Models for H isotope and He retention in irradiated tungsten

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- Threshold displacement energies for defect production in tungsten, can be found from simulations, experiments could be done using HVEM – could this be actually accomplished?

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Ab initio threshold displacement energies in iron

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Table 1. Threshold displacement energies from DFT-MD, AM04 and experiments.

TDE (eV)	Global minimum	$E_d(\theta,\varphi)$ ⟨100⟩	$E_d(\theta,\varphi)$ ⟨110⟩	$E_d(\theta,\varphi)$ ⟨111⟩	$E_d(\theta,\varphi)$ ⟨135⟩	E_d^{ave}
DFT Fe_{sd}	15	17	32	15	48	29
DFT Fe_{psd}	18	21	43	20	49	32
AM04	15	17	33	33	55	39
Experiment[a]	17	17	30–35	20		
Experiment[b]	20	20	30			
Experiment[c]	16–18					

[a]Direction specific experiments [24].
[b]Direction specific experiments [23].
[c]Global minimum experiment [25].

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Primary damage in tungsten using the binary collision approximation, molecular dynamic simulations and the density functional theory

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Table 1. Threshold displacement energies (in eV) for the different cohesive models along different crystal orientation of BCC tungsten.

Orientation	DFT	DFT-sc	MS-s	MS-h
⟨100⟩	40	58	31	43
⟨110⟩	63	>80	51	71
⟨111⟩	44	>80	45	65

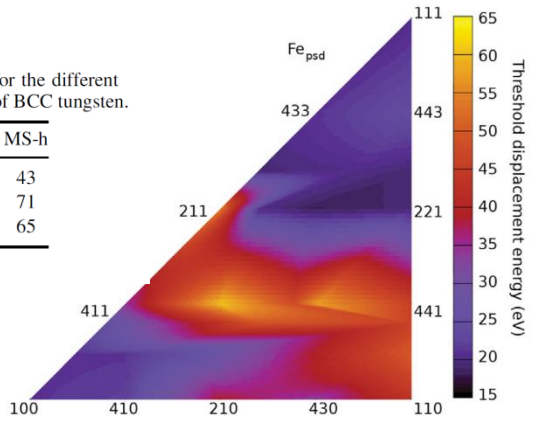

Figure 1. Angular anisotropy of the $E_d(\theta,\varphi)$ using Fe_{psd}.

United Kingdom Atomic Energy Authority

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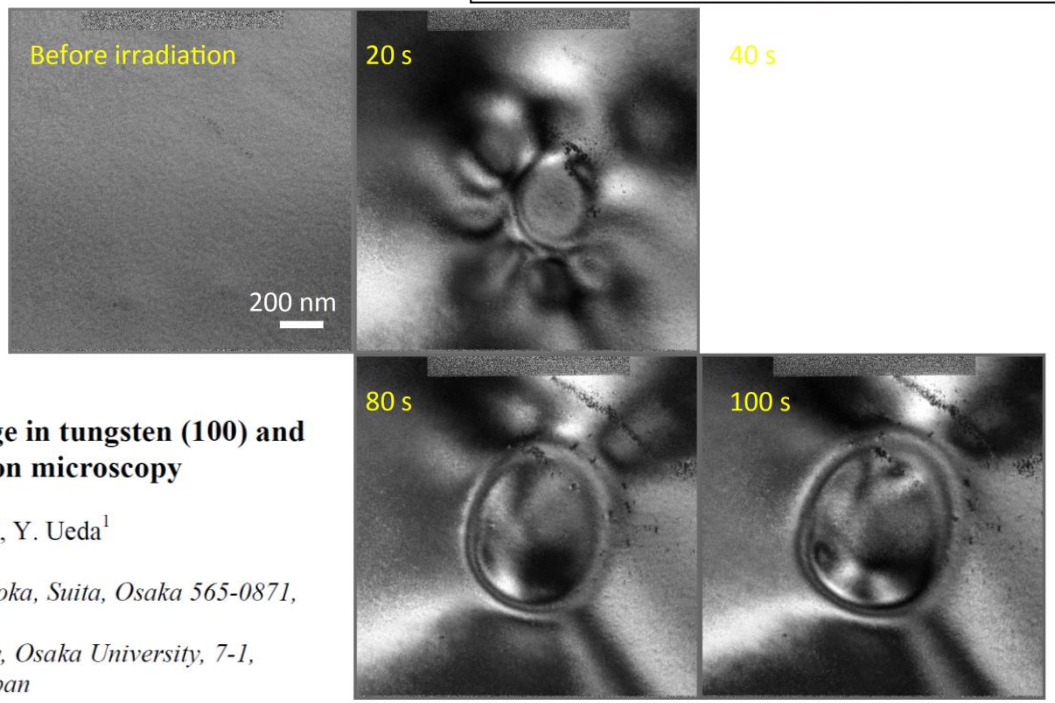
- Threshold displacement energies for defect production in tungsten, can be found from simulations, experiments could be done using HVEM – could this be actually accomplished?

