Molecular dynamics simulation of Fe plasticity in the presence of multiple defects

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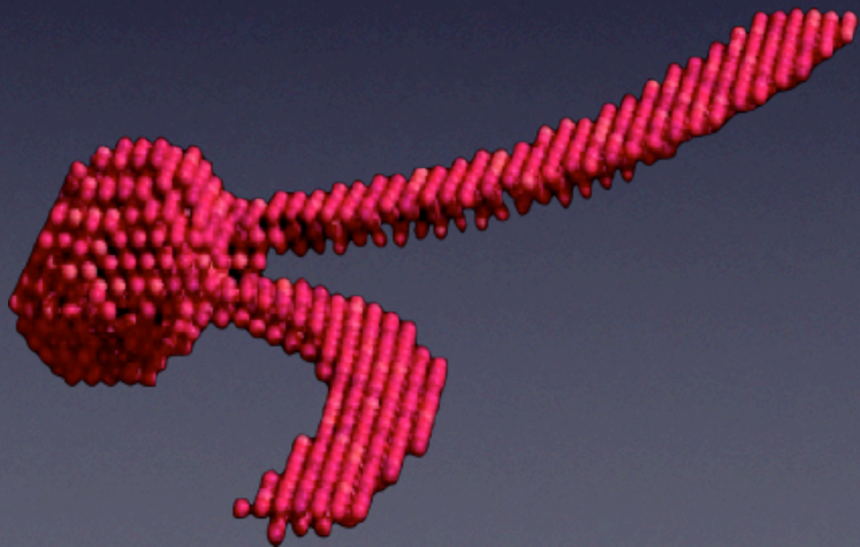

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Overview

- Introduction
- Molecular dynamics simulation technique
- Simulation conditions
- Edge dislocation–defect interaction
    - Interaction with void
    - Interaction with He bubble
    - Interaction with Cr precipitate
- Summary

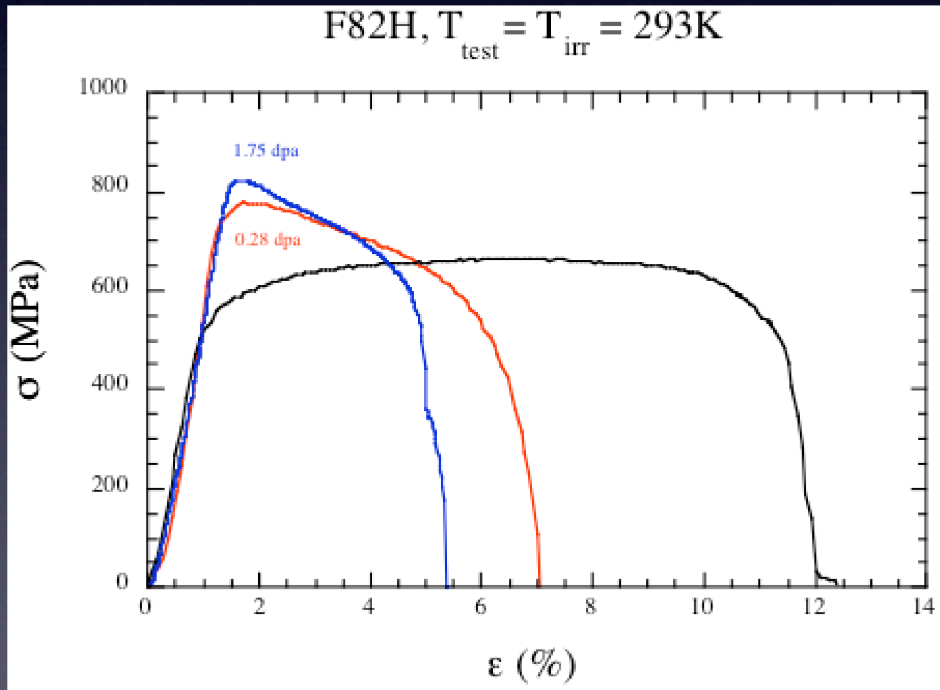
Introduction

- Irradiation-induced defects as voids, He bubbles and Cr precipitate → substantial hardening & loss of ductility below 400°C.

- Ferritic base steels → prime candidates for the plasma facing materials & the structural components of the future fusion reactors.

- Multiscale modeling → major tool in description of radiation defects in materials.

- Aim: to obtain a relationship between the irradiation defects and mechanical behavior by MD simulation & to get a physical concept of irradiation effects on Fe.



