The Abdus Salam International Centre for Theoretical Physics

United Nations Educational, Scientific and Cultural Organization
IAEA
International Atomic Energy Agency

2137-29

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

12 - 23 April 2010

Modelling helium effects in bcc iron

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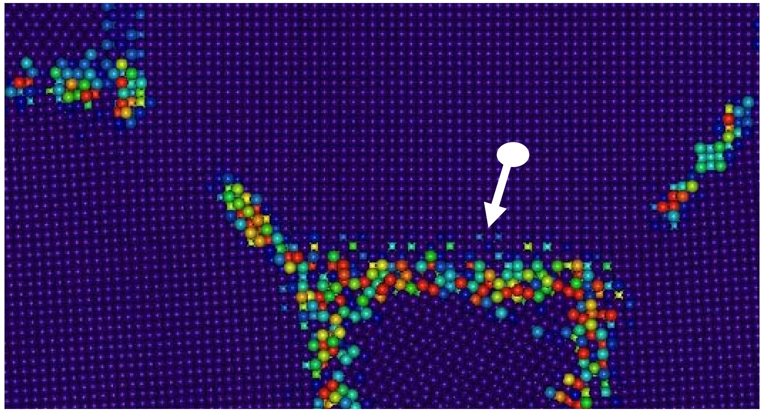


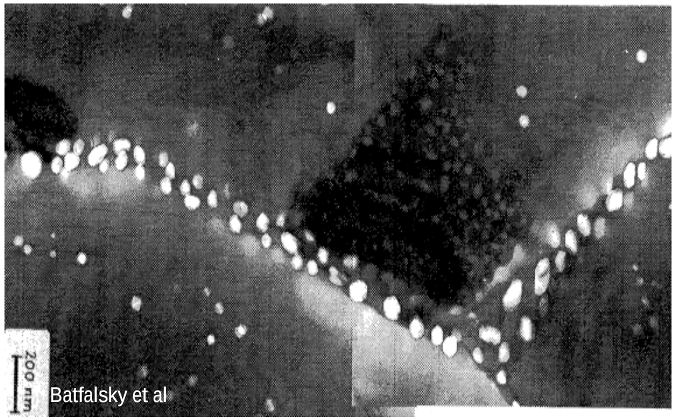


Table 1-1. Advanced fission and fusion operating conditions

	Fusion	Fission (Gen-IV)
Coolant	H_2O, He, Li, PbLi, FLiBe	H_2O(SC), He, Pb, PbBi, Na
Particle Energy	< 14 MeV	< 1–2 MeV
Temperatures	300-1000°C	300–1000°C
Max displacement damage	~ 200	15–200
He/dpa	10 appm/dpa	~ 0.1 appm/dpa
Stresses	Moderate, nearly constant	Moderate, nearly constant

Stoller

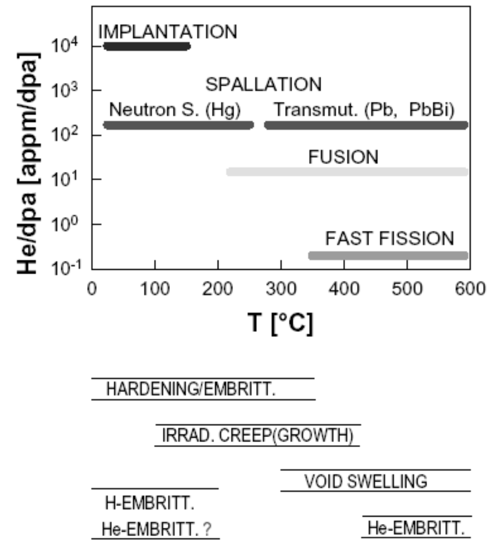
He Bubbles in Nuclear Environments

Bubbles can lead to material degradation

Bubble nucleation is still not well understood

Atomistic simulations provide possibility to study the dynamical processes in He clustering

Obtain insight into bubble nucleation and growth



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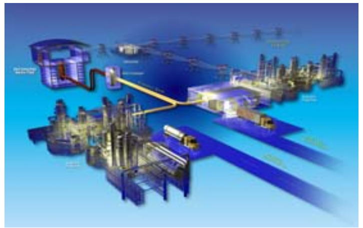
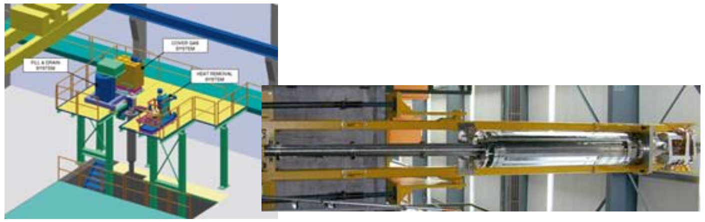
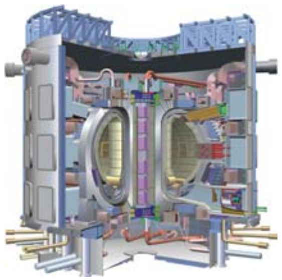






Key Issues of He in ferritic/martensitic steels

Ferritic/martensitic steels are:

very resistant to void swelling

Embrittlement is a problem

Range of temperatures 350 – 550 °C

- **lower value – embrittlement**
- **upper value - strong reduction in mechanical strength**

The role of He in the embrittlement is not clear

He Bubbles in Nuclear Environments

He is essentially insoluble

Interacts with and traps at nearly every atomic-nano-microscopic defect

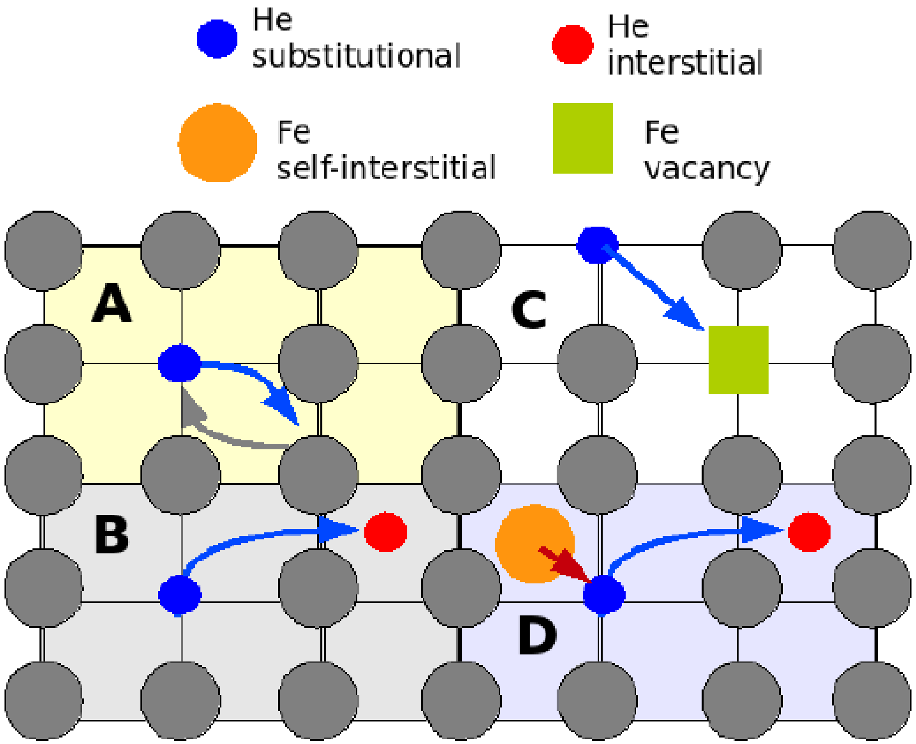
Precipitates as bubbles causing:
- irradiation hardening
- fast fracture
- creep rupture
- void swelling

Previous THDS of He implanted Fe reveal desorption events and activation energies (Ono et al, Sugano et al.,(2002 - 2004), Vassen et al. (1991)

Need to understand He transport (migration and defect trapping interaction kinetics), which governs He fate and overall microstructural evolution

Role of Helium

Diffusion
Trapping – position and method
Process of bubble nucleation and growth
Role of sinks on diffusion and bubble density and size



