Models of Helium Induced Surface Defects in Tungsten

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Abstract

Tungsten components facing helium plasmas show peculiar tungsten surface "fuzz" or "coral" after only a few hours.

Goals

- Hint at mechanisms of fuzz formation
- Determine time scale of fuzz formation

Mechanisms of interest

- Surface atom formation / sputtering
- Bubble formation / expansion / rupture

Tools

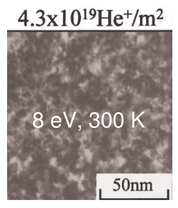
- Molecular dynamics simulations
- Kinetic Monte Carlo simulations (planned)

Results

Our simulations suggest that ad-atoms *can* form even at relatively low ion energies. However, we speculate that helium bubbles rupturing the surface form an important part of the mechanism of tungsten surface defect formation.

Surface Dynamics Under Plasma

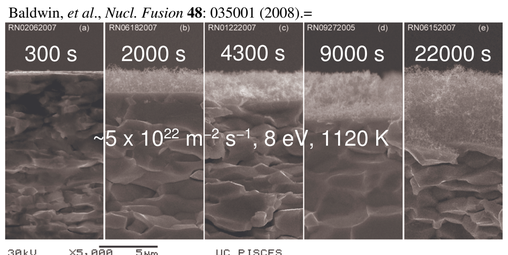
T < 700 K



H. Iwakiri, *et al.*, *J. Nucl. Mater.* **283–287**: 1134–1138 (2000).

non-specific damage

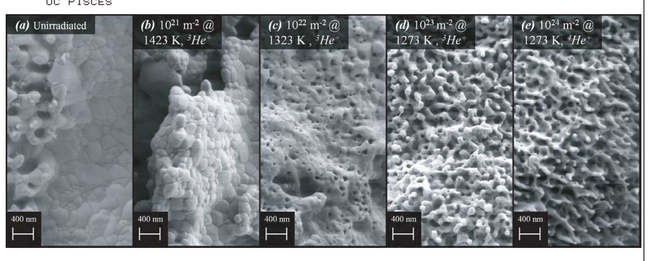
Baldwin, *et al.*, *Nucl. Fusion* **48**: 035001 (2008).=



900 K < T < 1900 K

fuzz / coral

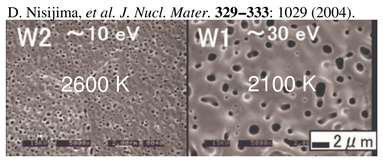
S. J. Zenobia and G. L. Kulcinski. *Phys. Scr.* **T138**: 014049 (2009).



