Plasma-Surface Interactions (PSI): Atomistic Insights into He Transport and Agglomeration in Plasma-Exposed Tungsten

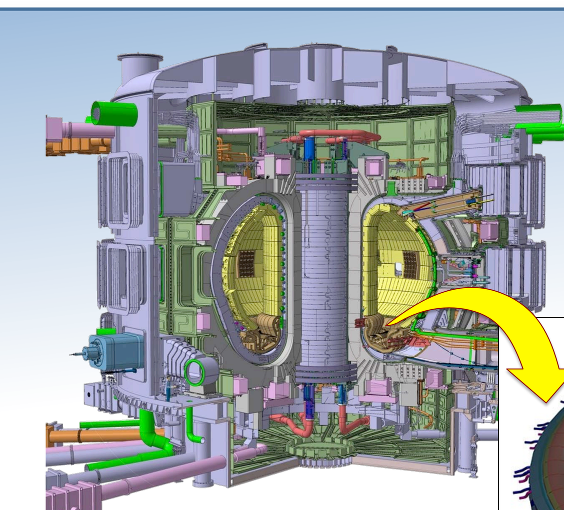
Presented on behalf of the PSI-SciDAC Team by Blas Pedro Uberuaga, LANL

Project web site: https://collab.mcs.anl.gov/display/PSIscidac/

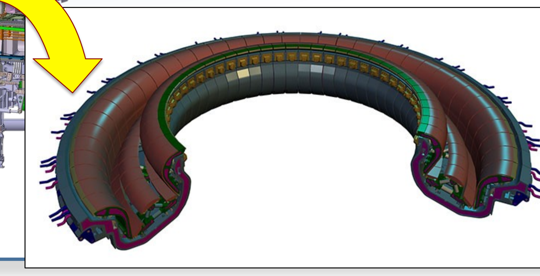
Motivation

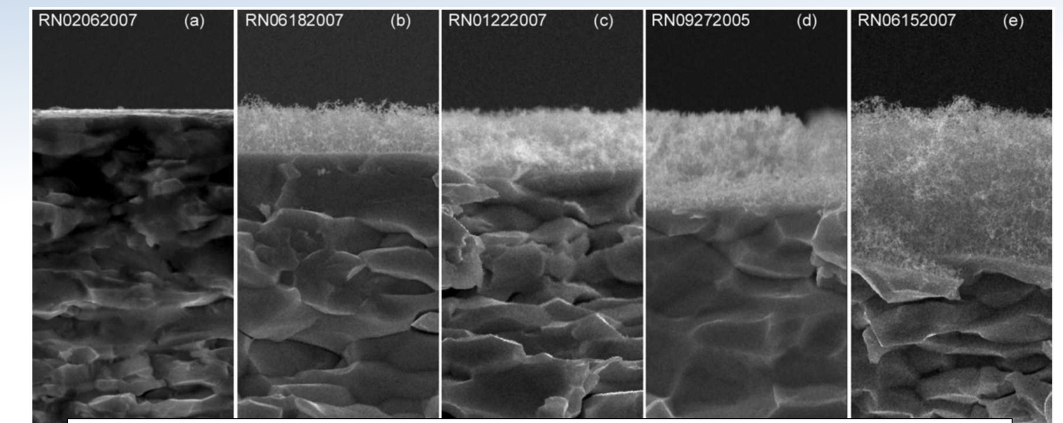
Nuclear fusion promises to be a clean and abundant energy source. The ITER demonstration reactor, with a tokamak design, is being built in Cadarache, France.

Countries collaborating on ITER.



In the tokamak, the divertor collects the ash from the fusion reaction, including He. Tungsten is a leading candidate material for the divertor.





Baldwin & Doerner, *Nucl. Fusion* **48**, 035001 (2008)