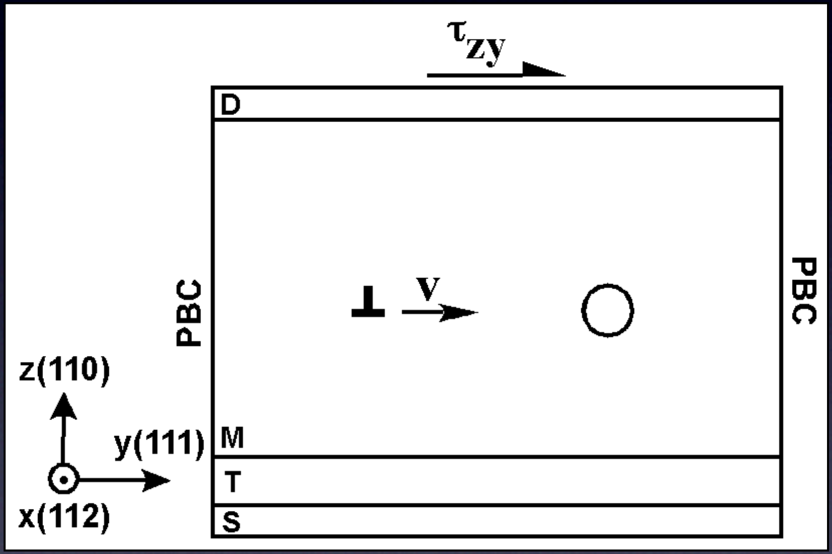
F82H, a ferritic/martensitic steel,
P. Spätig, R. Schäublin, S. Gyger and M. Victoria
Journal of Nuclear Materials, 258-263 (1998) 1345-1349

Molecular Dynamics simulation

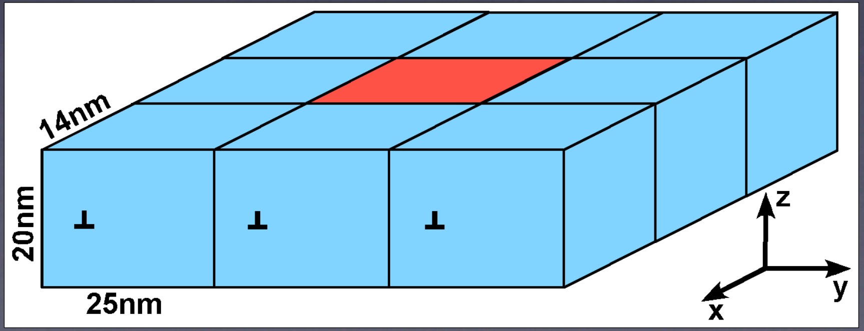
- MD simulation: solving the Newton equation of motion for particles of a system using empirical interatomic potentials, which gives trajectory of atom displacement
- Simulation steps :
  - Sample creation → describes the atomic configuration of dislocation (Disloc)
  - Deformation → allows the dislocation to move, using the embedded atom method (Moldy)
- Deformation mode: shear due to an applied stain rate in the upper region of sample.
- Material: bcc-Fe, single crystal

MD simulation sample

- A box including an edge dislocation in [112] direction & a defect on the dislocation slip plane, (110)



- The box is built up in several regions:
  - The mobile region: atoms follow Newton equation
  - Upper region: atoms to control the deformation of sample and are forming a free surface
  - Bottom region 1:   the thermal bath
  - Bottom region 2: static atoms to anchor the specimen



- Periodic boundary condition applied along dislocation line direction & slip direction

Simulation conditions

- The many-body interatomic potentials:
  - Fe-Fe → Ackland 1997, Mendelev 2003, Dudarev-Derlet 2005
  - Fe-He → Wilson-Johnson 1972
  - He-He → Beck 1968
  - Fe-Cr & Cr-Cr → Olsson 2005

- MD simulation parameters:
  - Defect type → void, He bubble, Cr precipitate
  - Temperature → 10, 100, 200, 300, 500, 700 (K)
  - Defect size → 1, 2, 3, 4, 5 (nm)
  - He density → 0, 1, 2, 3, 4, 5 (He/v)

Size of box	(14-17)×25×20 nm^3
No. of Fe atoms in the box	566586
Dislocation speed	60 $m \cdot s^{-1}$
Time step	1 fs
Annealing before straining	5 ps
Total simulation time	480 ps

Dislocation – void Interaction

- Each passage of dislocation shears the void by one Burgers vector.

