Radiation damage and H/D retention studies on ion-irradiated tungsten and its alloys – Plans for experiments and modeling

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Plasma-Wall Interaction with Irradiated Tungsten and Tungsten Alloys in Fusion Devices
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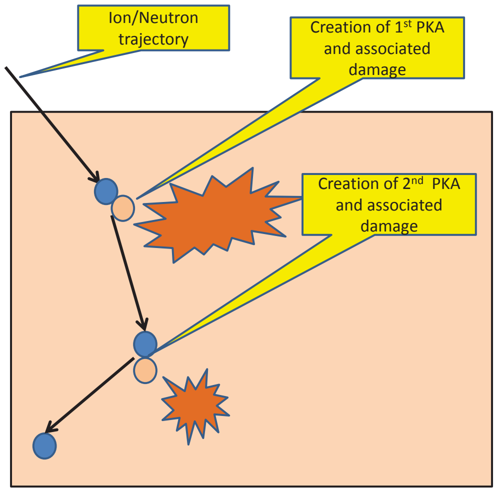
Fusion Research in India

- At present we have two tokamaks (ADITYA and SST-1) where experiments are being carried out
- We are also participating in ITER and a few other collaborations
- Our aim is to develop fusion technologies for exploitation in future
- One of the key elements of these is the development of plasma-facing components and the required materials
- We will use carbon-based materials in the beginning on SST-1. But later, we plan to modify the FW and Divertor with tungsten
- Understanding H-retention is an important issue for steady state
- On a longer time scale, the next step machines (SST-2, DEMO) will need to have a reliable database and a good understanding of the behavior of PFM under strong irradiation condition
- Such behavior not only affects plasma-wall interactions but creates boundary conditions for service, replacability and effectiveness

Motivation

- Radiation Damage due to 14 MeV Neutrons and 3.5 MeV Helium and its effect on retention and transport of H isotopes needs to be understood
- In the absence of 14 MeV high Flux Neutron source, surrogate Ion Irradiation study is useful even with its own limitations.
- Even after extensive studies and their reports many gap areas need to be probed for details, to remove contradictions and to bring new insights in
- Mechanisms for the defect formation due to energetic Neutrons, Heavy ions, Helium and plasma.
- Microstructural changes on microscopic levels and their correlation with the mechanical, thermal and other properties.
- Dependence of radiation damage and retention on different irradiation parameters such as fluence, energy and irradiation temperature



- The PKA will create a cascade of displacements which may relax into a configuration with trap sites
- A population of H atoms can be imagined to build within the tungsten (as a result of exposure to plasma and to some extent that created due to transmutations)
- H-atoms can get trapped/de-trapped and move through the grain
- There is a need to understand what is the extent of saturation and how it is going to affect the recycling at the wall
- With increasing dose, it may become necessary to know if the properties of W have changed and in what way they impact the performance

Objective

To study the dependence of H/D transport and retention on various aspects such as:

1. structural and microstructural changes
2. presence of Helium and Helium Bubbles
3. impurities/alloying elements
4. Irradiation parameters and substrate-temperature

We plan to carry out experiments and modeling for the above

Scientific Scope

- The interaction of the PKA with the W lattice will be simulated by using energetic heavy ion beams in the particle accelerators
- The structure-specific aspects in a single/polycrystalline samples (micro-crystallites and grain-boundaries) of tungsten which can influence the cascade size will be explored
- The kind of defects that are generated due to irradiation and the corresponding trap energies and their abundances will be quantified by different diagnostic techniques and modeling
- The effect of stress fields/gradients formed due to the helium bubbles on H-transport will also be examined by modeling

Modeling Plan

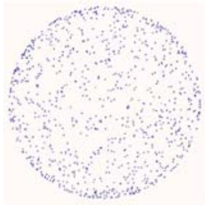
- Modeling the radiation cascade: Creation and relaxation of Frenkel pairs
- Modeling the trap locations and energies
- Modeling the dynamics of H/D within a damaged lattice
- Ultimately, establish the correlation with experiments on TDS

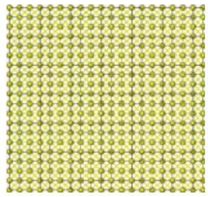
Plan (cntd)

- For obtaining PKA energy spectrum in W, SDTRIM-SP will be used
- MD code ParCas/LAMMPS: for the damage of W on W
- Calculations for the diffusion coefficients (Interstitialcy and grain boundary) will be done using LAMMPS
- Long term evolution of FP
- Modeling of the trap energies by MD/Potential Energy Surface technique
- Model the diffusive recombination and transport by KMC