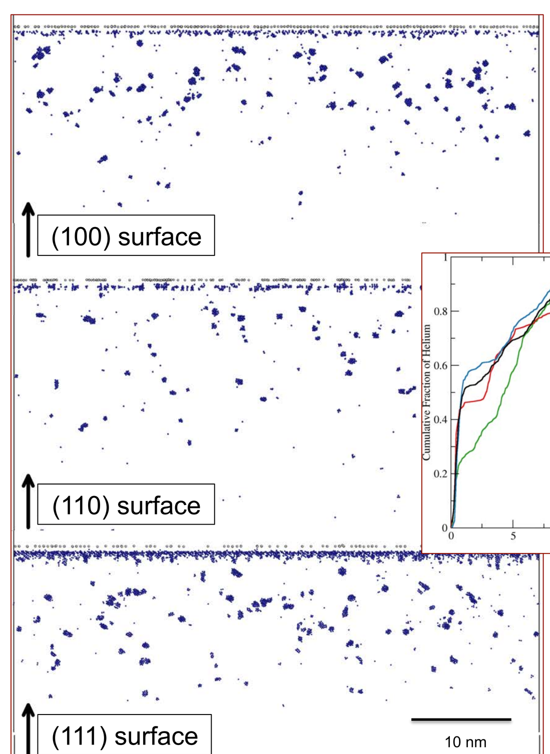
When W is exposed to He plasma, a fuzzlike nanostructure forms. This fuzz Increases retention of tritium and production of dust, degrading plasma.

Our Goal: understand and predict the response of W to He plasma to develop mitigating strategies for fuzz.

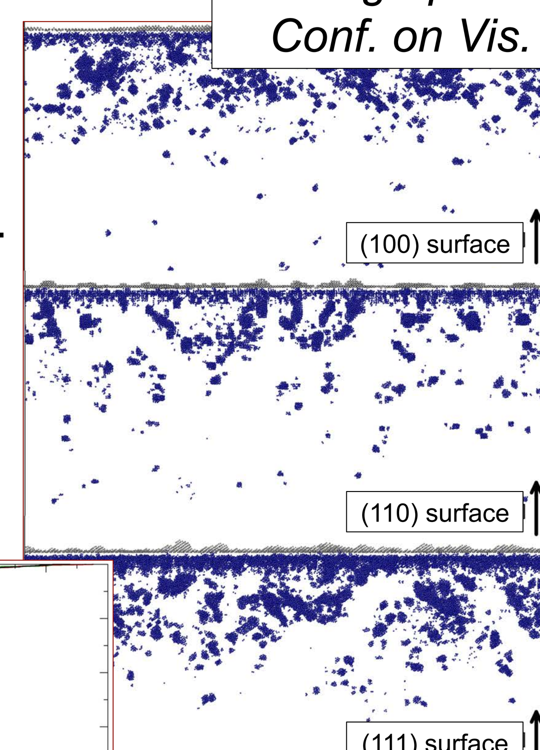
Surface Effects (U. Missouri)

Refs: *JAP* **116**, 143301 (2014); *Eurographics Conf. on Vis.*

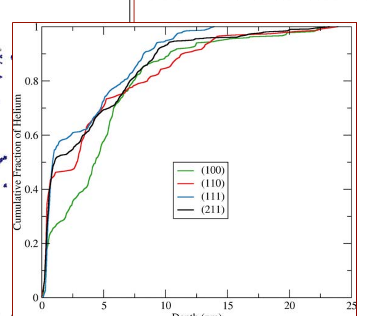
He profiles at W surfaces after exposure to 100 eV He plasma at a flux of 4×10^{25}/m^{2}s using molecular dynamics (MD).



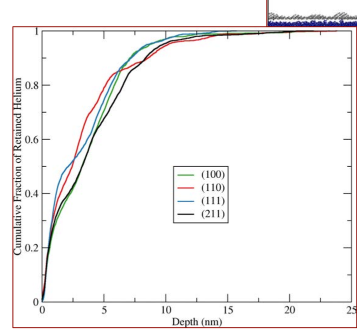
Low fluence (4×10^{18}/m^2; 100 ns)



High fluence (3.3×10^{19}/m^2; 830 ns)



Left: At low fluence, significantly more He retained in 111 surface.

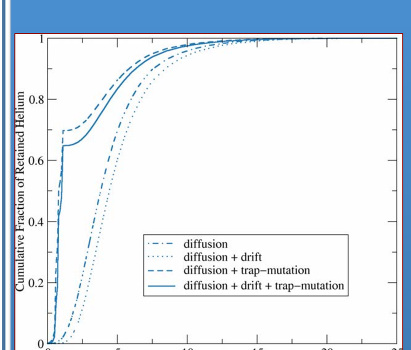


Right: At high fluence, differences in retention are less significant.