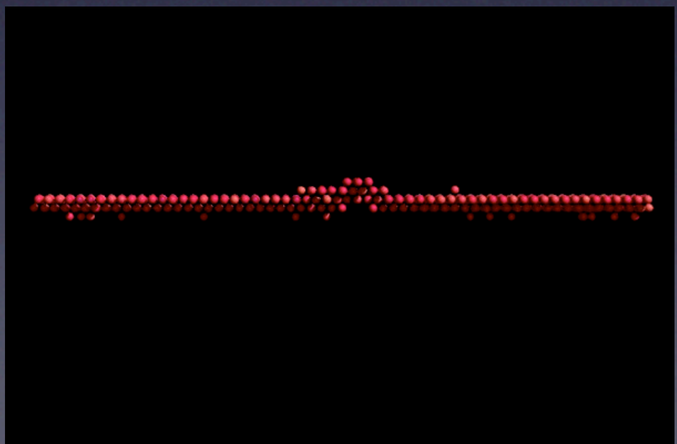
Main interaction mechanism

↓

Climb & Cross-slip

↓

Jog formation

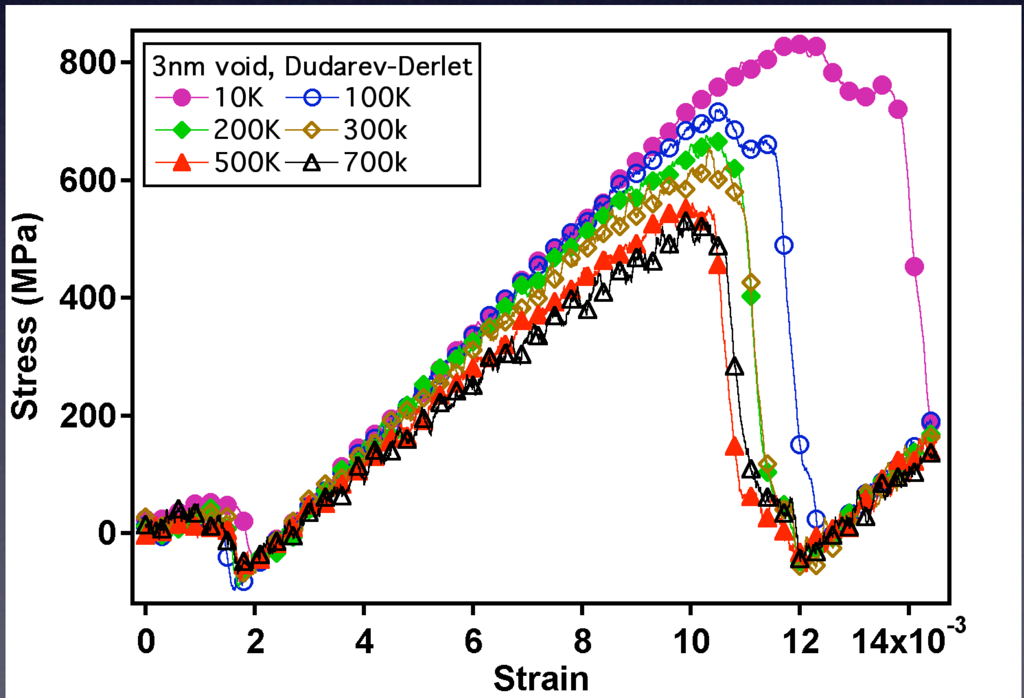


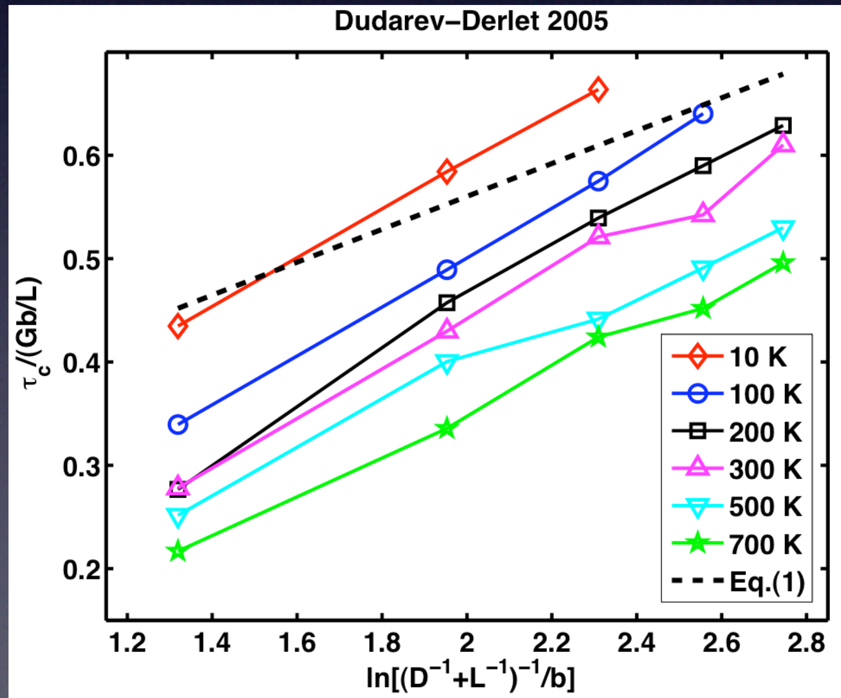
S.M. Hafez Haghighat and R. Schaeublin, Journal of Computer-Aided Materials Design 14 (2008) 191.

