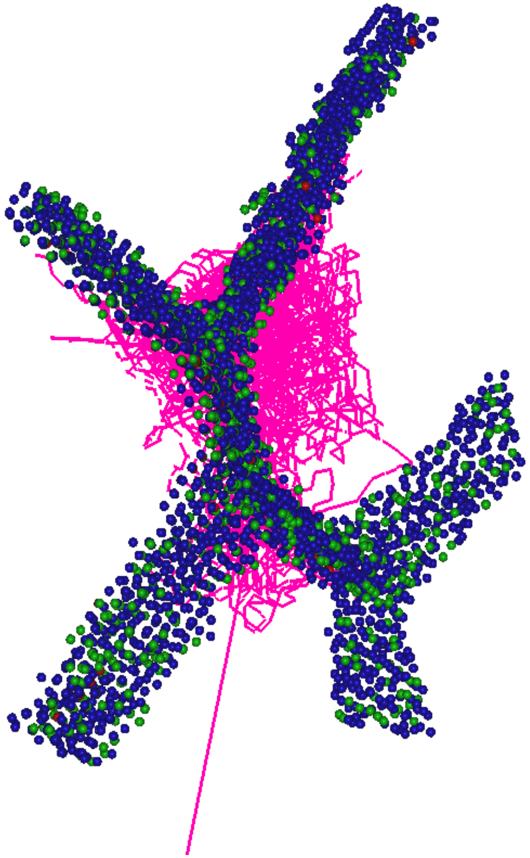
Easier formation of truncated SFT

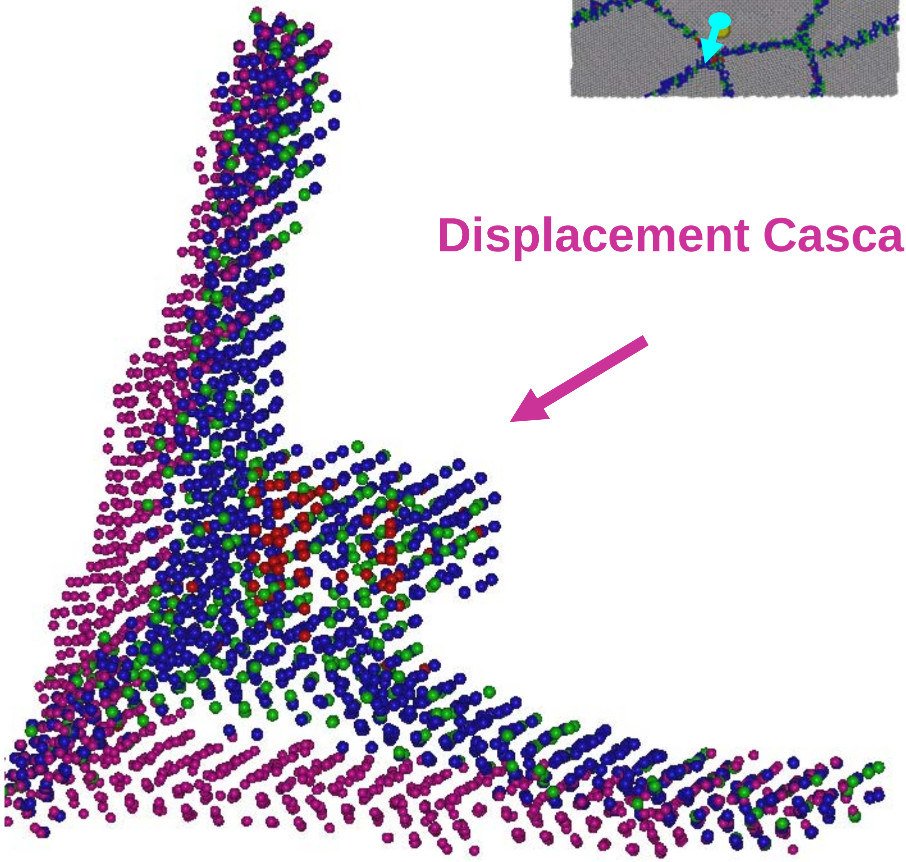
Cascade directed towards the GB