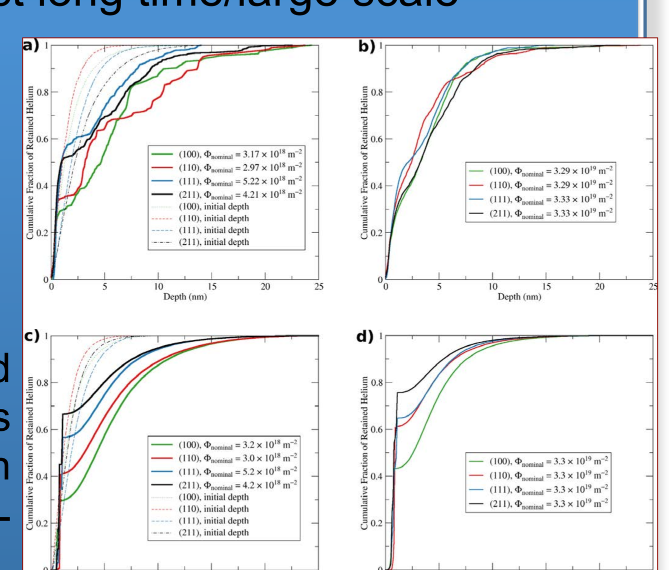
Xolotl-PSI

(ORNL, U. Tennessee)

Xolotl-PSI is a cluster dynamics code that incorporates atomistic information to predict long time/large scale behavior.



Left: Ability to turn on/off near-surface effects in Xolotl provides insight into the importance of various physics.

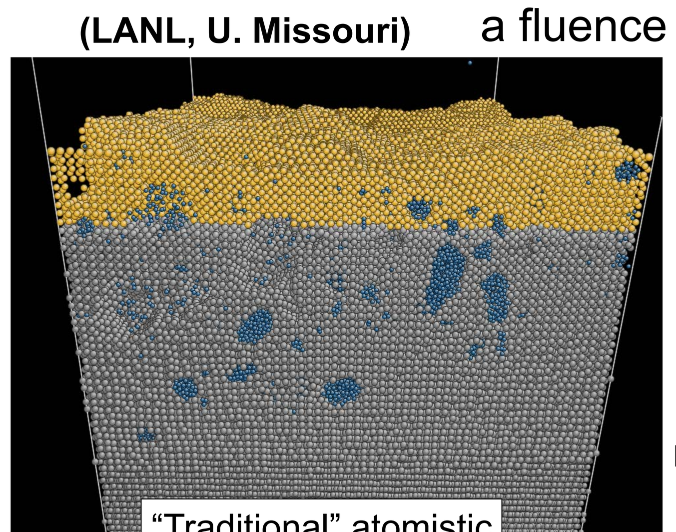


Right: He profiles depend strongly on near-surface effects at low fluence, but at high fluence, Xolotl currently over-estimates near-surface effects.

Visualization

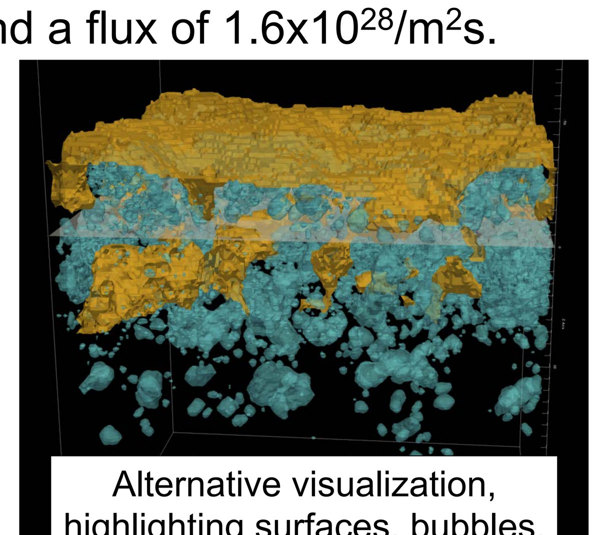
(LANL, U. Missouri)

(100) W surface after exposure to 100 eV He plasma to a fluence of 4.7×10^{21}/m^2 and a flux of 1.6×10^{28}/m^{2}s.



"Traditional" atomistic visualization

Blue atoms/ surfaces indicate He, yellow atoms are created adatoms, and yellow surfaces represent surfaces.



Alternative visualization, highlighting surfaces, bubbles, and voids

Key finding: modified damage mechanisms near the surface trap He at low fluence. Bubbles near the surface do not grow appreciably at higher fluence. The amount of trapped He depends on the surface orientation.