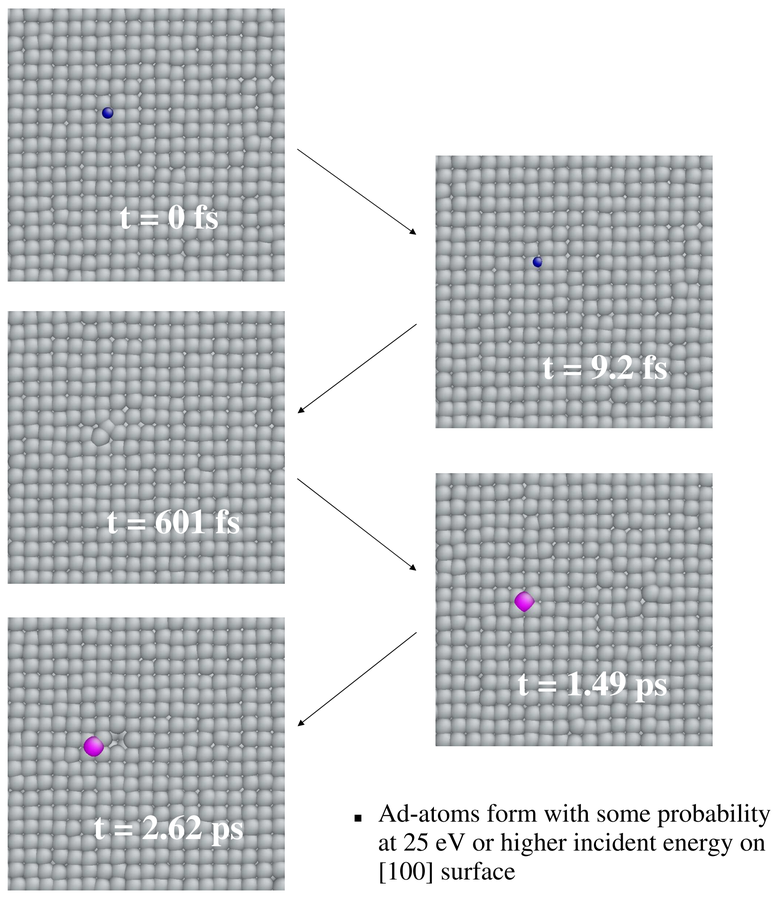
T > 2000 K

holes

D. Nisijima, *et al. J. Nucl. Mater.* **329–333**: 1029 (2004).



Mechanism 1: Ad-Atom Formation



- Ad-atoms form with some probability at 25 eV or higher incident energy on [100] surface
- Probability decreases noticably on [110] surface

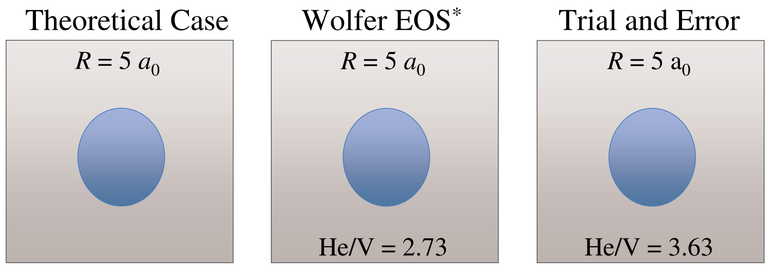
Mechanism 2: Bubble Rupture

Bubble Bursting Mechanism: Loop Punching

- Bubble pressure exceeds $P^{2\gamma/R + \mu b/R}$
- Bubble punches out dislocation loops.
- The dislocations reach the surface and create a hole

Periodic Loop-Punching Simulations at 500 K

- Equilibrium He/V = 2.73 from Wolfer equation of state*
- Computed bubble pressure was 30% lower during MD
- Adjusting He/V to 3.63 yields a pressure matching the theoretical pressure.
- We assume $He/V^{loop} = 3.63$ is required for loop punching



$P_{gas}^{\frac{2\gamma}{R}+\frac{\mu b}{R}} = 3.66\ \text{GPa}$ $< P_{gas} >= 2.1\ \text{GPa}$ $< P_{gas} >= 3.71\ \text{GPa}$

* W. G. Wolfer. *Phil. Mag. A* **58**: 285–297 (1988).