Temperature and size effects

- Temperature ↑ ⇒ release stress and strain ↓
- Void size ↑ ⇒ release stress ↑
- Results are compared to elasticity of continuum:

$$\tau_c = \frac{Gb}{2\pi L}\left[\ln\frac{(D^{-1}+L^{-1})^{-1}}{b} + B\right]$$

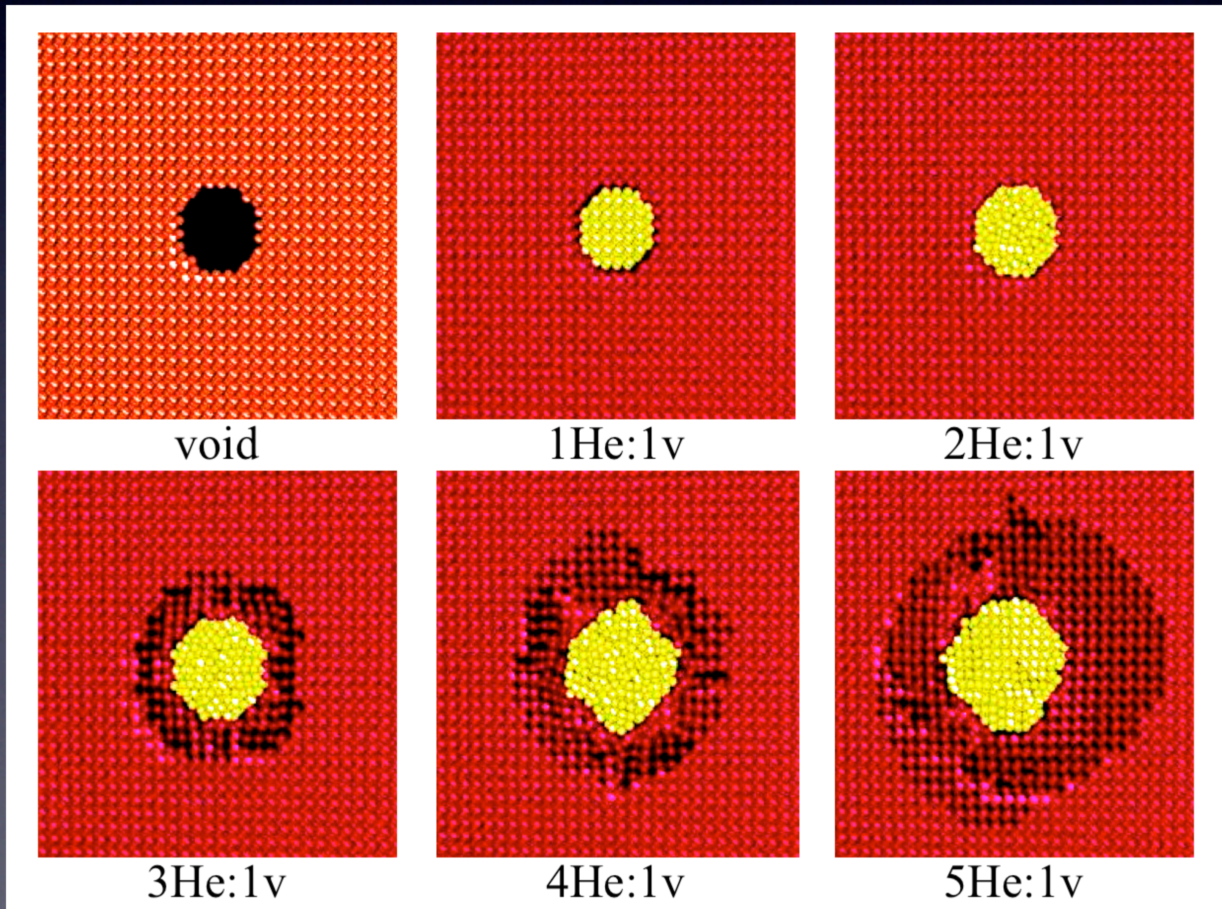




S. M. Hafez Haghighat, J. Fikar, and R. Schaeublin, Journal of Nuclear Materials 382 (2008) 147.

He bubble in Fe

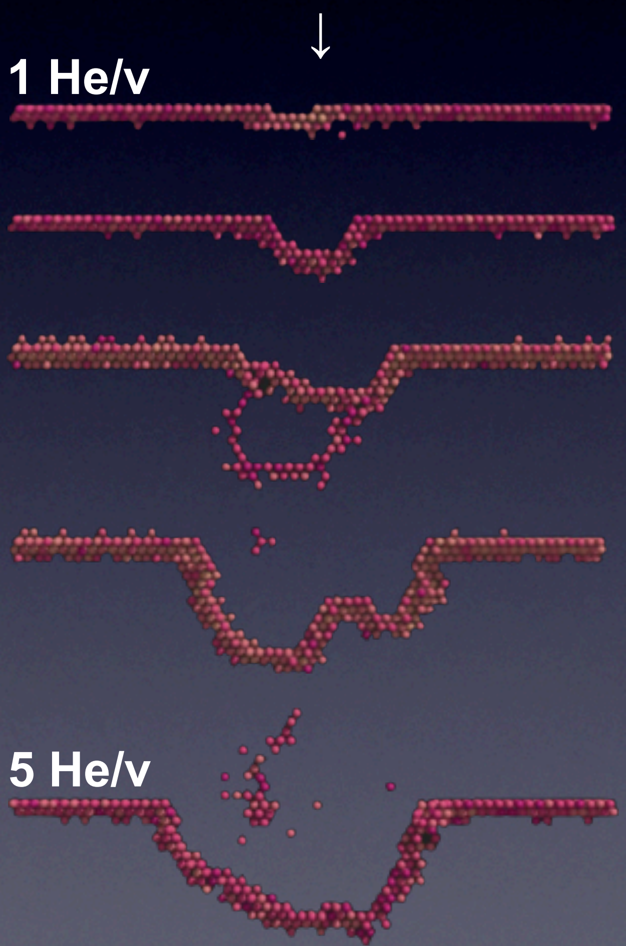
- According to *ab initio* calculations He ratio of 1–5He:1v is reachable
- Initial cavity size: 2 nm
- Atomic structure of He atoms and surrounding Fe atoms after relaxation