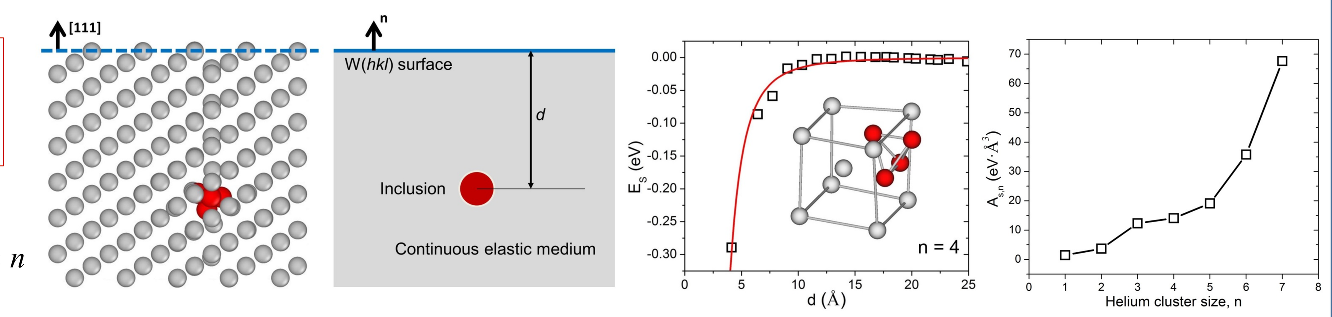
Drift Effects (UMass)

Refs: *Surf. Sci.* **626**, L21-L25 (2014); *JAP* **115**, 173512 (2014); *JAP, submitted; J. Phys.: Condens. Matter, submitted.*

Small mobile He clusters, from aggregation of implanted helium in tungsten, migrate to the surface by Fickian diffusion and drift due to a thermodynamic driving force for surface segregation originating from the elastic interaction between the cluster and the surface. Interaction energy: $E_s(d)$

$$E_s(d) = -\frac{A_{s,n}}{d^3}$$

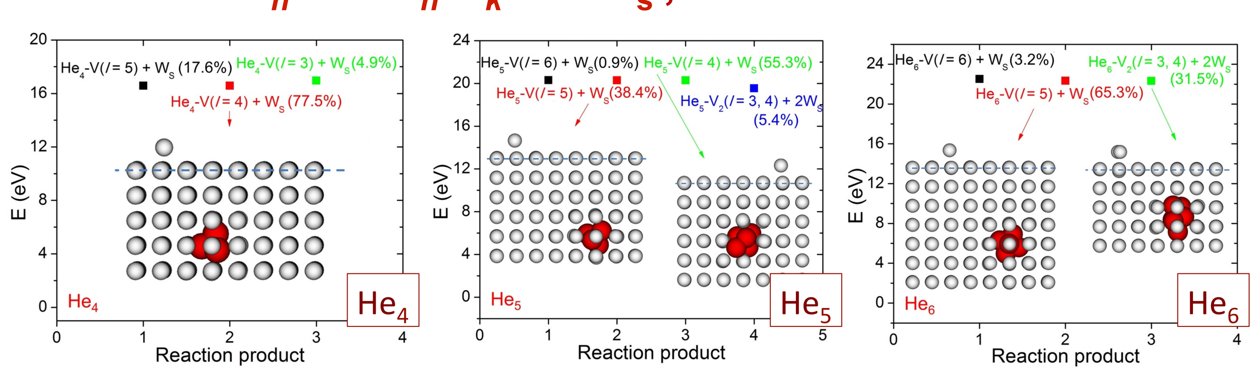
$A_{s,n}$ increases with increasing cluster size n