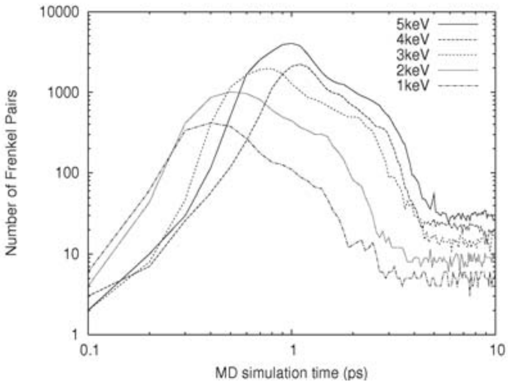
Earlier Work (Warrier et al) on Fe-Cr will be extended

- Concentration dependent EAM potential for FeCr used
- PKA from center of cubic domain launched in 1000 random directions at 0.1, 0.5, 1, 2, 3, 4, 5 keV
- PBCs along X-Y-Z, 10 ps NPT at 300 K, 10 ps collision cascade
- ns runs for 1 PKA at 0.1, 0.5, 1, 2, 3, 4, 5 keV in Fe(90%)-Cr(10%)
- Channeling fraction?



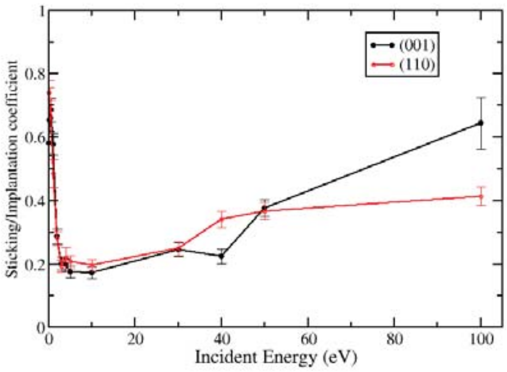


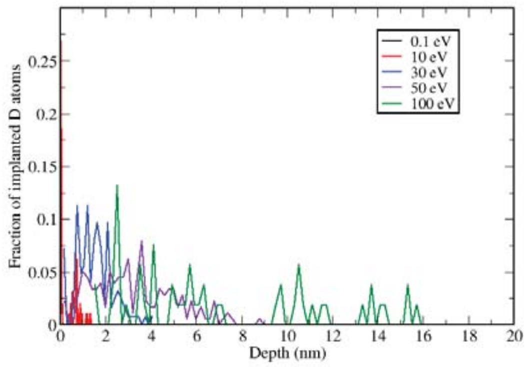
Cascade evolution with time in Fe-Cr



Preliminary Trials

- ParCas Code *(K. Nordlund et al. PRL 77 (1996) 699)*
  - Potential: W-W and W-D *(Liu et al. Jnl. App. Phy. Vol.112, 013518 (2012))*
  - Energy 0.005-100 eV
  - [100] and [110]
  - N=1000
  - Xyz= 4.5 x 4.5 x 20 nm^3 (x-y periodic+ B thermostat)





Self-Diffusion coefficient in single crystal and bicrystal Tungsten: MD (preliminary)

➢**Molecular dynamics Code: LAMMPS (S. Plimpton, J. Comp. Phy. 117 (1995) p.1-19)**

➢**Domain size:** 10x10x10 unit cells

➢**Boundary conditions:** Periodic boundary conditions

➢**Timestep used:** 1 femto-second

➢**Potential:** W-C-H potential developed by Juslin et al, J. App. Phy., 98 (2005) 123520. This potential has been used by several workers (Yu et al, JNM 441 (2013) 324-330, Juslin et al, JNM 438 (2013) S1221-S1223)

➢The system is first relaxed at 300 K and 0 bar pressure and then NVE simulation has been performed.

Elastic Constants obtained from MD simulations for W-C-H potential

Elastic constants at 300 K

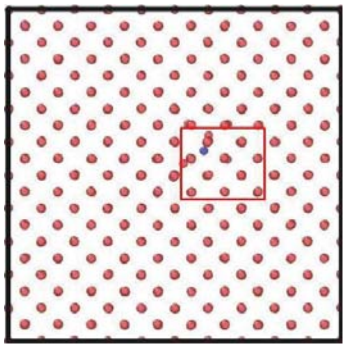
Material constants		Experiments			Our results
C (GPa)	c_{11}	521	501	513	504.38
	c_{12}	201.4	199	207	201.30
	c_{44}	160.4	151	153	166.55
Ref.	-	[21]	[22]	[23]	

[21] D I Bolef and J De Klerk, "Elastic constants of single crystal mo and w between 77 and 500 k," *J. Appl. Phys.*, vol. 33, no. 7, pp. 2311, 1962.