A – exchange

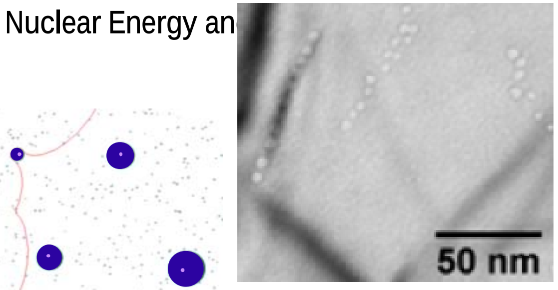
B – Dissociative

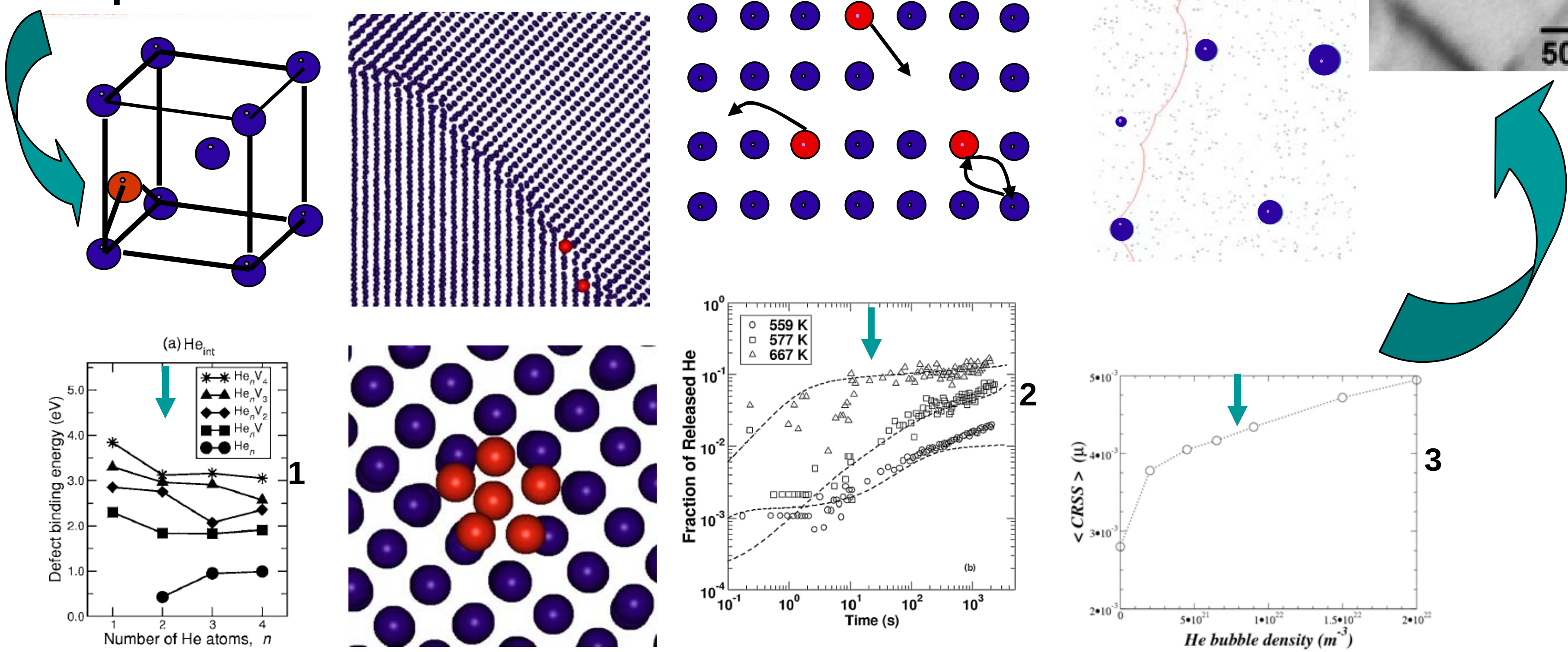
C – Vacancy

D - Replacement

Caturla

Computer facilities





ab initio	Molecular Dynamics	KMC/ Rate Theory	Dislocation Dynamics	TEM sample

Time + Length

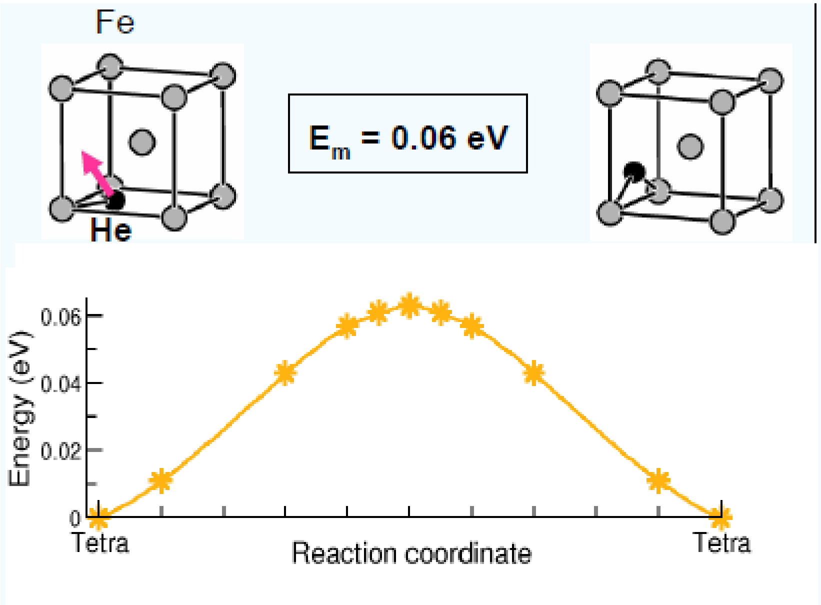
Small clusters **Bubble nucleation**

Non-ideal bubble growth **Ideal bubbles**

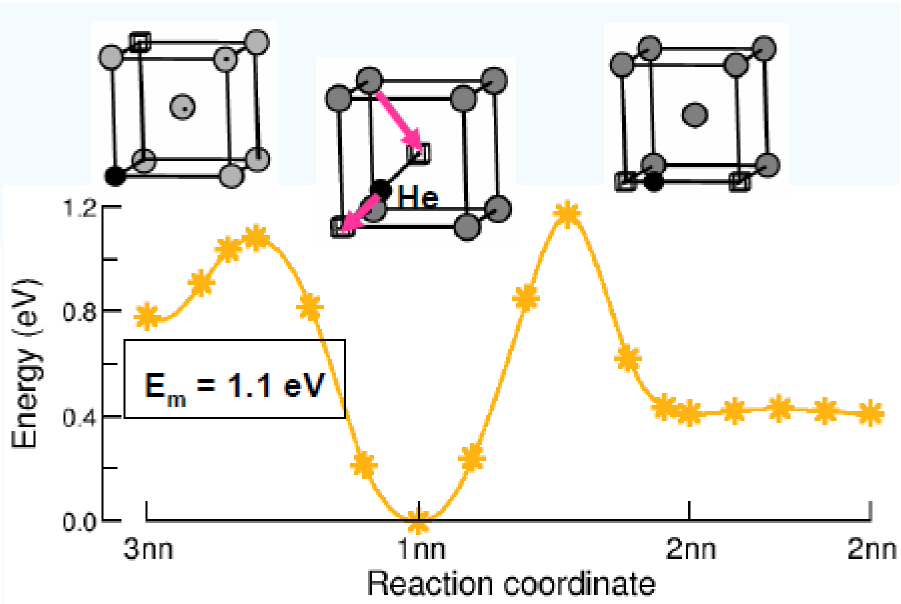
Fu (2005)

He migration in Fe DFT Calculations

Interstitial He



Substitutional He

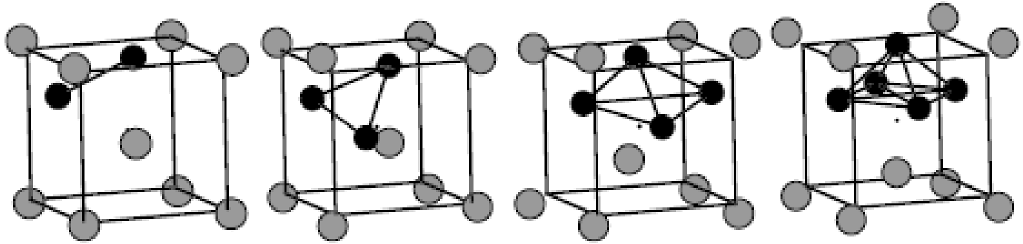


Dissociation and kick-out mechanism

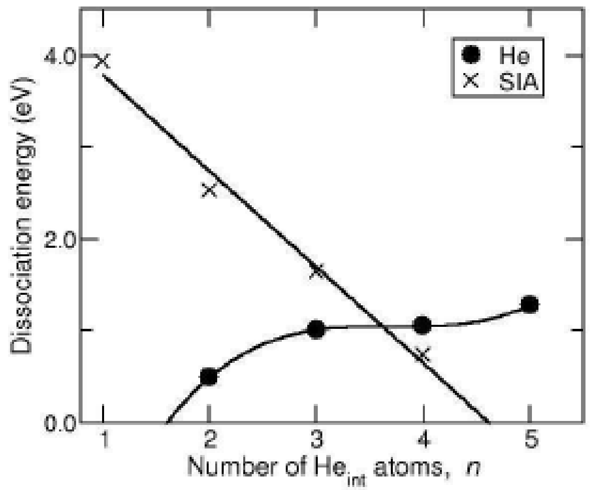
Vacancy mechanism

He-V Nucleation DFT

Fu et al (2007)