10keV PKA

12nm





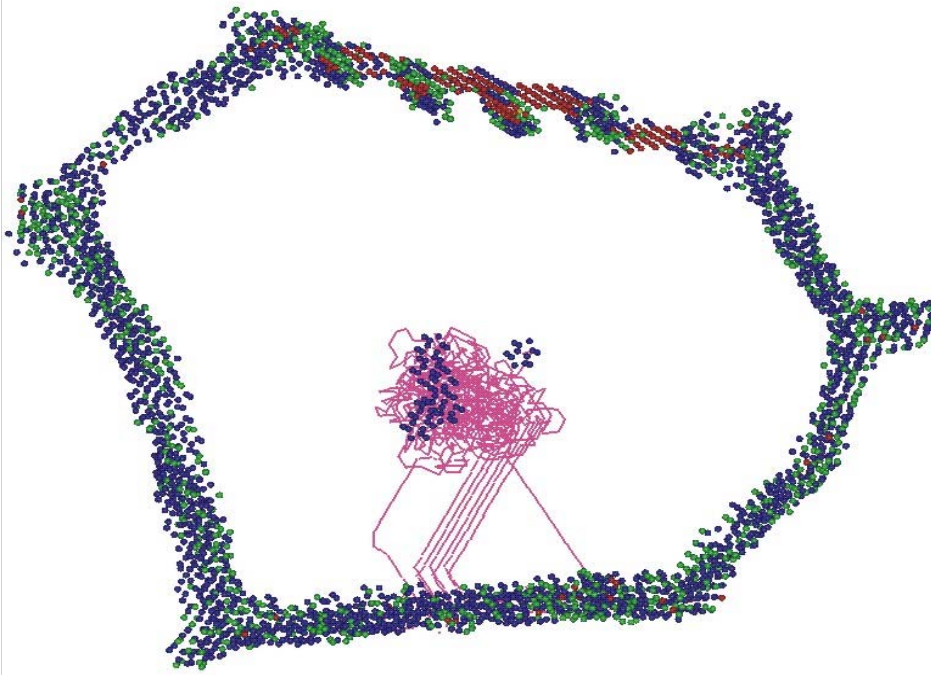
Displacement Cascade

Case 1:

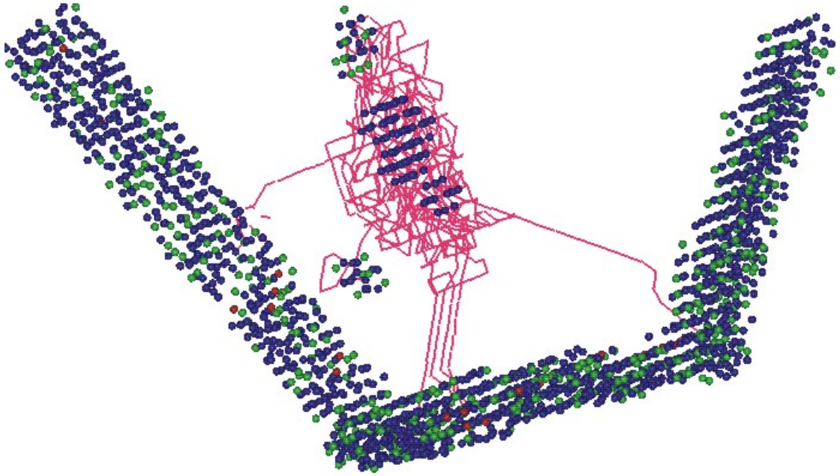
Case 2:

Size Effects

fcc nc Ni



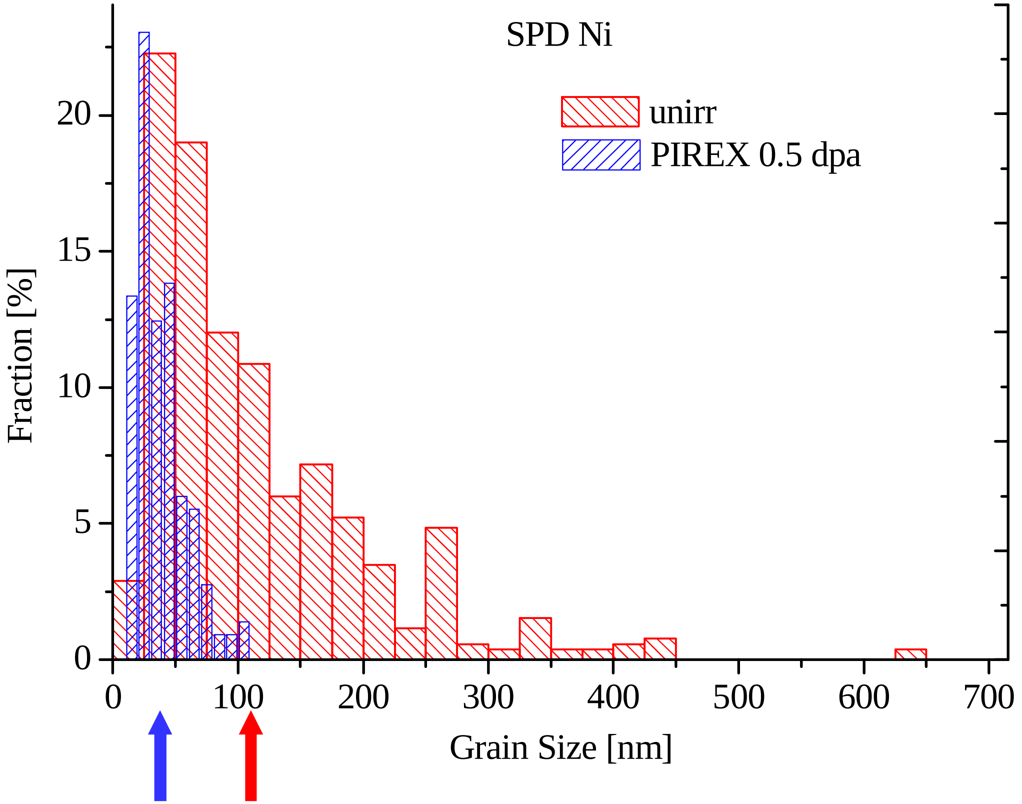
12nm grains



20nm grains

Experimetally irradiated HPT Ni

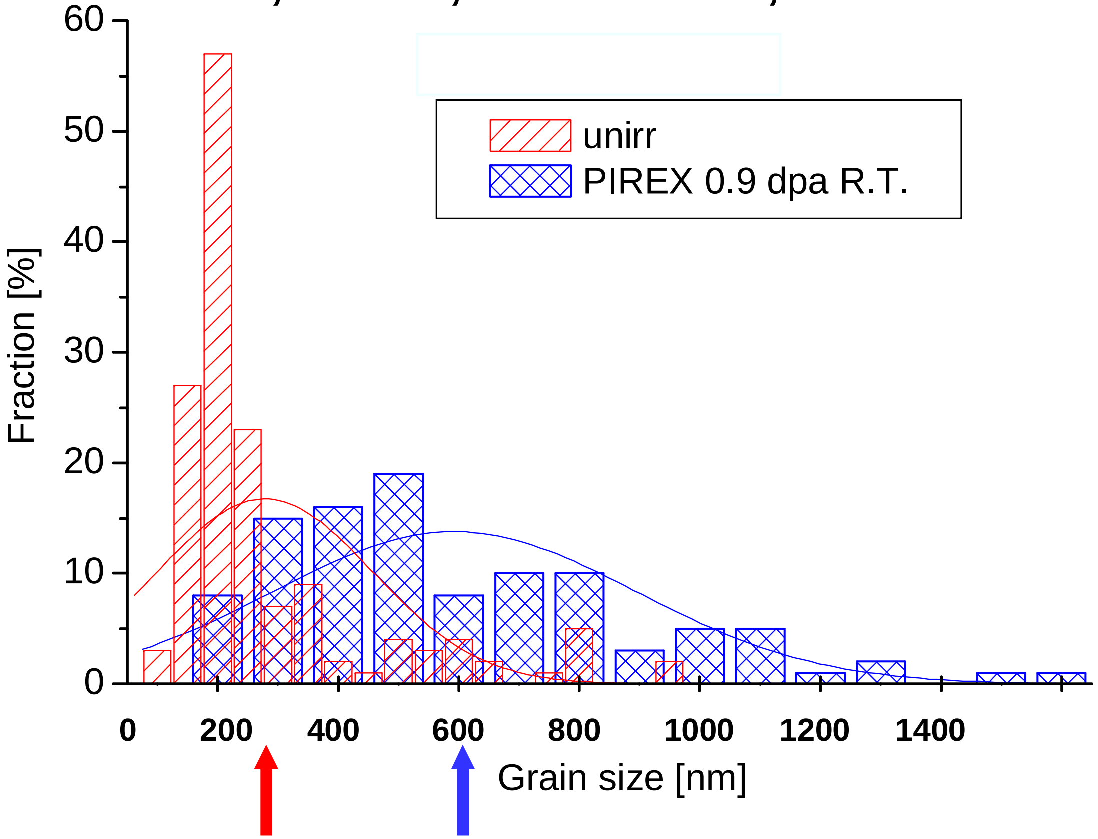
M. Victoria, N. Nita, R. Schäublin, R. Z. Valiev



Average grain size decreases from 115 nm (unirradiated, 34 nm by XRD) to 38 nm (irradiated)