[22] S J Wright, "The elasticity of pintsch crystals of tungsten," *Proc. Roy. Soc. (London)*, vol. A126, pp. 613, 1930.

[23] P W Bridgman, "Certain physical properties of single crystals of tungsten, antimony, bismuth, tellurium, cadmium, zinc, and tin," *Proc. Am. Acad. Arts Sci.*, vol. 60, no. 6, pp. 329, 1925.

Interstitialcy diffusion in Single crystal Tungsten



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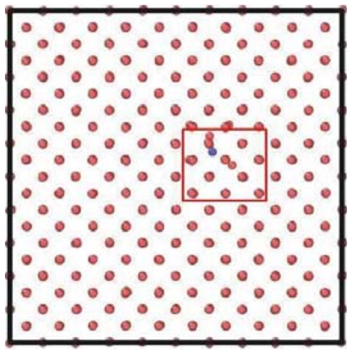

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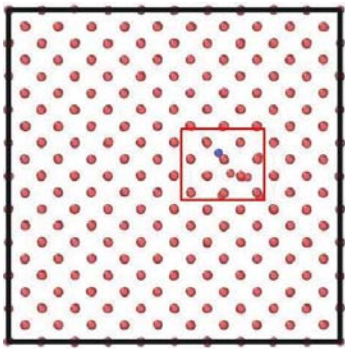

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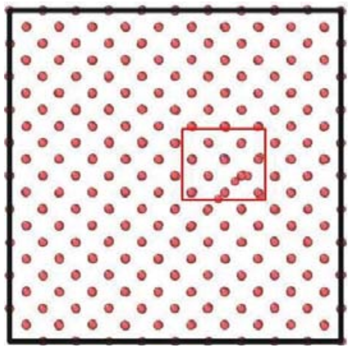
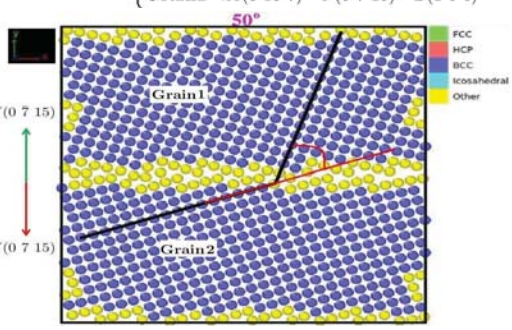


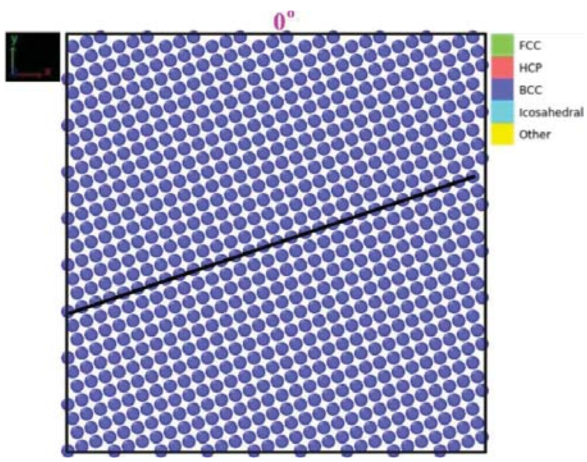
Bicrystal

Angle of misorientation: $\cos\theta = \dfrac{h_1h_2+k_1k_2+l_1l_2}{\sqrt{h_1^2+k_1^2+l_1^2}\sqrt{h_2^2+k_2^2+l_2^2}}$

$< h_1k_1l_1 >$ and $< h_2k_2l_2 >$ are grain boundary normals

$$Bicrystal: 50.03^\circ \begin{cases} \text{Grain1} & : X(0\ 15\ 7) \quad Y(0\ \bar{7}\ 15) \quad Z(1\ 0\ 0) \\ \text{Grain2} & : X(0\ 15\ \bar{7}) \quad Y(0\ 7\ 15) \quad Z(1\ 0\ 0) \end{cases}$$





Plan for Experimental study

- Irradiation of W by
  - Heavy ions (W)
  - W + H/D
  - He
  - W + He
  - W + He + H/D
- Structural and micro-structural and morphological changes- by XRD, TEM and SEM
- Depth Profiles and Migration Energies
- Techniques for depth profiles of H/D and He in un-irradiated and irradiated Tungsten -
  - NRA, ERDA, SIMS
- For Migration Energies and total retention of H/D
  - TDS
- For W-La_2O_3 chemical information and segregation, if any
  - XPS, EDX/EPMA

Thank you