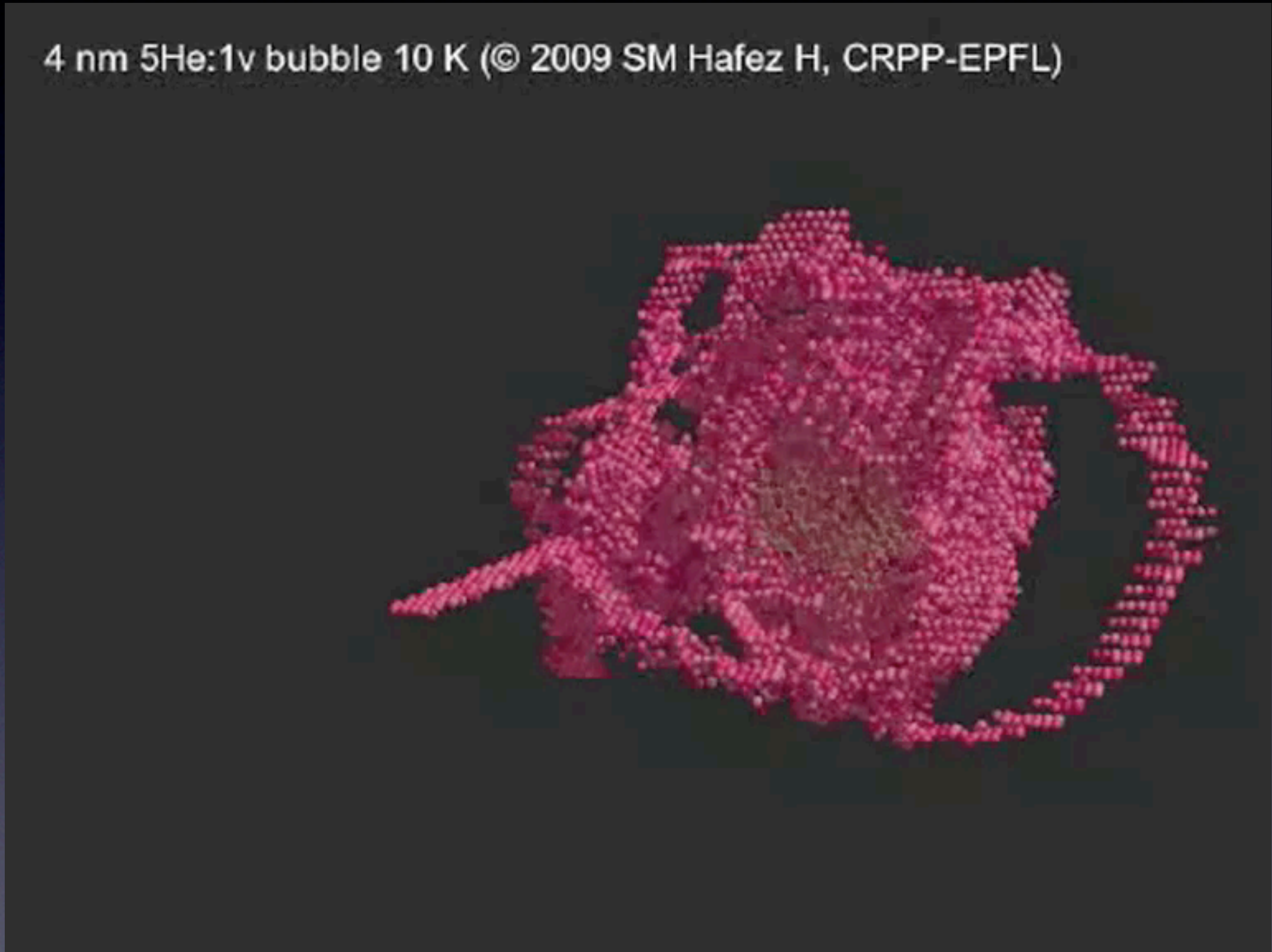


S. M. Hafez Haghighat, G. Lucas, and R. Schaeublin, Europhysics Letteres 85 (2009) 60008.

Dislocation – He bubble Interaction

Jog formation on edge dislocation due to interaction with He bubble

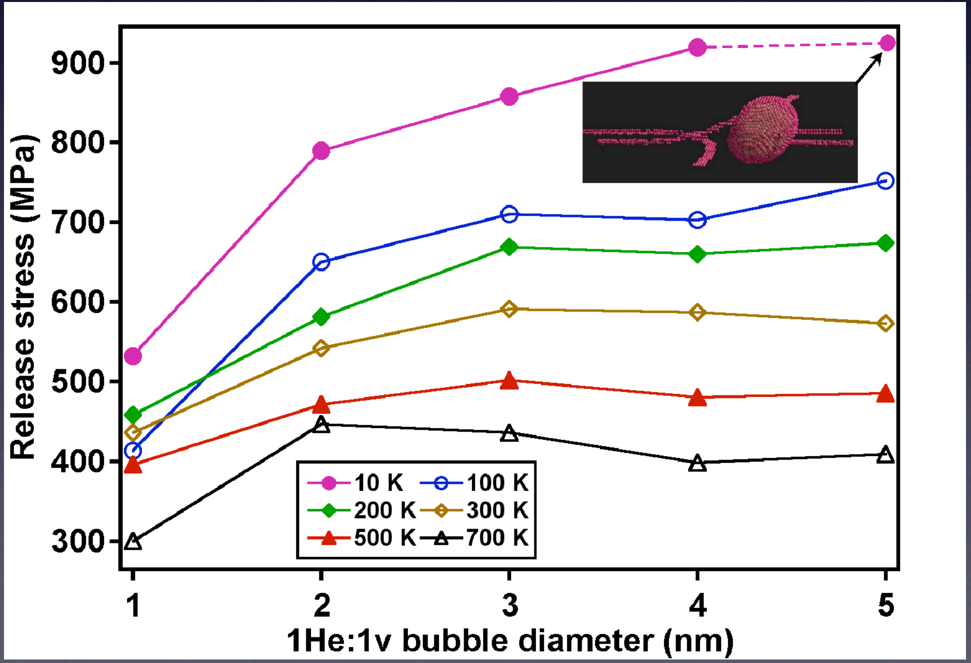


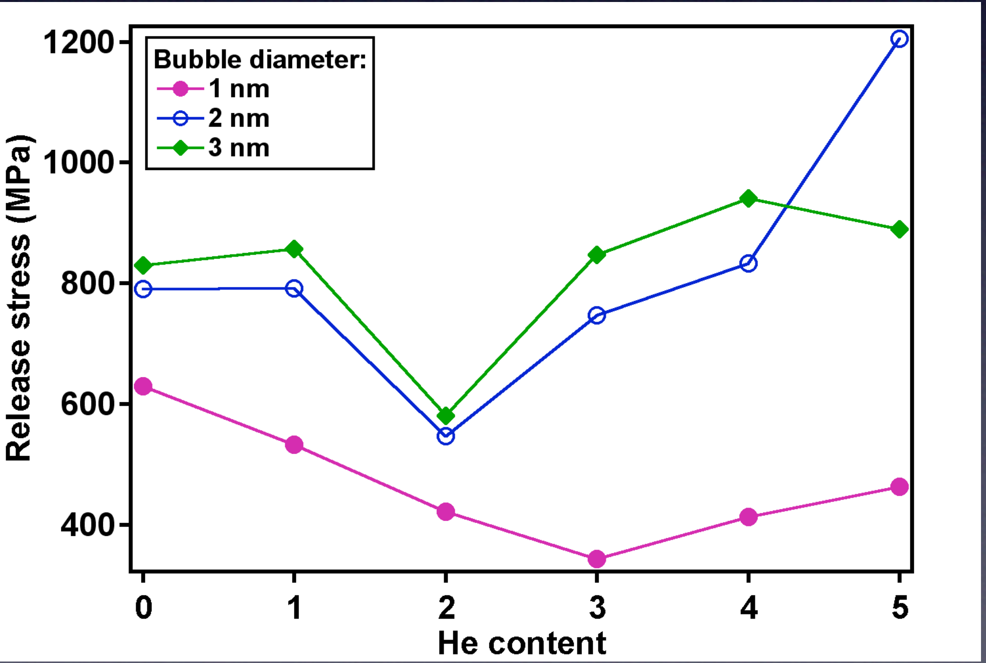


- He content ↑ ⇒ loop punching (emission of interstitials or dislocation segments from bubble)

Temperature and size effects

- Bubble size ↑ ⇒ release stress ↑, strengthening rate ↓
- Drop at moderate He contents (densities) due to surrounding stress field
- High He contents ⇒ the largest obstacle strength due to loop punching