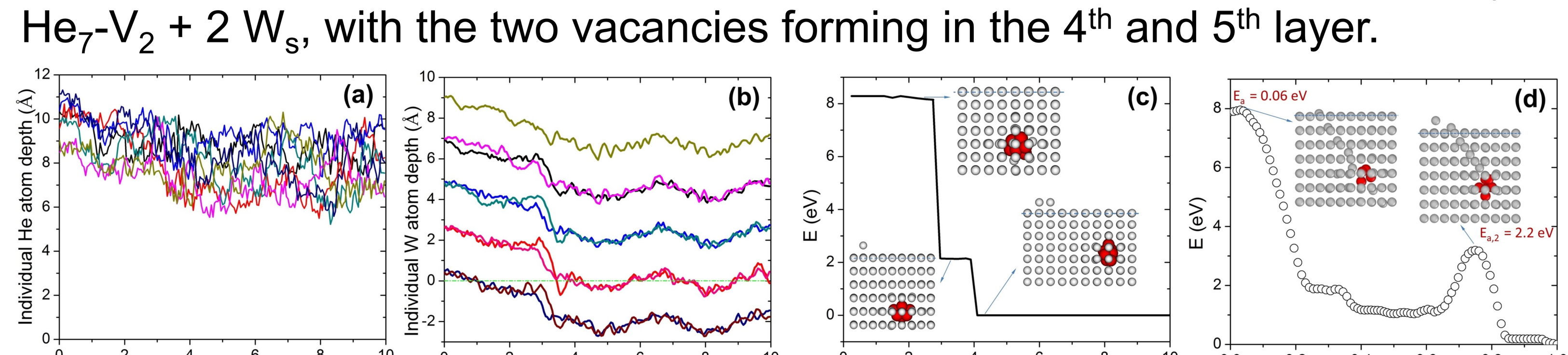
As the clusters approach the surface, cluster reactions are activated with rates much higher than those in the bulk. The dominant ones are trap mutation (TM) reactions, generating immobile helium-vacancy complexes a few layers below the surface plane and tungsten surface adatoms:

$$W + He_n \rightarrow He_n\text{-}V_k + k\, W_s\,;\ k \geq 1$$

Examples: He_4, He_5, and He_6 near W(110)



Analysis of a MD trajectory capturing the trap mutation reaction $W + He_7 \rightarrow He_7\text{-}V_2 + 2\, W_s$, with the two vacancies forming in the 4th and 5th layer.



Evolution of depth below the surface of all seven He atoms of the He_7 cluster during the trap mutation reaction.

Evolution of subsurface W displaced during the trap mutation reaction, forming two adatoms W_s (indicated by the negative values in the bottom two trajectories).

Energy evolution along the quenched MD trajectory during the trap mutation reaction.

CI-NEB pathway for this reaction. Silver and red spheres denote W and He atoms; the dashed line indicates the surface.

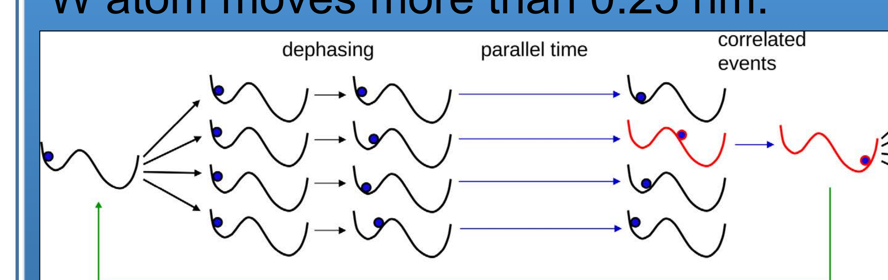
Key finding: elastic interaction potentials based on elastic inclusion theory provide an excellent description of cluster-sink interactions and explain cluster drift transport toward the surface. Trap mutation is the dominant reaction near the surface. Multiple W adatoms and vacancies are formed in TM reactions of larger clusters (typically, n ≥ 4). Such cluster dynamics contribute significantly to surface morphology, near-surface defect structures, and He retention.

Rate Effects (LANL)

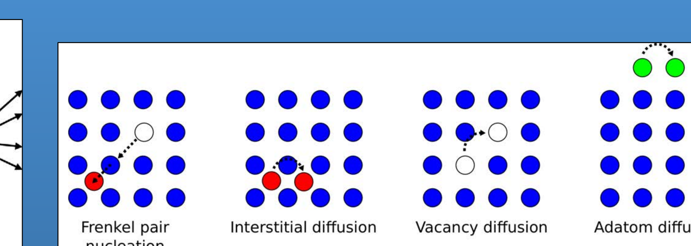
Ref: *PRL* **114**, 105502 (2015)

MD necessarily uses rates much higher than experienced in ITER. To understand the effect of the He absorption (growth) rate on bubble evolution, we perform accelerated MD simulations (parallel replica dynamics (ParRep)).