2.0 MeV
(110)

- Clearly visible formation of defect clusters
- Data suggests E_d < 70 eV for (110)



Crystal orientation dependence of displacement damage in tungsten (100) and (110) probed using in-situ high voltage electron microscopy

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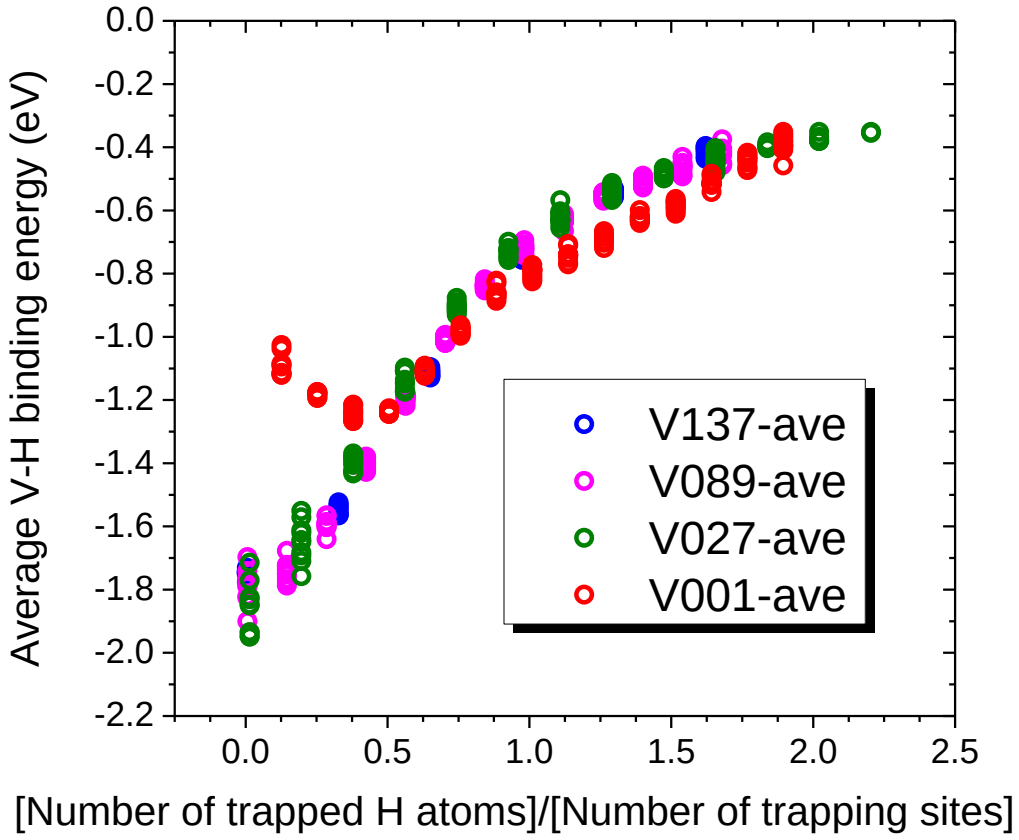
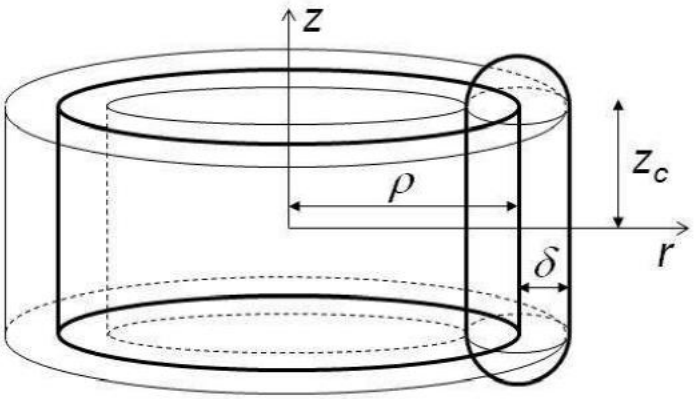
- Binding and trapping energies, involving not only single defects but also defect complexes – e.g. vacancy clusters: it is clear that accurate values can only be derived from DFT. TDS experiments show that there are only a few binding energy values that characterise the desorption curves. [this is incorrect - SLD]