He clusters

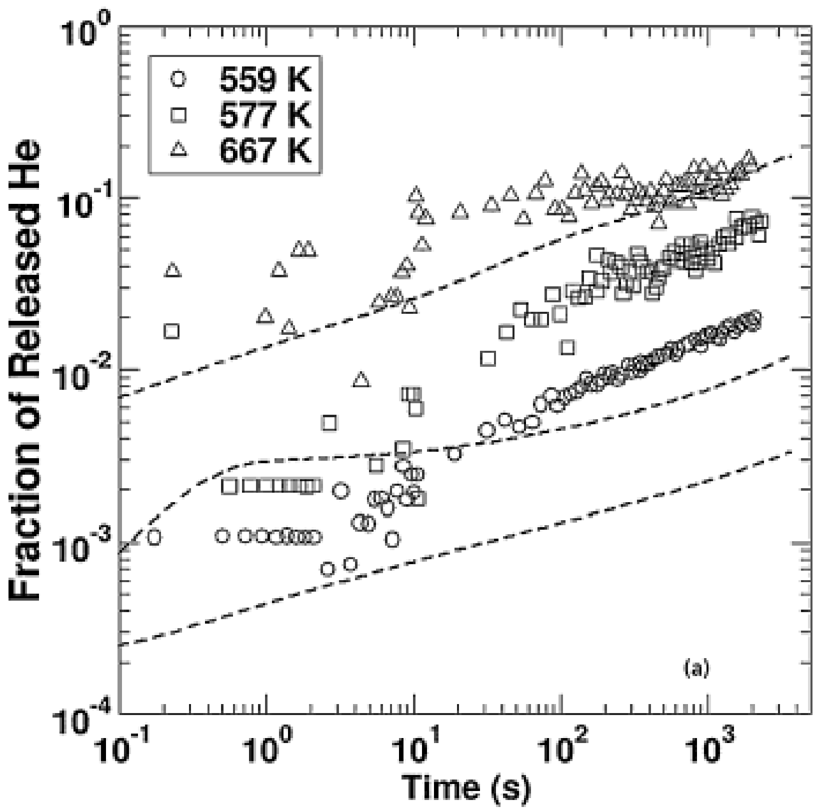


Spontaneous emission of SIA from He$_n$ when n >4

Desorption Experiments KMC

Caturla et al

Input DFT data for pure Fe



Discrepancy between model and experimental measurements, thought to be due to impurities

Role of Carbon

Fu Ortiz Caturla et al

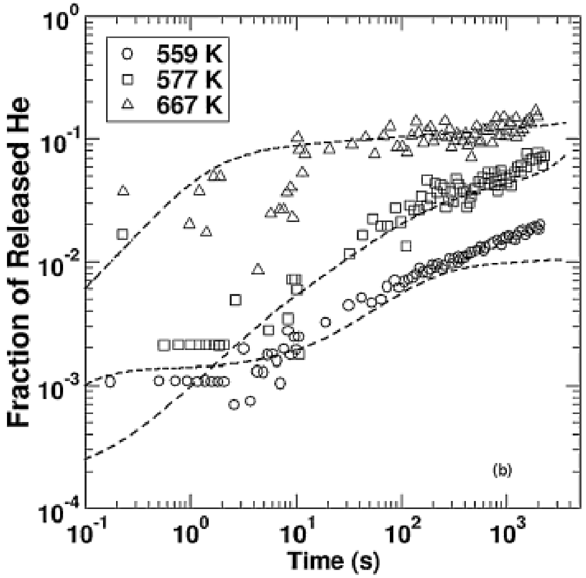
Ab initio results:

C reduces the effective migration energy of vacancies

C reduces He-V binding energy

C traps V and reduces He_nV_m formation leading to kick-out He_{sub} + SIA = He_{int}

Information used in KMC modelling and provides a good comparison to desorption experiments

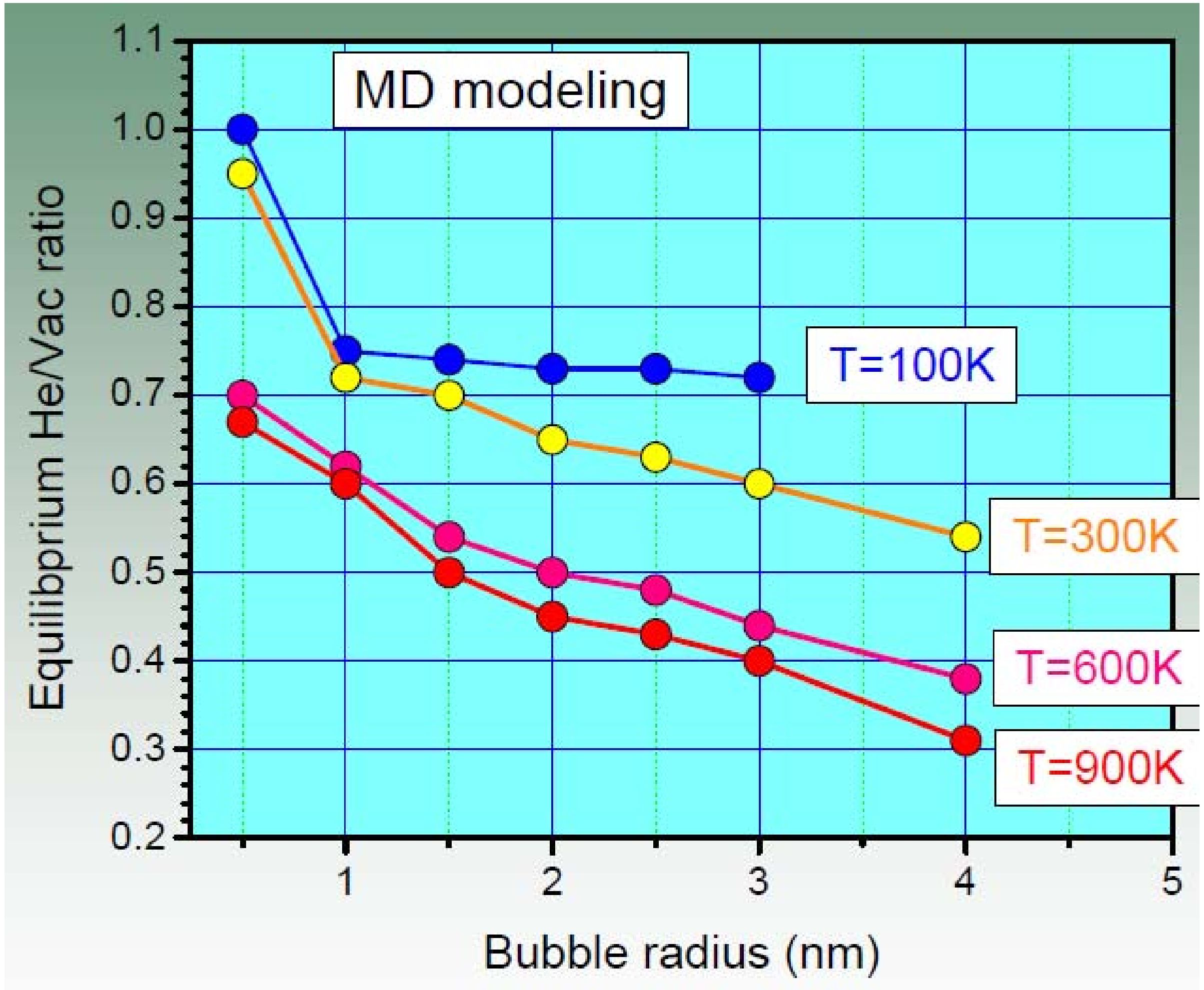


fitted values of vacancy migration energy, V–He and V–HeV binding energies

Formation Energies DFT vs MD

		Fe-Fe	*Oct*	*Tetr*
DFT	Seletskaia		4.60 H	4.37
	Fu		4.57 H	4.39
MD	JN	AMS	4.512 H	4.385
	JN	DUD_O	4.444 H	4.326
	Gao	DUD_N	4.529 H	4.423
	JN	FS	4.406 H	4.290
	Wilson	FS	5.25 L	5.34
	Seletskaia	FS	4.54 H	4.5
	Yang	FS	5.25	
	Morishita	FS	5.25 L	5.34
	Venteleon		L	