Experimentally irradiated SPD Cu-0.5Al_2O_3

M. Victoria, N. Nita, R. Schaublin, R. Z. Valiev

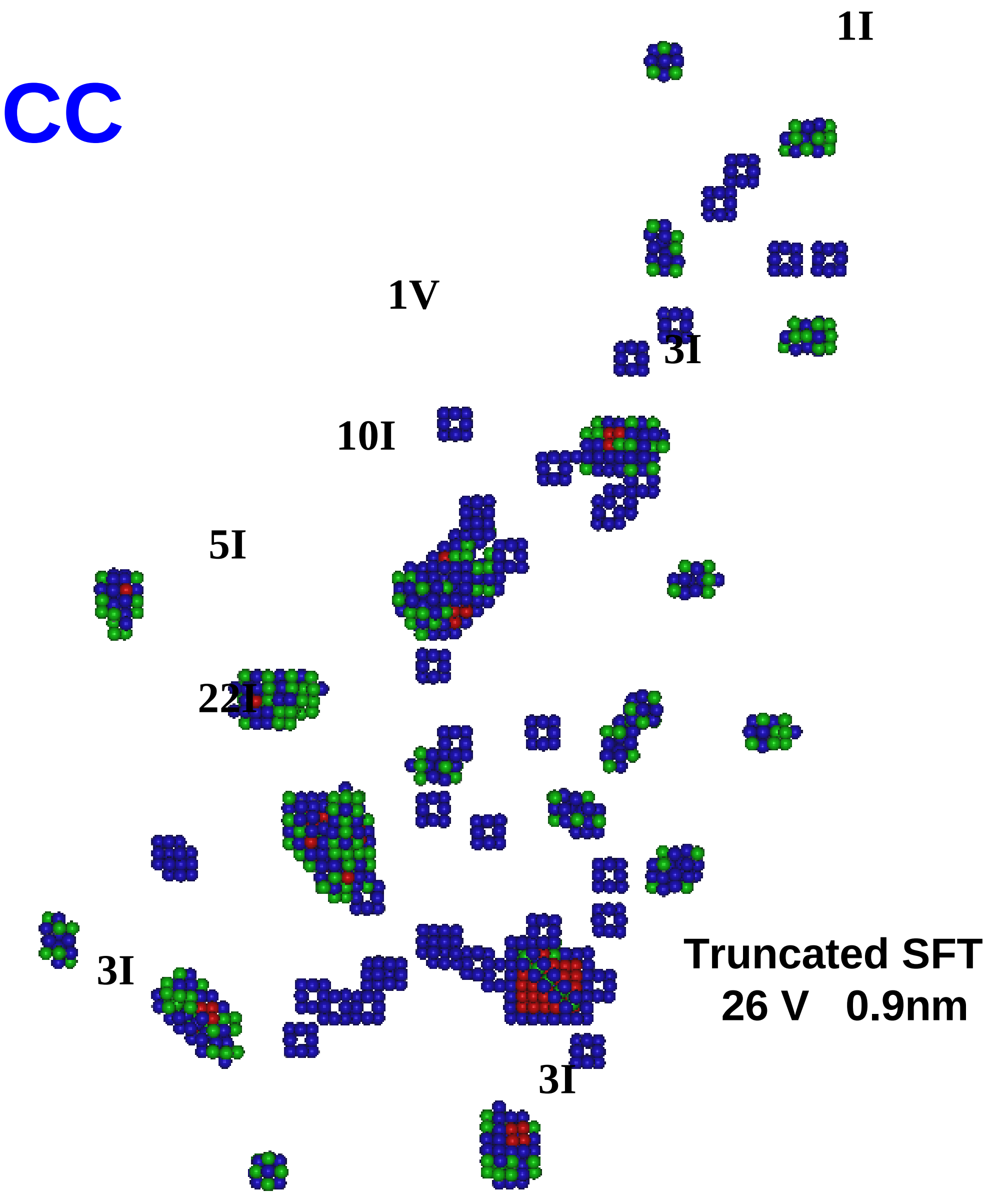


Average grain size increases

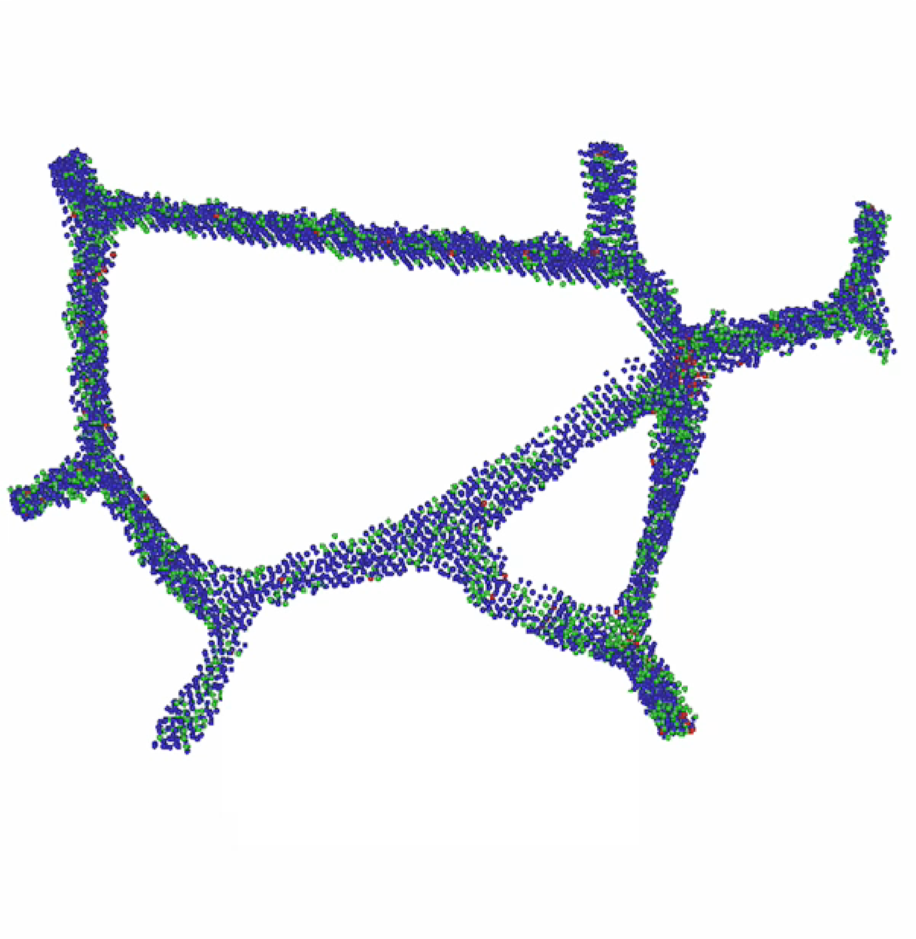
Single crystal FCC

After 4 cascade-overlaps of 20keV 1 truncated SFT forms.