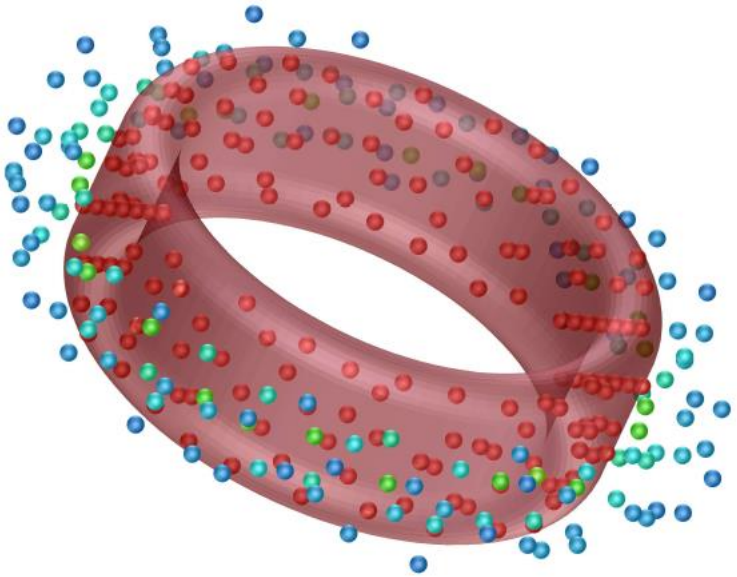


- Interpretation of macroscopic TDS experimental data necessarily requires the use of rate theory type, or kMC, or both approaches. So far information about defect, dislocation and grain boundary microstructure is not included in such simulations.

a)



b)



$$N_{loop} = 2\pi\rho\, n_{core} + \frac{2\pi}{3\Omega_H}\xi_c \left[A \frac{-\Omega_{rel}^H}{k_B T \ln c_H} \frac{\mu b}{3\pi} \frac{1+\nu}{1-\nu}(1-\xi_c^2) - 6\rho\delta z_c \right]$$

A. De Backer *et al.*, submitted to Nuclear Fusion (2017)

- Relating TDS measurements to microstructure is probably a reasonable overall objective for the modelling effort.

Has not been achieved. (too difficult?)

- Standard tungsten samples

Has been achieved, by Dr T. Schwarz-Selinger and Dr H.-T. Lee

- Standard preparation of the samples: annealing, implantation, followed by characterization (PAS), for the comparison of TDS curves – possibly for hydrogen and helium

Has been achieved, by Dr T. Schwarz-Selinger and Dr H.-T. Lee

- Comparison of TDS experiments, accompanied by comparison of interpretations using various codes (TMAP, kMC). Are the effective trapping/activation energies derived from various experimental TDS curves going to be the same?

Has been achieved.

- Comparison of software for the interpretation of TDS experiments. Need a “standard” TDS curve, for hydrogen, and for helium desorption.

Status unclear, comparison of software is in progress.

- TDS experiments – a range of experiments with variable desorption rates.

Has been achieved.

- Depth distribution of hydrogen and deuterium and tritium – as a likely source of uncertainties

It still remains the likely source of uncertainties.

- Specifically a modelling task: the development of potentials for MD of tungsten, comparison of potentials with DFT, for various configurations.

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Interatomic potentials for modelling radiation defects and dislocations in tungsten

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- Specifically a modelling task: the development of potentials for MD of tungsten, comparison of potentials with DFT, for various configurations.

Comparison of potentials – equilibrium properties

	$E_{cohesive}$	Lattice Constant	C_{11}	C_{12}	C_{44}	E_v	E_{100d}	E_{110d}	E_{111d}	E_{octa}
	(eV)	(Å)	(GPa)	(GPa)	(GPa)	(eV)	(eV)	(eV)	(eV)	(eV)
Expt.	-8.90 [*]	3.1652[#]	522.4[#]	204.4[#]	160.6[#]	3.7			9.06	
DFT		3.18					11.513	9.84	9.55	11.7
FS	-8.90	3.1652	522.44	204.41	160.61		8.652	Not stable	7.805	8.524
AT	-8.90	3.1652	522.43	204.41	160.61		9.783	Not stable	8.883	9.968
Juslin (EAM)	-8.90	3.1652	522.47	204.45	160.64	3.554	10.277	10.157	9.50	10.393
DNMD	-8.90	3.1652	523.10	204.67	160.81	3.557	11.334	9.768	9.472	11.7
DNMD+ZBL (Bjorkas)	-8.90	3.1652	523.10	204.67	160.81	3.557	11.332	9.766	9.472	
DNMD+ZBL (Fikar)	-8.90	3.1652	523.10	204.67	160.81	3.557	11.333	9.768	9.472	
Li-ABOP	-8.86	3.1652	515	203	162	3.52	12.01	9.53	9.33	12.05
Juslin-ABOP		3.165	542	191	162	1.77	8.93	8.77	9.62	9.92
Zhou et al	-8.757	3.165				3.567				

Displacement energy

E_d (eV)	Expt. [**]	AT	AT+ZBL	DNMD	DNMD+Fikar	DNMD+ Bjorkas
Min.	~40-50	64	48	55±3	55	41±1
Avg.	~80	166	128	88.3±0.7		84.5±0.9

[*] Table 3, Kittel (1976) [#] P. Bujard, Thesis, University of Geneva (1982)
[**] Maury et al. Radiat. Eff. 38 (1-2) (1978) 53-65

Dr. S. Deshpande (2015)