He Bubble Stability MD

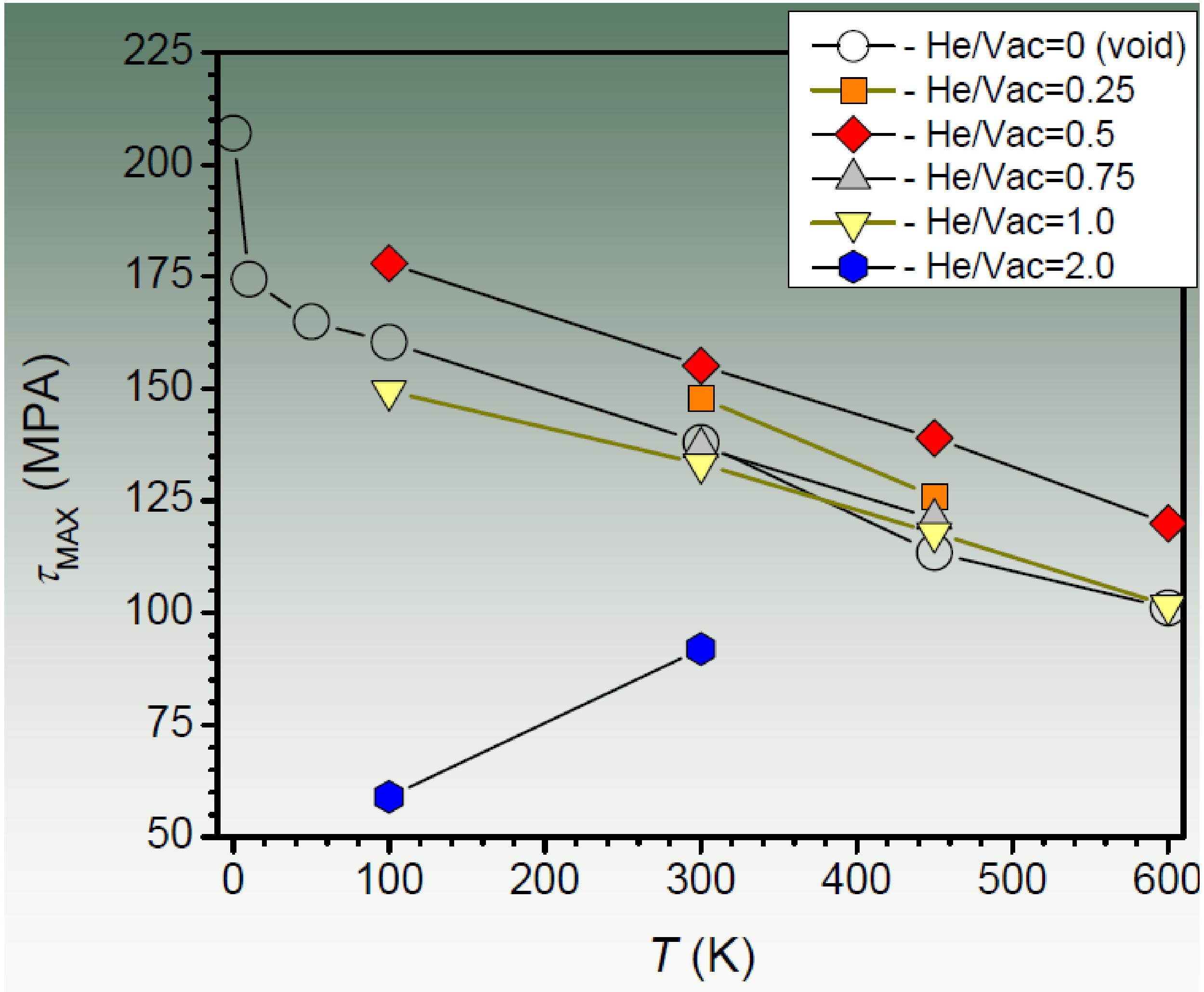


Osetsky et al

He/V ratio in the bubble is very low

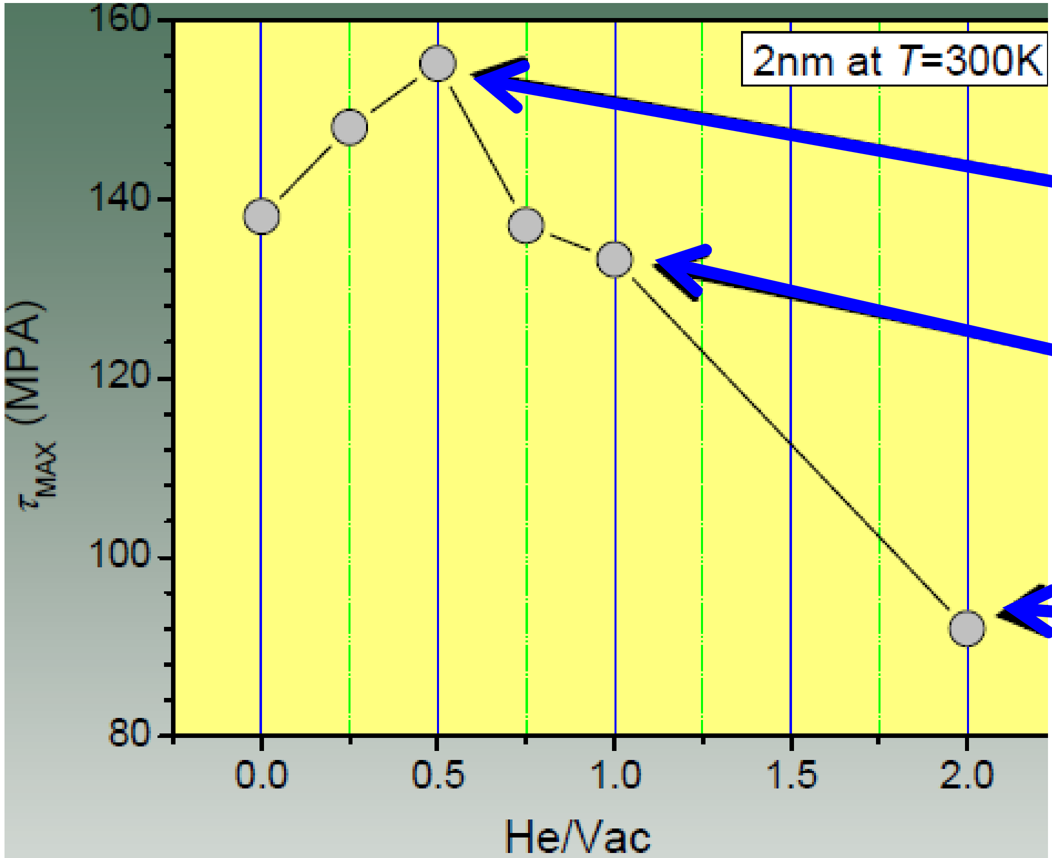
Dislocation-bubble interaction MD

Osetsky et al



Dislocation-bubble interaction MD

Osetsky et al



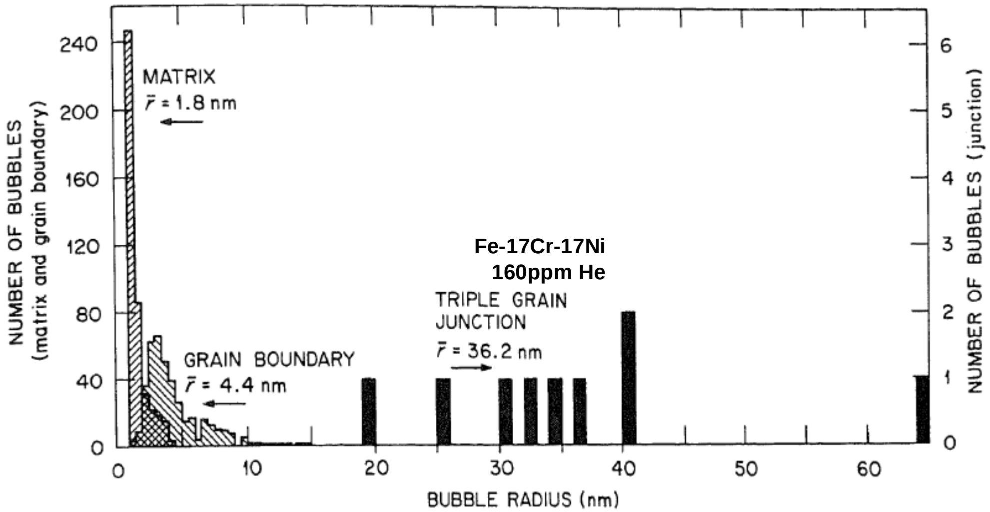
Strong obstacle

medium obstacle

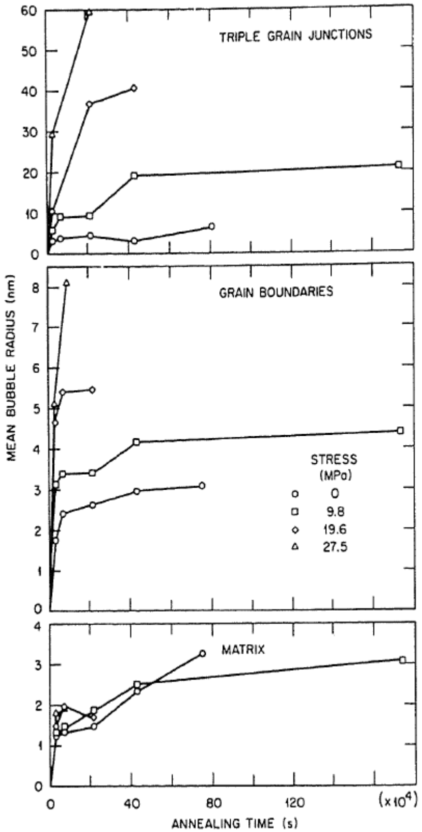
weak obstacle

Helium Bubbles at GBs

Ullmaier et al 1980



Braski et al 1979



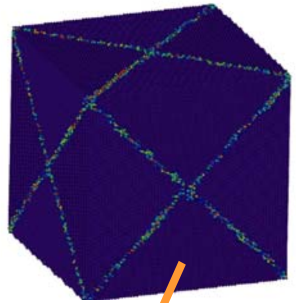
Braski et al 1979

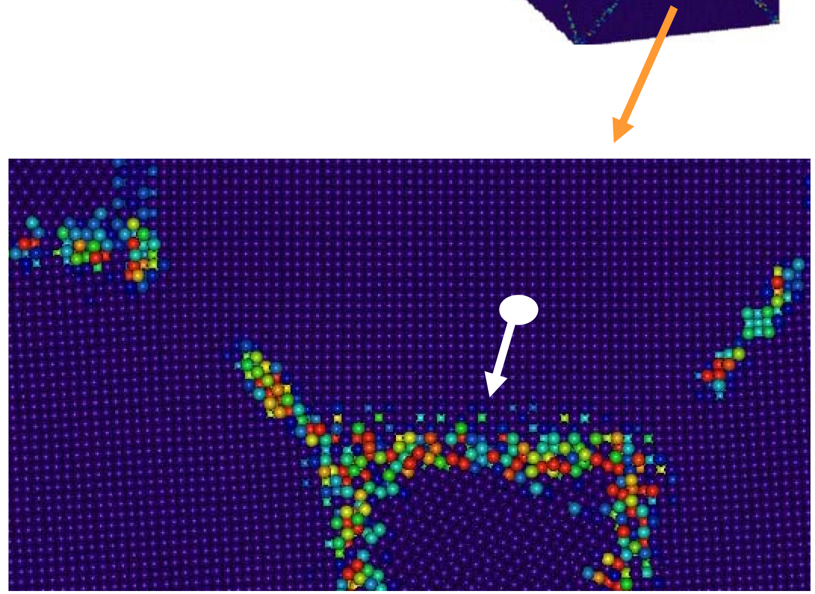
He bubbles formed in GBs lead to GB decohesion which leads to embrittlement