fcc nc Ni



Cascade Overlap

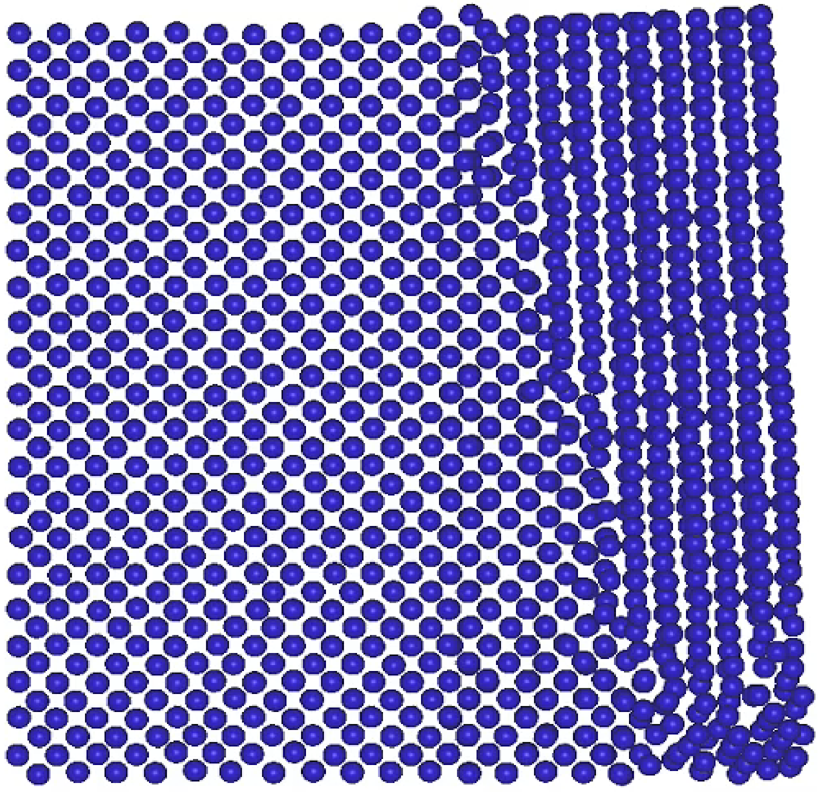


movie

4 PKAs 20keV 12nm grains

Cascade Overlap

bcc nc Fe

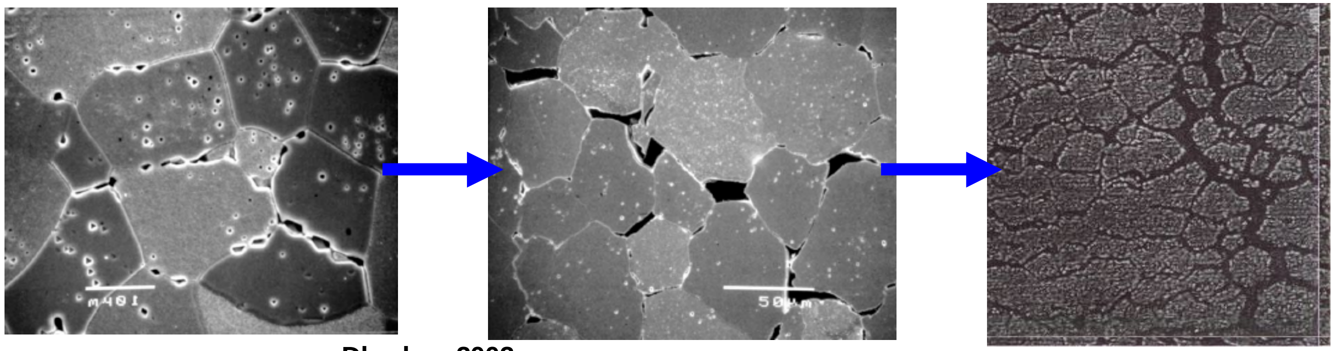


Experiment: Voids produced preferentially along actively climbing dislocations (Kitajima *et al.* JNM 1979)