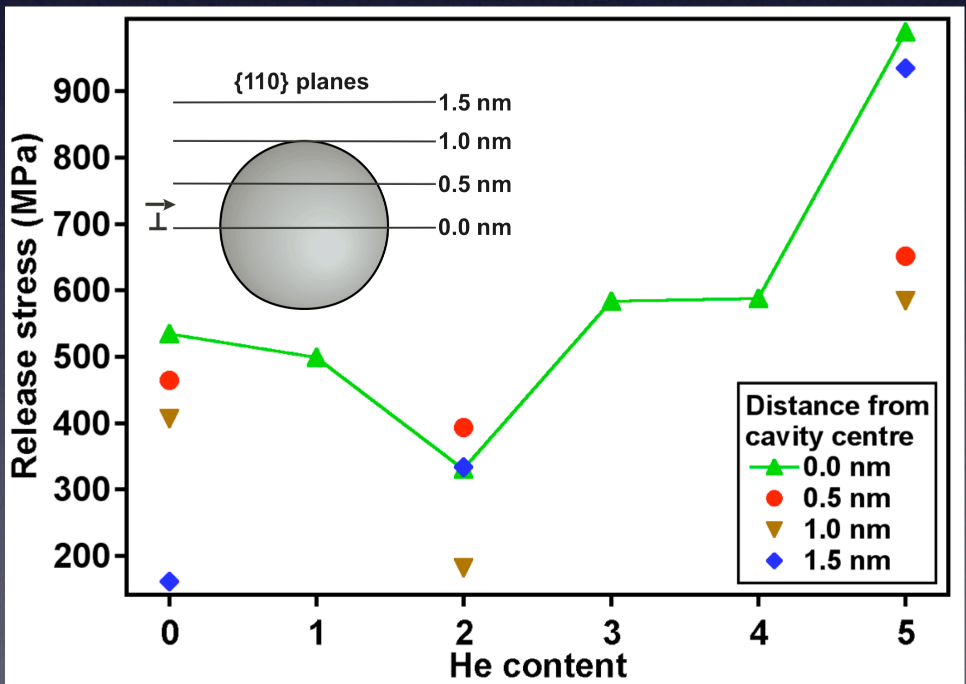


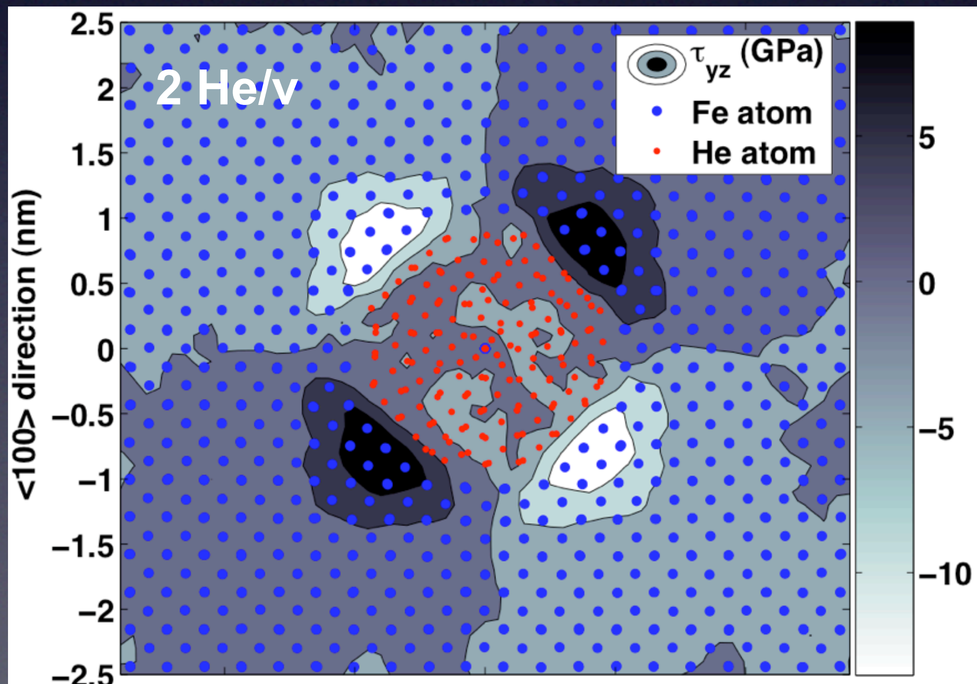


S. M. Hafez Haghighat, G. Lucas, and R. Schaeublin, Proceeding of Dislocation 2008, Hong Kong.

Dislocation – bubble geometry effect

- Low He content : dislocation height ↑ ⇒ monotonous softening ⇒ shearing area effect
- Moderate He content : dislocation height ↑ ⇒ non-monotonous variation ⇒ stress field effect
- High He content : dislocation height ↑ ⇒ non-monotonous variation ⇒ loop punching effect