The creep lifetime expectancy of a metal is also affected by the accumulation and fast diffusion of helium in GBs

MD Simulation of He in nc alpha Fe

- 0K + 300K
- Periodic Boundary Conditions
- Fe-Fe: Dudarev-Derlet (MP-CS2) potential
- He-He: Beck Potential
- Fe-He: Juslin-Nordlund (nc sample);
  MP-CS2-He Potential (bicrystal)
- Bi-crystal: Σ3, Σ5; 12,000 atoms
- NC: high, low angle and close to Σ3 GBs; 700,000 atoms
- Free volume in sample calculated by mesh-grid calculation





Collaborators

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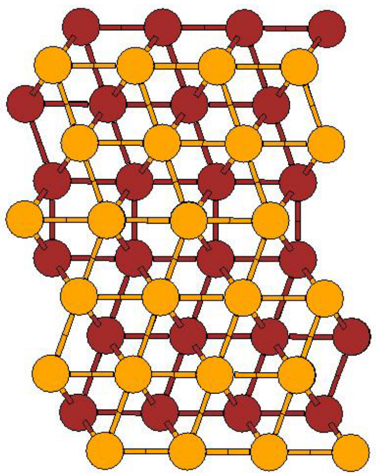
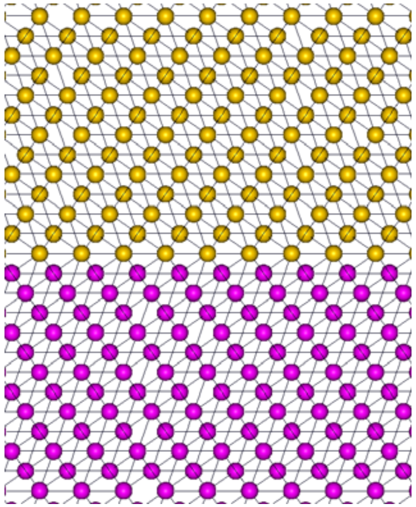
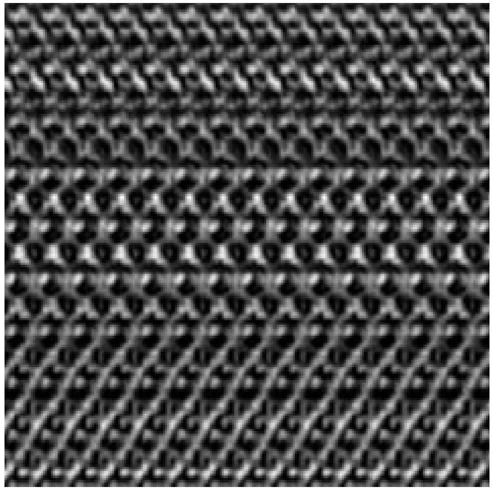
Bi-crystal Σ 3 {112}