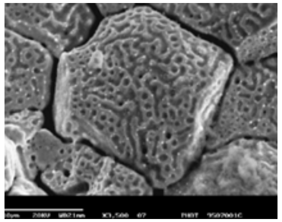
movie

4 PKAs 20keV 12nm

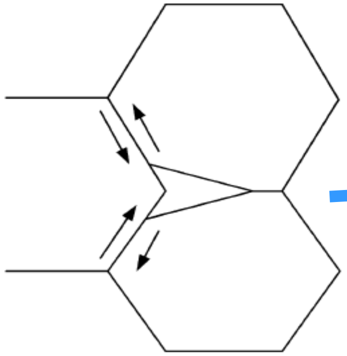
Voids, Swelling and Cracking

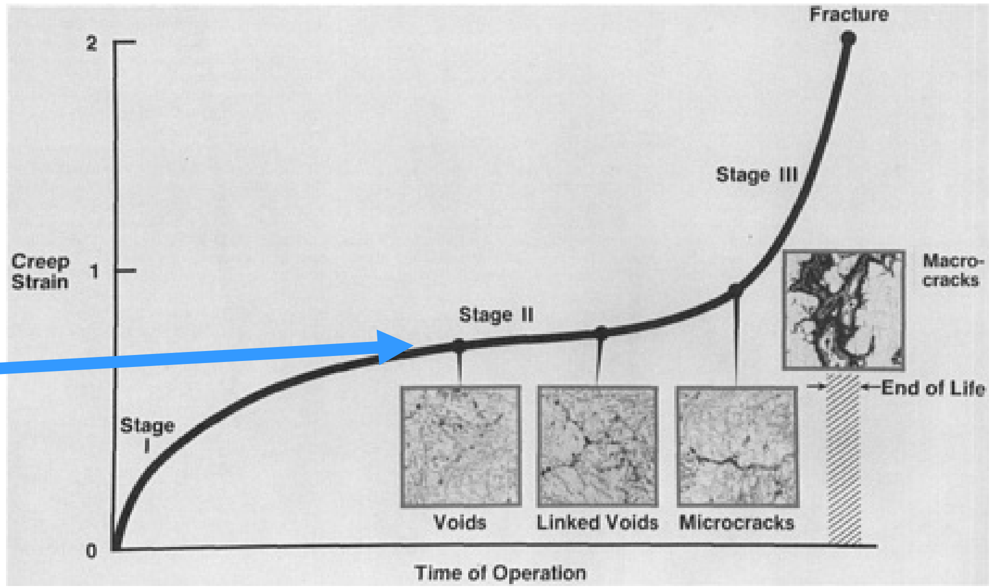


Dherbey 2002



White 2004

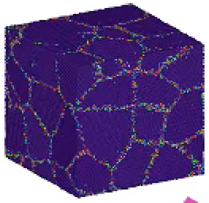


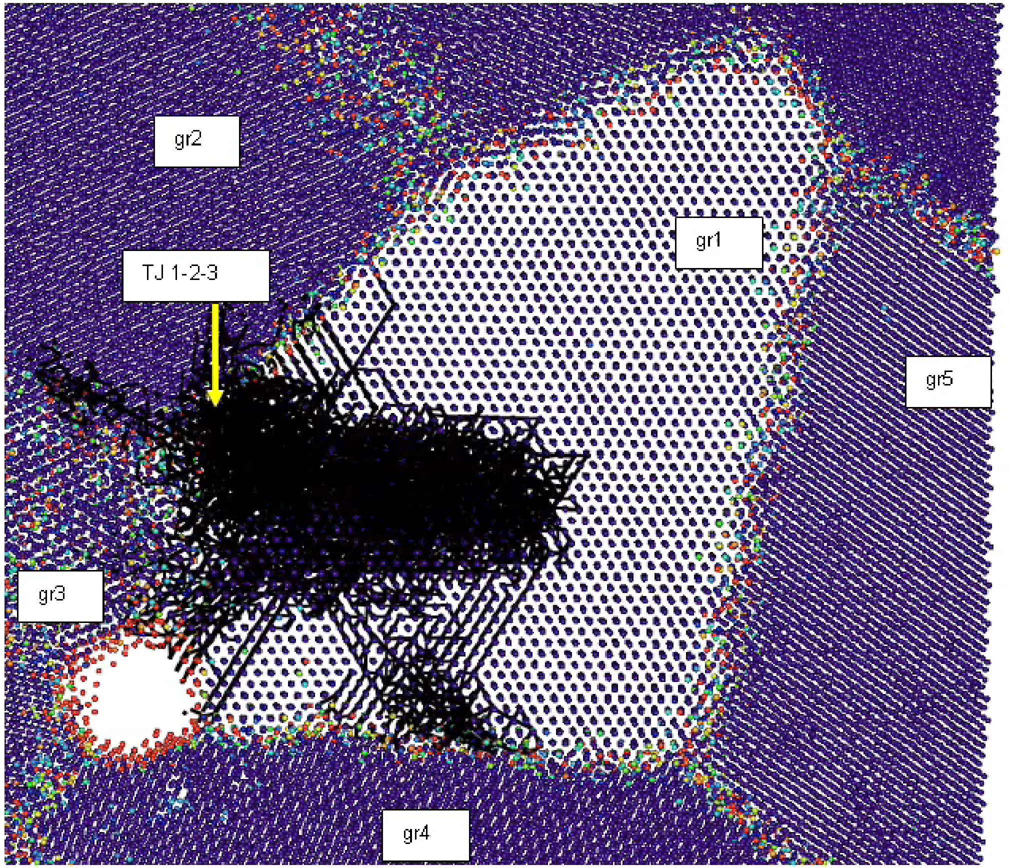


ASM Materials Handbook, online version 2005

Pre-existing Voids - MD

20keV





bcc nc Fe

Defects attracted to GBs and void

movie

The `Empirical-Potential´ Issue

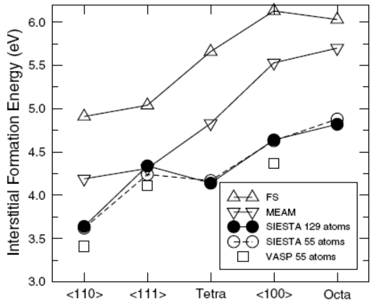
Difference in interstitials formed:

bcc nc Fe

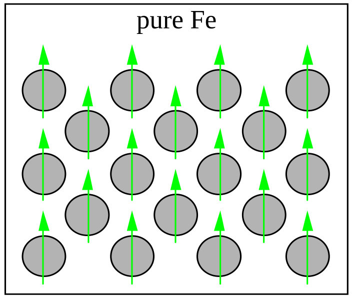
Non-magnetic potentials predict similar energies for the <110> and the <111> SIA dumbbells which contradict experiment.