Non Periodic Loop-Punching Simulations at 500 K

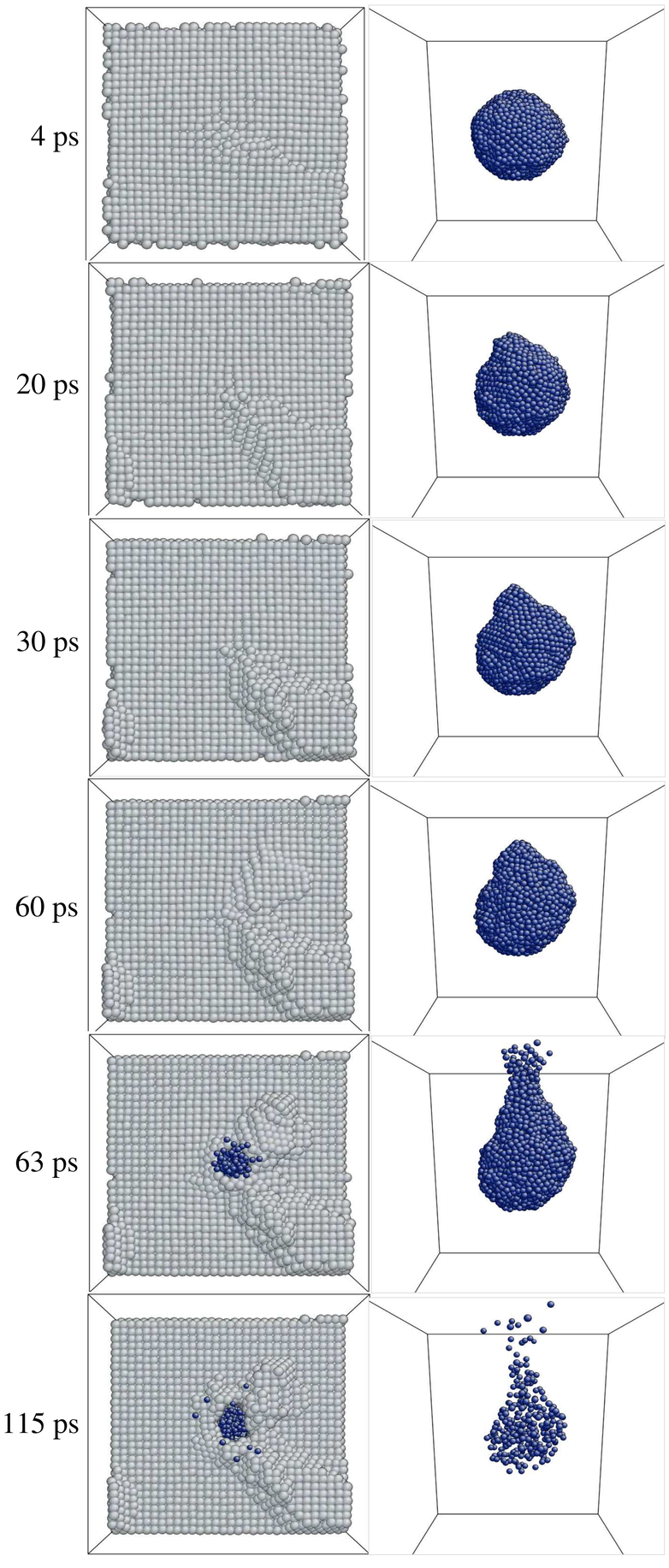
Idea: Put bubble below the surface and see how much pressure it takes before it ruptures.

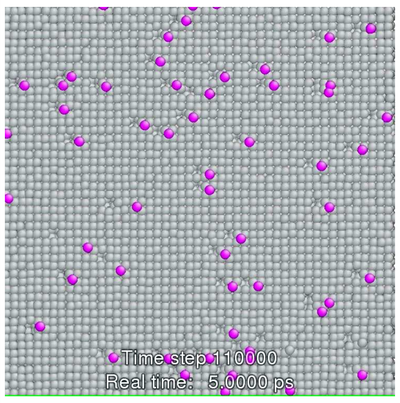
Bubble stability as a function of d, depth

He/V	1.43	2.74	3.07	3.85	4.08
$d = a_0$	bursts				
$d = 2\ a_0$	stable	bursts			
$d = 3\ a_0$		stable	bursts		
$d = 5\ a_0$			stable	bursts	
$d = 10\ a_0$				stable	stable

- $d < R$ → bubble bursts for $He/V < He/V^{loop}$
- $d = R = 5\ a_o$:
  Number of He for $P^{2\gamma/R+\mu b/R}$ is 3787 and He/V=3.63
  Number of He for bursting is 4025 and He/V=3.85
  (4025-3727)/3727 = 6% discrepancy in number of heliums between loop punching pressure and bubble bursting
- $d = 2\ R = 10\ a_0$ → bulk behavior (no surface effect)

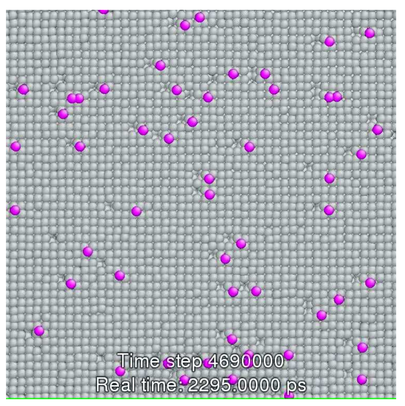
Snapshots of a bubble rupturing with $d = 5\ a_0$





Time scale is too short in molecular dynamics

Need model involving diffusion, formation, and aggregation of defects on long time scales and long length scales



Conclusions

- Ad-atom formation on [110] surface much less likely than [100] surface
- Ad-atom migration is very slow, much too slow for molecular dynamics
- Further work is needed to simulate ad-atom migration on the appropriate length scales

- Helium bubbles leave significant damage on the surface after they rupture
- Loop punching seems to be the underlying bubble bursting mechanism
- Longer scale simulations need to be conducted to explain how the bubbles form, diffuse and reach the loop punching pressure