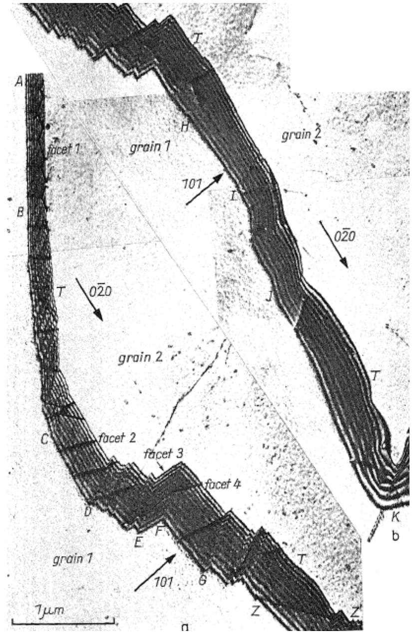
ab-initio



MD

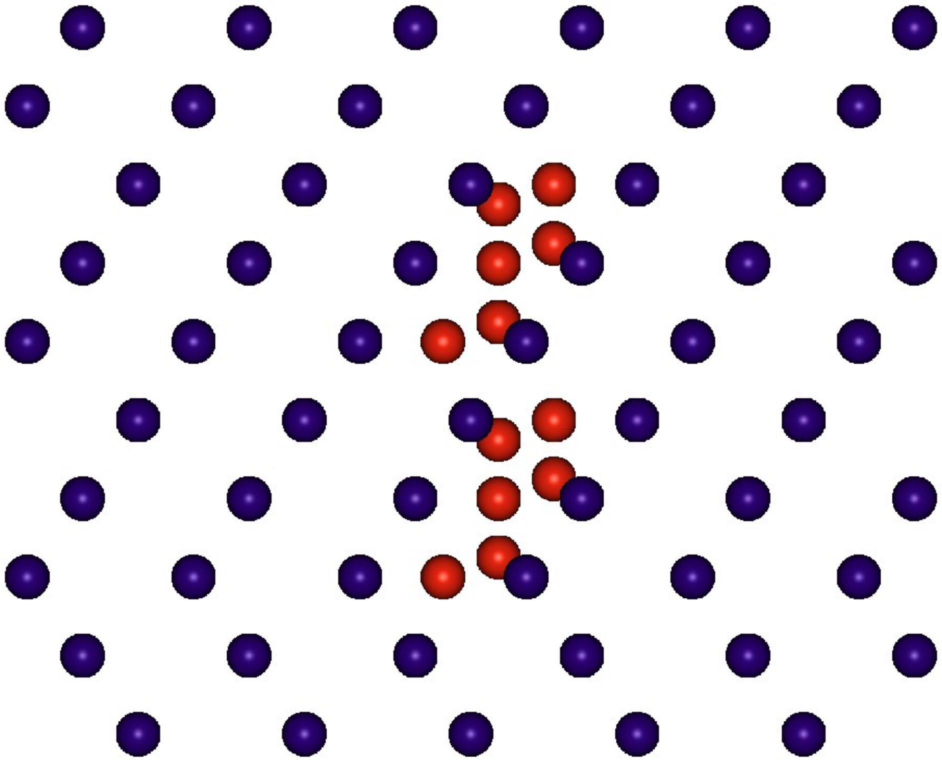


TEM simulation

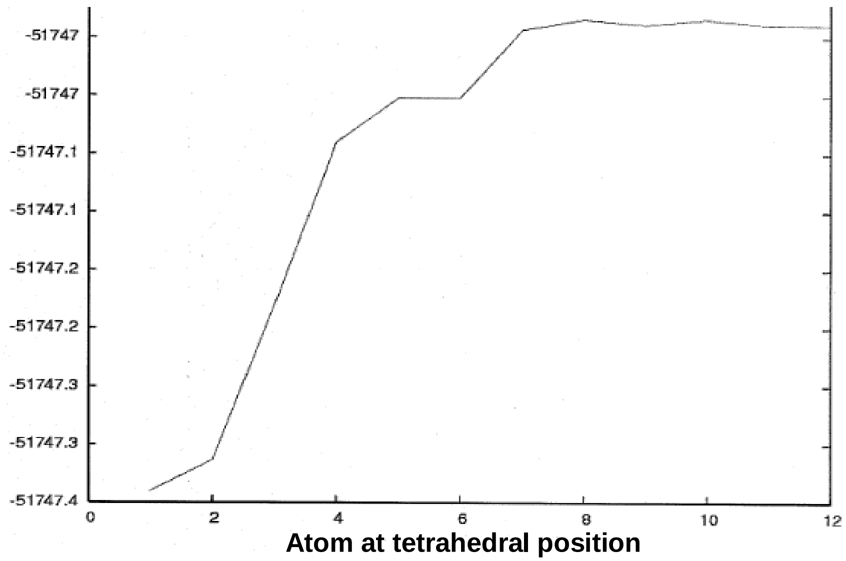


TEM experiment:
Forwood *et al* 1988

He in bi-crystal Σ 3 {112}

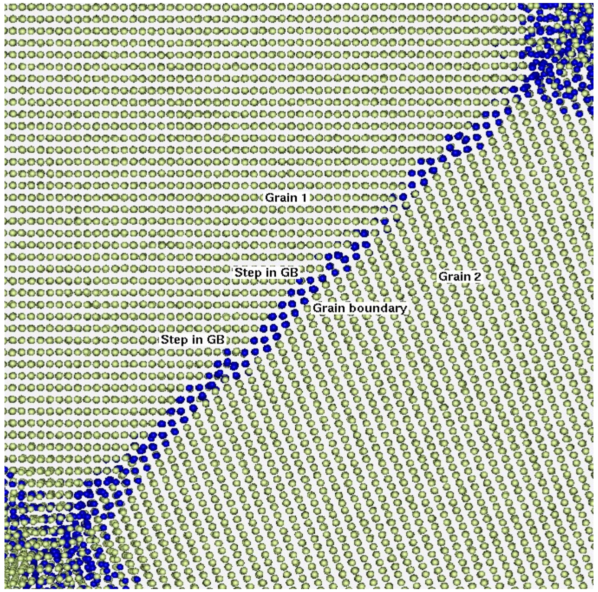


● He

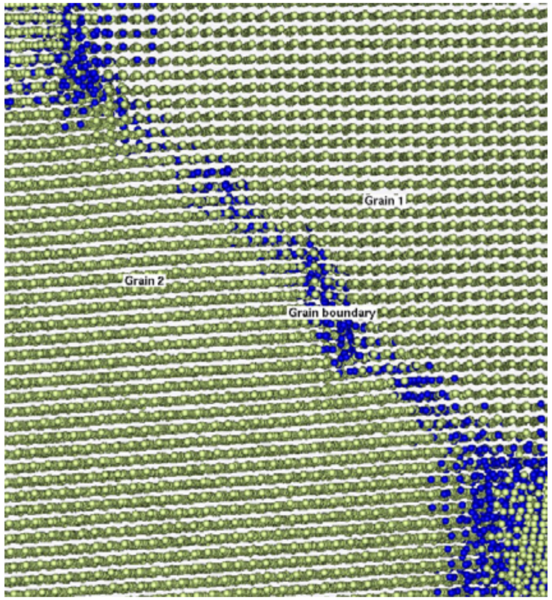


Σ3 {112} GB is not a strong sink for He atoms; also seen *ab initio* calculations