Ab initio calculations (Fu 2004) show a 0.7eV difference between configurations with:

<110> dumbbell the most stable configuration
<111> dumbbell almost unstable
results are comparable to experiment

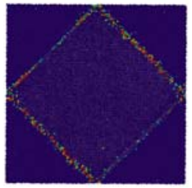


Fu et al 2004

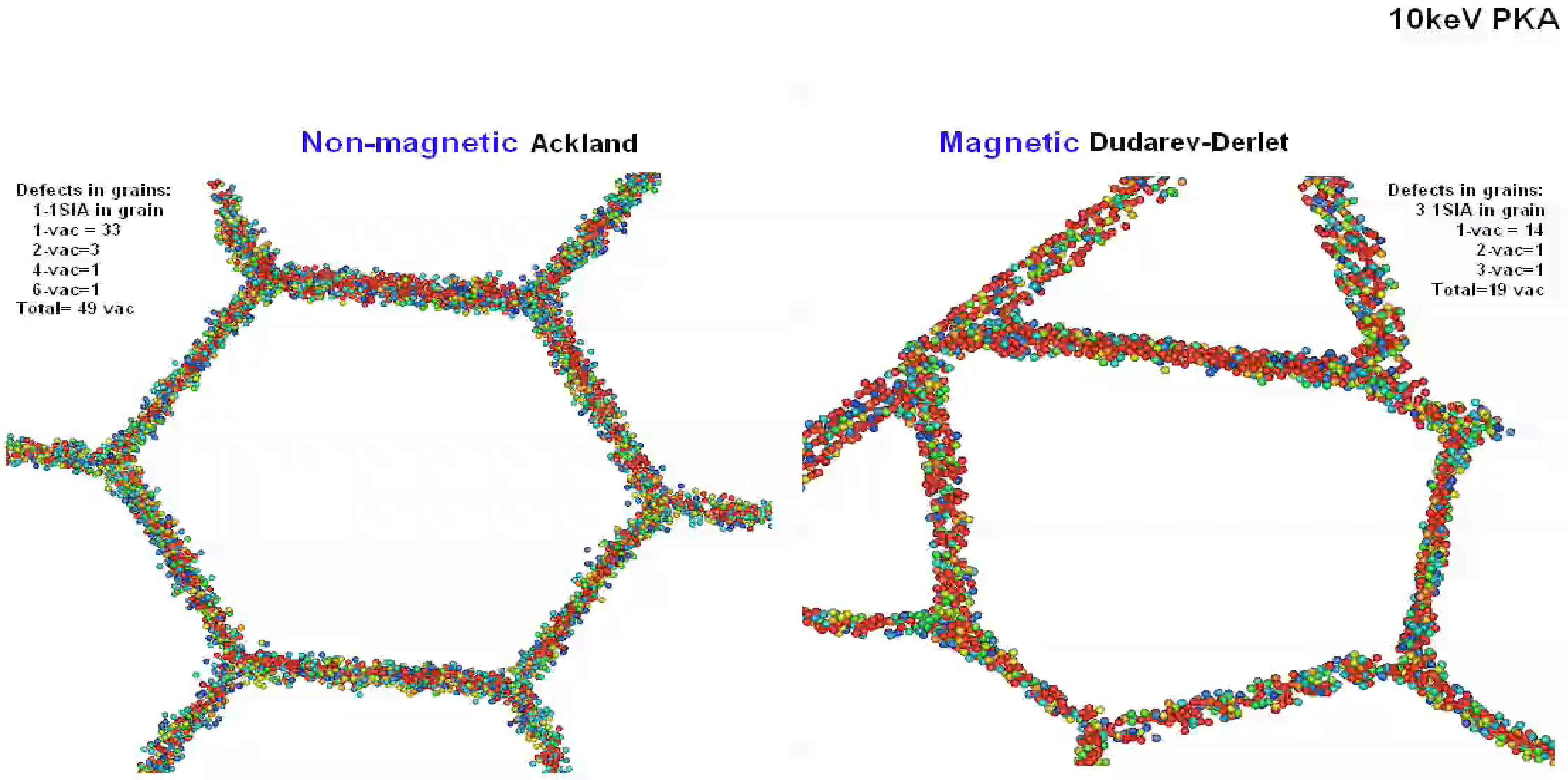


Dudarev-Derlet potential includes magnetism produces the correct interstitial

Mendelev potential is non-magnetic and has been fitted to produce the correct interstitial