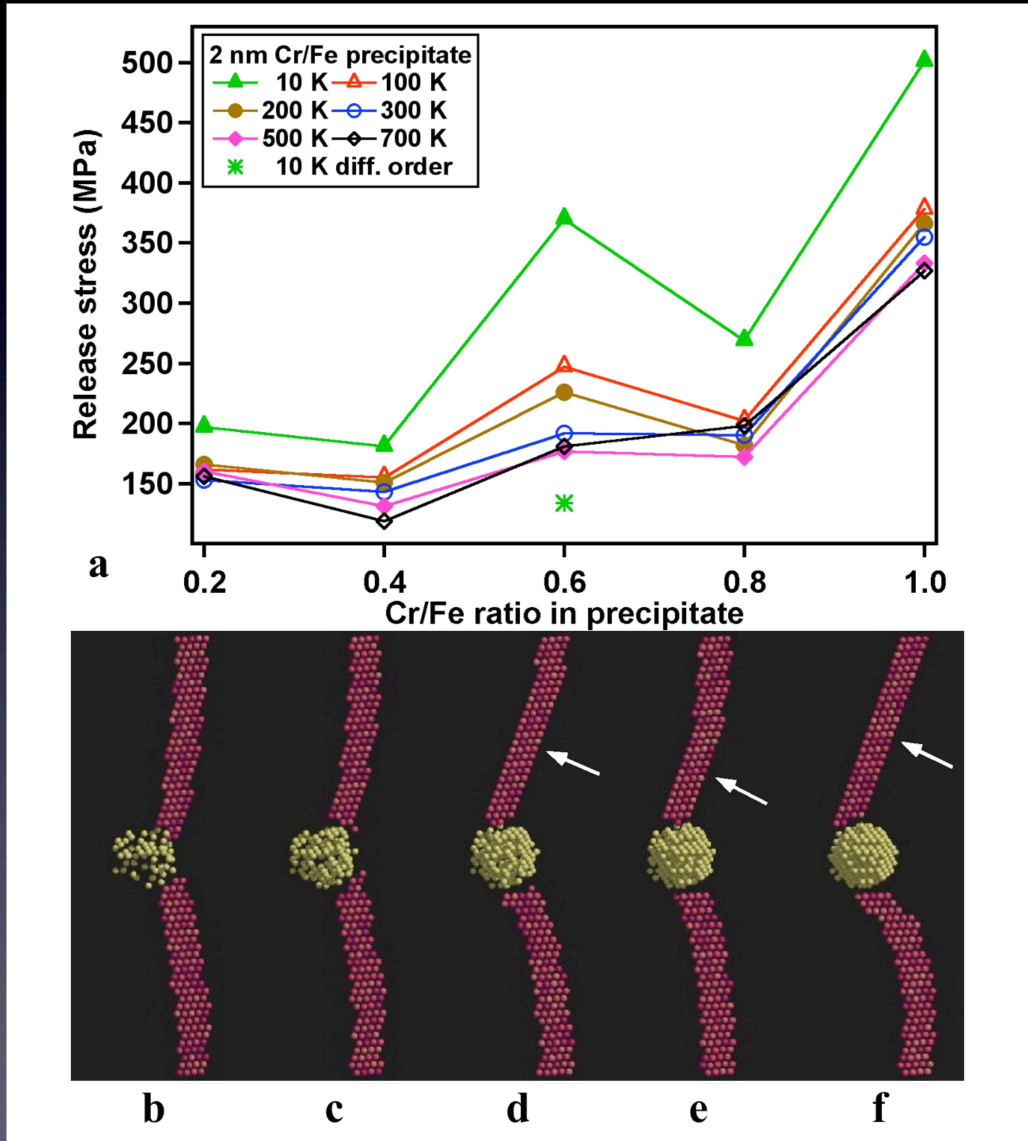
S. M. Hafez Haghighat and R. Schaeublin, Philosophical Magazine, accepted for publication, 2009.

Dislocation – Cr precipitate Interaction

- Cr precipitate is coherent with surrounding Fe.
- No jog formation was observed after dislocation–precipitate interaction
- Shearing of precipitate by one Burgers vector similar to void.

Effect of Cr/Fe ratio

- With increasing Cr/Fe ratio the strength of the precipitate increases non-monotonously.
- A different Fe-Cr atomic arrangement in 0.6 Cr/Fe precipitate shows a significant change in release stress.
- The length of straight mixed dislocation increases with the strength of precipitate.



Summary

- Interaction of an edge dislocation with void, He bubble and Cr precipitate were investigated using MD simulation in bcc-Fe.
- Interaction mechanism may differ from one to other by forming an upper jog, a lower jog or no jog formation, respectively.
- With increasing temperature, the release stress decrease for all defects.
- Pressurized He (inert gas) bubbles : the surrounding stress field generated by the bubble has a strong influence on its strength.
- The dislocation loops punched out from the pressurized He bubble interact with the mobile dislocation.
- Cr atomic configuration in Cr precipitates has a strong effect on strengthening.
- For a given size and temperature, a void and a He bubble (even at moderate contents) are stronger obstacle for an edge dislocation than a Cr precipitate.