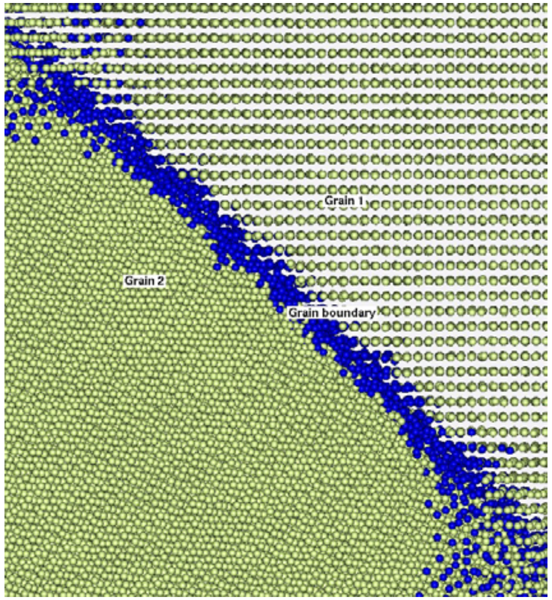
GB structure in nc α Fe



Symmetrical GB with steps

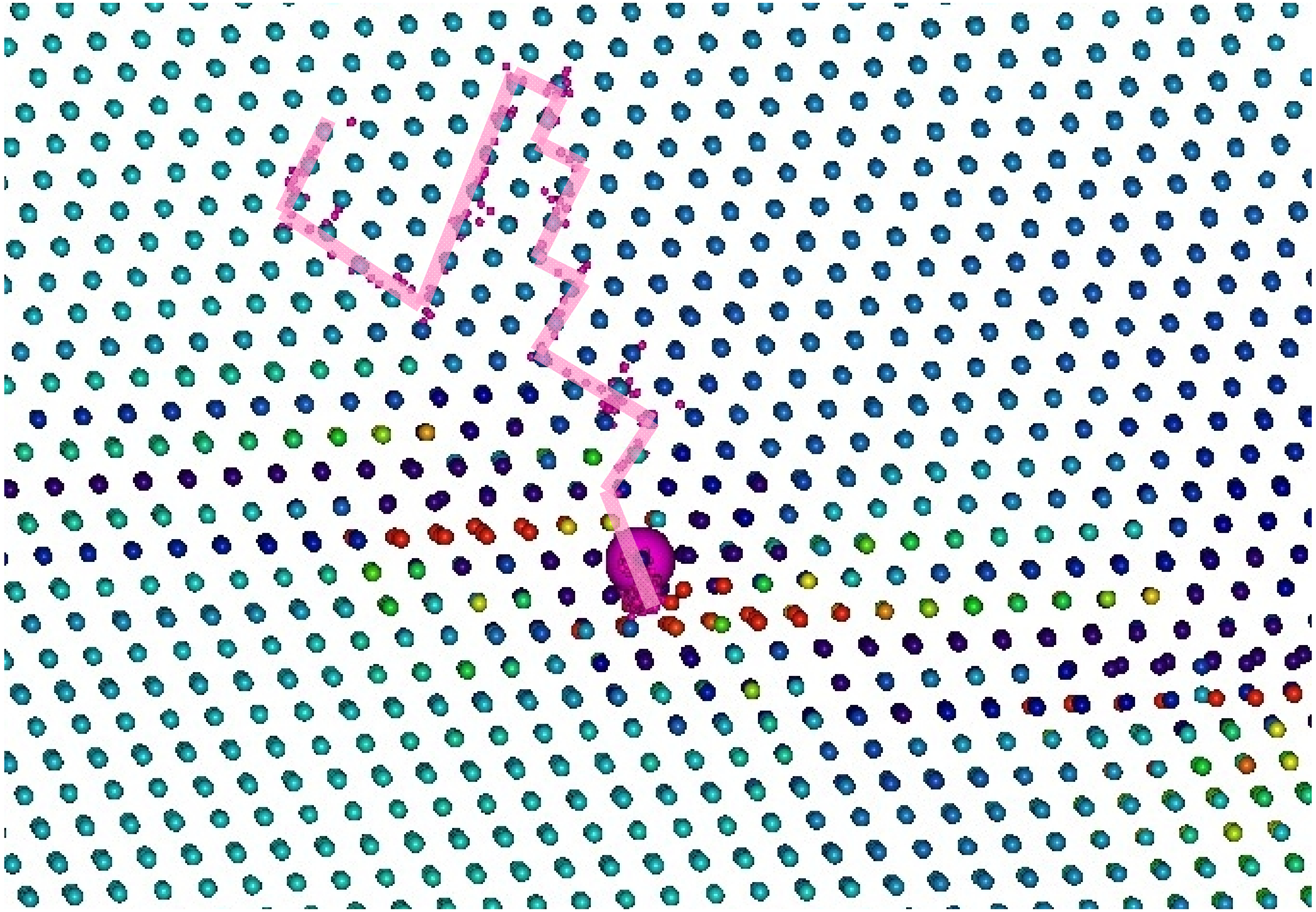


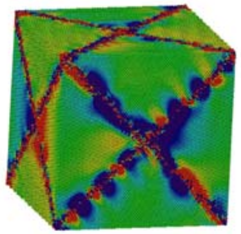
Low angle GB



High angle GB

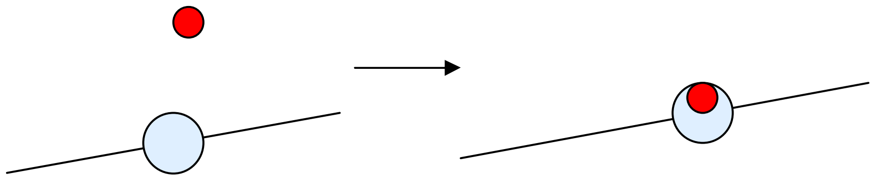
He movement in nc α-Fe





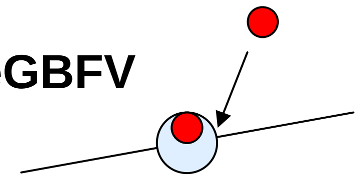
He moves to step within the non-ideal symmetrical GB

Step 1:
He inserted into matrix



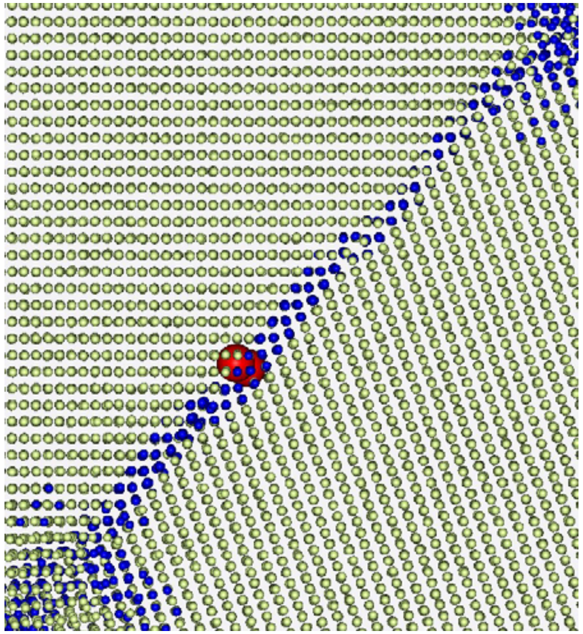
He moves to free volume in GB
-HeGBFV (free volume) formed

Step 2:
Insert He at tetrahedral position in HeGBFV

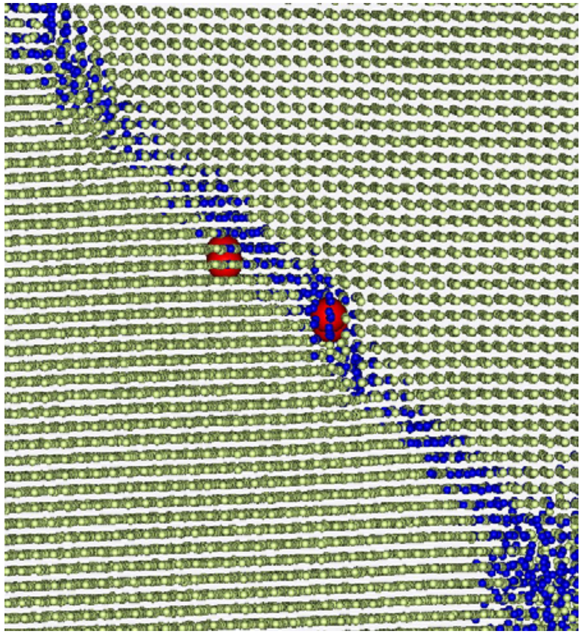


Geometrical insertion of He

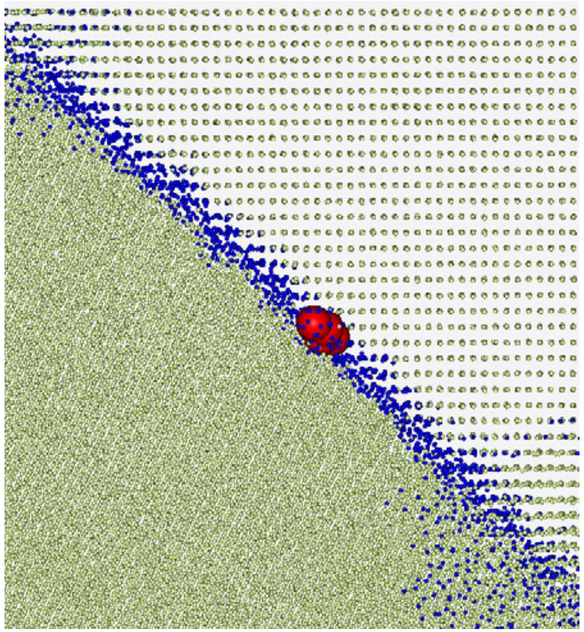
He inserted near pre-existing trapped He



Symmetrical GB with steps



low angle GB

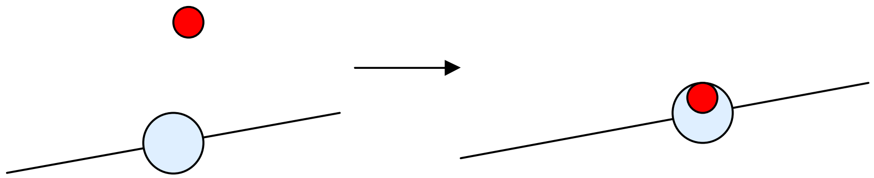


High angle GB

He atoms form He_2V cluster

Step 1:

He inserted into matrix

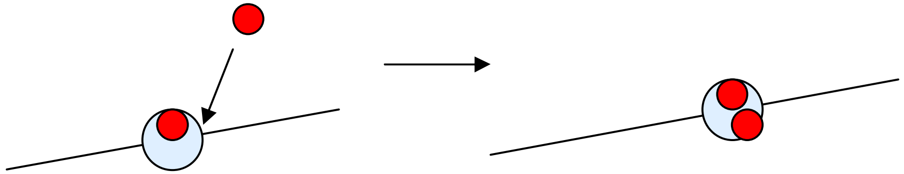


He moves to free volume in GB

-HeGBFV (free volume) formed

Step 2:

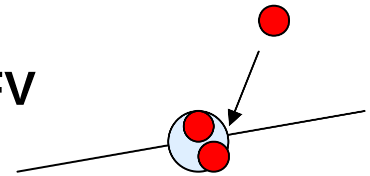
He at tetrahedral position in HeGBFV



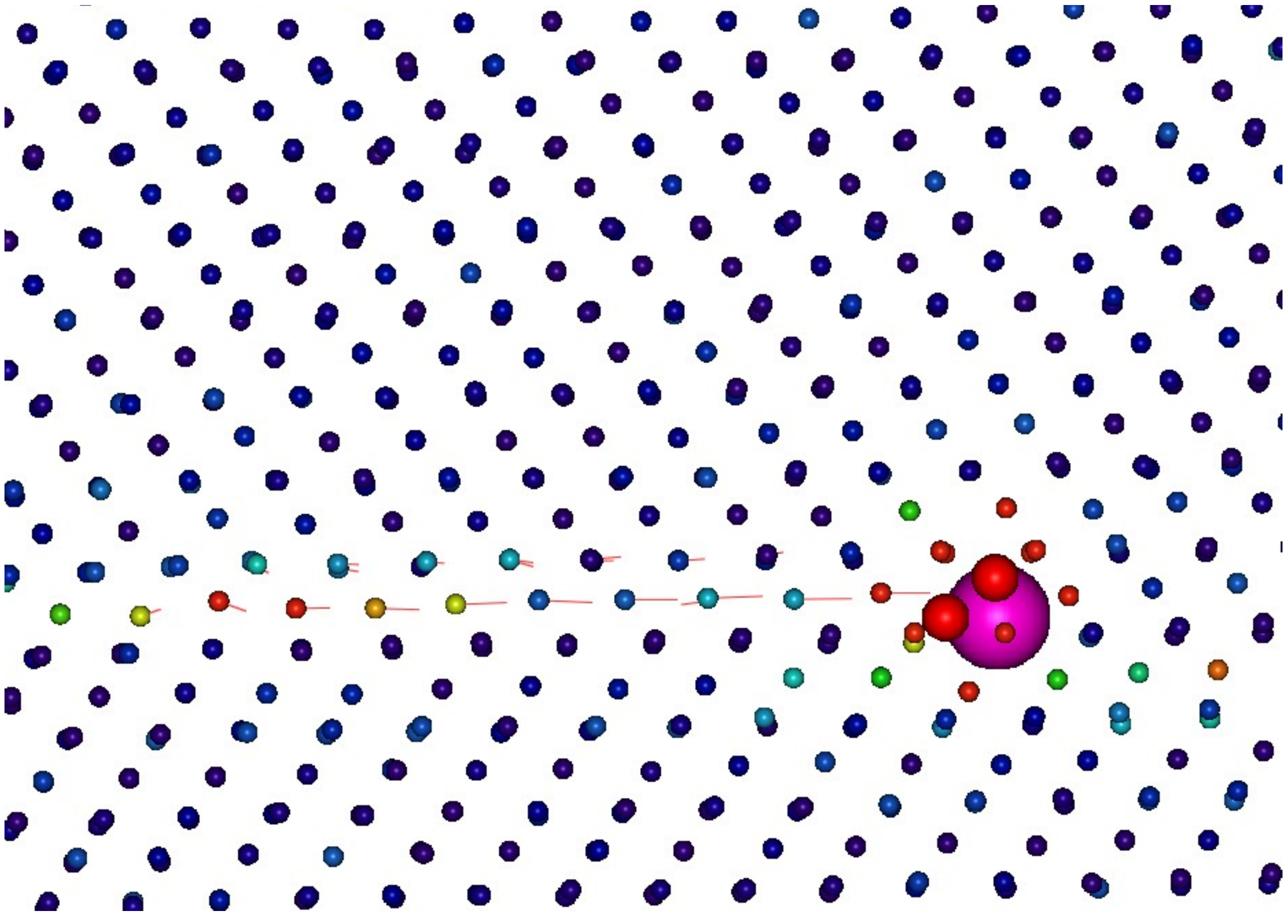
-He_2GBFV formed

Step 3:

He at tetrahedral position in He_2GBFV



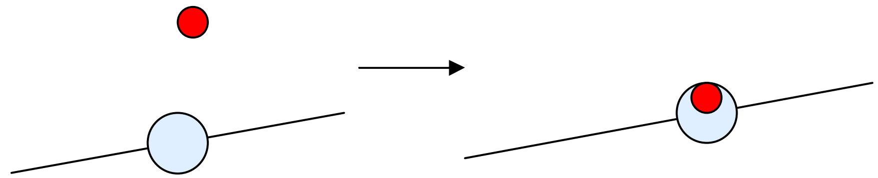
Geometrical insertion of He part 2



Fe atom movement to accommodate He cluster

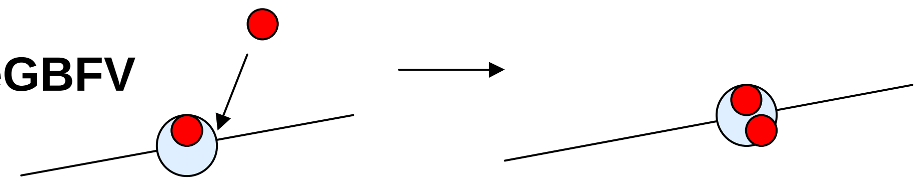
Step 1:
He inserted into matrix

He moves to free volume in GB
-HeGBFV (free volume) formed

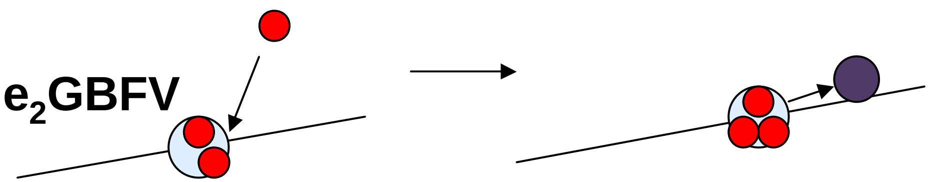


Step 2:
Insert He at tetrahedral position in HeGBFV

-He_2GBFV formed

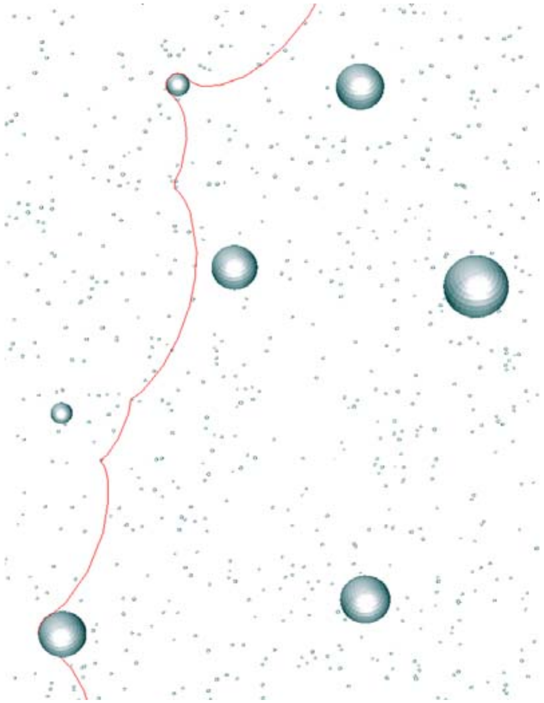


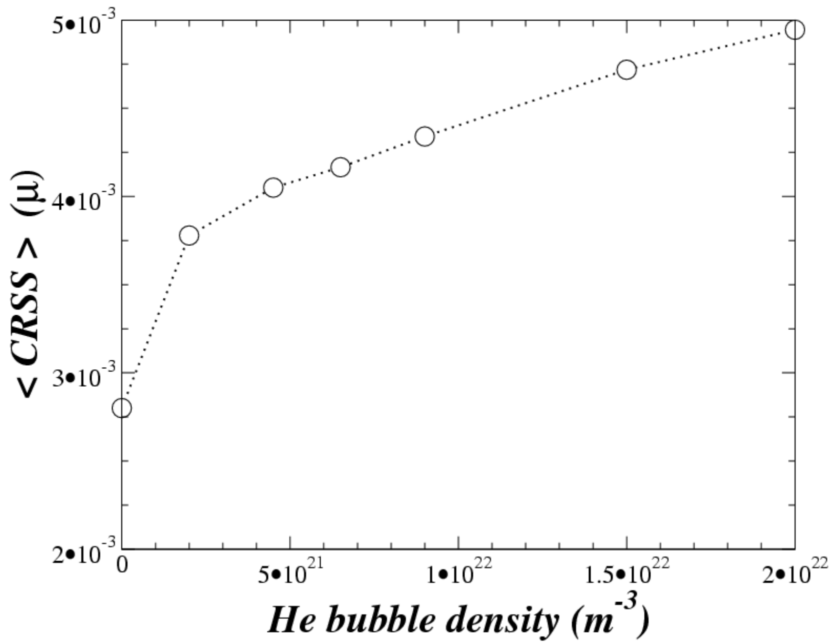
Step 3:
Insert He at tetrahedral position in He_2GBFV



-He_3GBFV formed
-Fe atoms reaccomodate within the GB
-He-kickout in GB with smaller number of He atoms than in matrix

Helium-dislocation-dispersoid interaction in Fe- 3D DDD





Inclusion of helium causes a dramatic increase of the CRSS, a factor of 2 relative to the non-irradiated samples

Modelling provides insight in a much shorter time than experiment

Summary

-He nucleation in the matrix and at GBs is still not well understood

-Atomistic + mesoscale simulations provide the ability to study the dynamical processes involved in He-clustering.

- Electronic structure calculations reveal stability of tetrahedral Hei

- MD/MS studies of He binding with atomic/nanoscale defects

- KMC studies of HemVn cluster diffusion

- Rate theory/cluster dynamics modeling of He desorption, and transport and fate of He in neutron irradiated steels

- Prospects of He management by ODS-type nano-scale precipitates

Free Codes

LAMMPS: ***lammps.sandia.gov (C program)***

? MOLDY Cask (LLNL) (Fortran)

Moldy: http://www.ccp5.ac.uk/moldy/moldy.html

Visualisation: ***www.ks.uiuc.edu/Research/vmd/***

Books:

http://www.ebookpdf.net/
___The-art-of-molecular-dynamics-simulation-free-download_ebook_.html