20nm 4-grain sample



10keV PKA

Non-magnetic Ackland

Defects in grains:
1-1SIA in grain
1-vac = 33
2-vac=3
4-vac=1
6-vac=1
Total= 49 vac

Magnetic Dudarev-Derlet

Defects in grains:
3 1SIA in grain
1-vac = 14
2-vac=1
3-vac=1
Total=19 vac

Very little damage, GB accomodates the cascade, local movement of GB

movie

Atomistic simulations in β-SiC

Ab initio	***Ab initio* - GB**	**Empirical Potentials**	**MD**	**MD- rad dam Single crystal**	**MD- rad dam Bi-crystal**
Lucas *et al* 2005-8 Frenkel pairs 3C-SiC 96 atoms Quantum Espresso	Koyama *et al* 2002 Tensile stress, fracture sigma 9	Tersoff 1989 Brenner type Bond-order reactive potential	Yip *et al* 1997-9 heat capacity, thermal conductivity	Diaz de la Rubia *et al* 1995-6 5keV, 200000 atoms	Moriani *et al* 2006 Sigma 5 3keV
Bockstedte *et al* 2004-7 Vac, diffusion migration and diffusion FHI96SPIN, 64 atoms	Rulis *et al*	Gao *et al* 2002 Brenner type include bond order and bond conjugation	Szlufarska *et al* 2005-8 Nanoindentation-amorphorous,	Perlado *et al* 1997-2005 5-10keV 300,1300K 800000 atoms	
Windl *et al* 1998 displacement-threshold energies 64 atoms, Fireball		Belko *et al* 2003 Tersoff with improved repulsive part	Kohler *et al* 2002 Tilt GBs	Farell *et al* 2009 10keV, 0-2000K 1M atoms	
Kinoshita *et al* 2007 Shear deformation VASP	*Ab initio* Review: Silicon Carbide, pg27, Bockstedte et al.	Vashita *et al* 1999, 2007 two-body and three-body covalent interactions	SiC nanowires	Devanathan, Gao *et al* 1998-2007 0.25 to 50 keV 6M atoms	
Jiang *et al* 2002 Ground state properties CASTEP, 84 atoms		**Tight Binding** Koyhama *et al* 1990 Self-consistent tight binding	Mura *et al* 1998, Amorphisation and order	Yuan *et al* 2001-2 Alpha SiC 512 atoms, 25 ns	
# atoms	**types of GBs**	**Fitting various properties; Rad dam – repulsive part**	**Properties that can be modelled**	**Time and length scale**	**Type of GBs**

Red= limitations

Beta SiC Fe

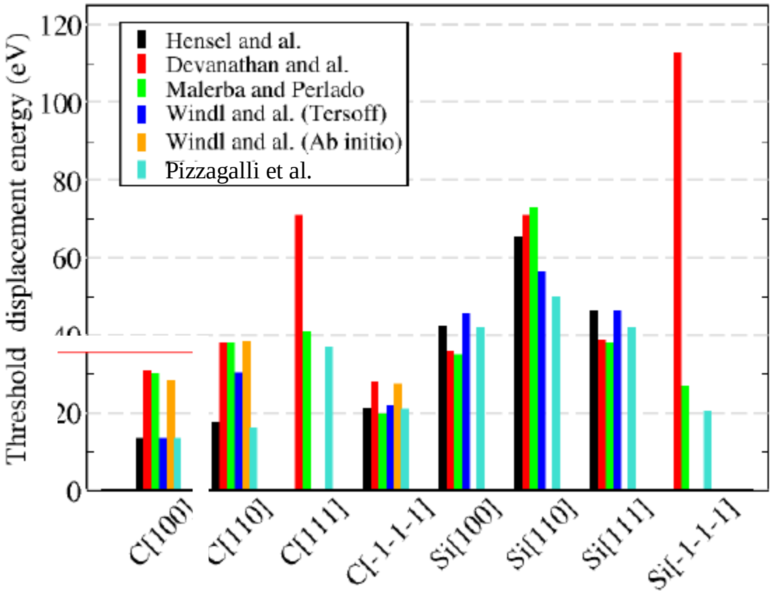
The `Empirical- Potential´ Issue

Beta SiC Fe

Radiation Damage:

Different potentials lead to different estimates of displacement energies

Uncertainty due to the use of potentials and/or techniques in calculations ?



Ref: Pizzagalli et al

Difference in interstitials formed:

- Tersoff potential: CTSi interstitials

- Modified Tersoff (including Ziegler et al corrections- (green)): dumbbells

Conclusions

MD comparison simulations of bcc and fcc structures show the

formation of truncated SFT of 2nm comparable in size to

experimental 2-4nm SFT formation

formation of voids in bcc Fe rather than SFTs (fcc metals)

attraction of SIAs to sinks present as GBs in nc bcc and fcc

Cascade volume is: comparable when the GB not directly involved

differs when GB is inside the cascade

Size of the grain affects the damage produced. Smaller grains seem to be more radiation resistant by producing less damage.

Inclusion of GBs affects the damage produced during irradiation