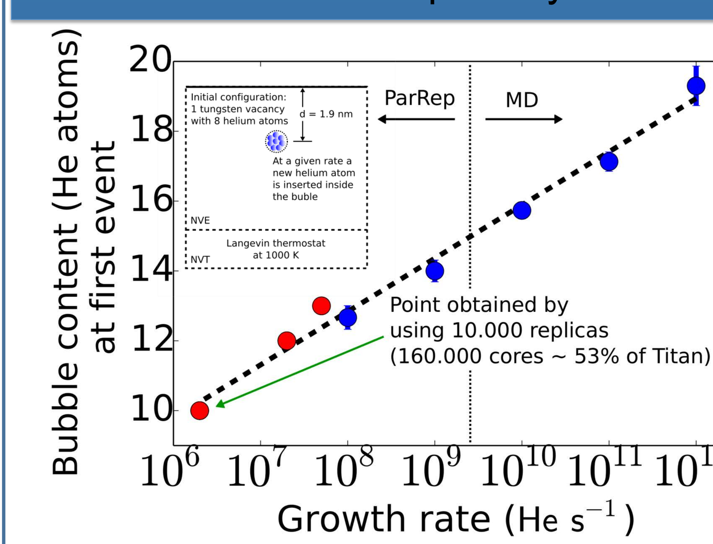
ParRep parellelizes the time evolution of the dynamics, greatly increasing the time scales of direct simulation. Here, events are triggered when at least one W atom moves more than 0.25 nm.



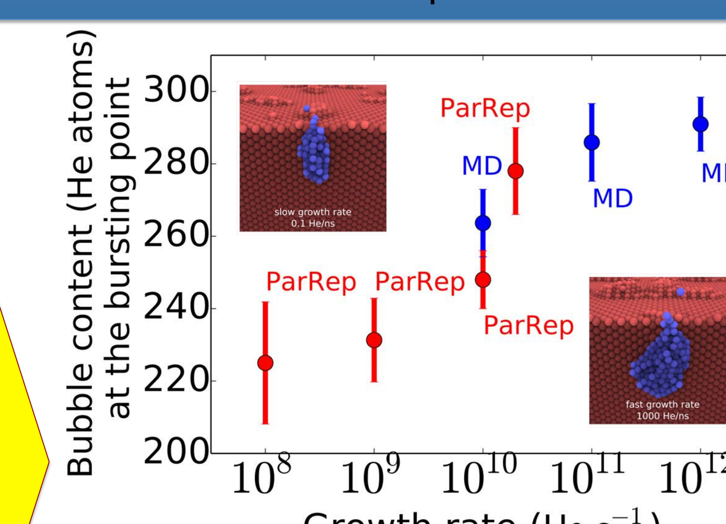
Parallel replica dynamics



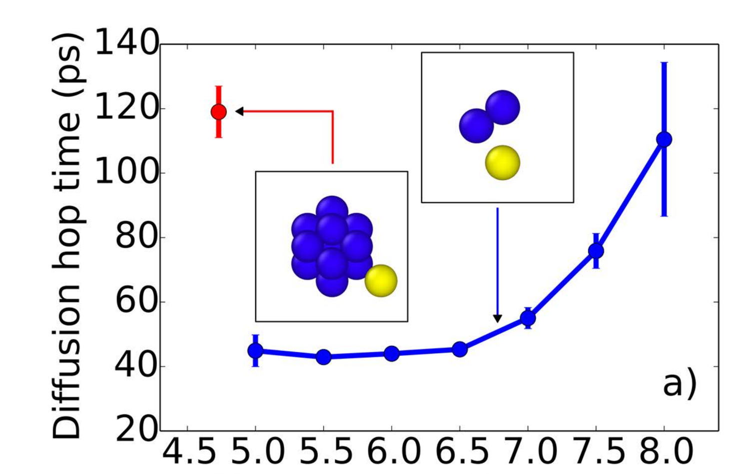
ParRep events



As the growth rate is decreased, the pressure at which events occur also decreases → the matrix has time to respond to the pressure.

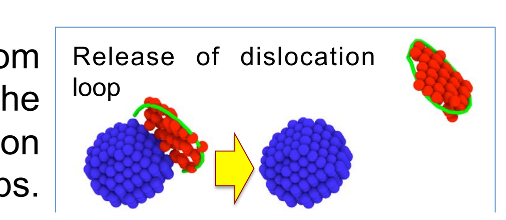


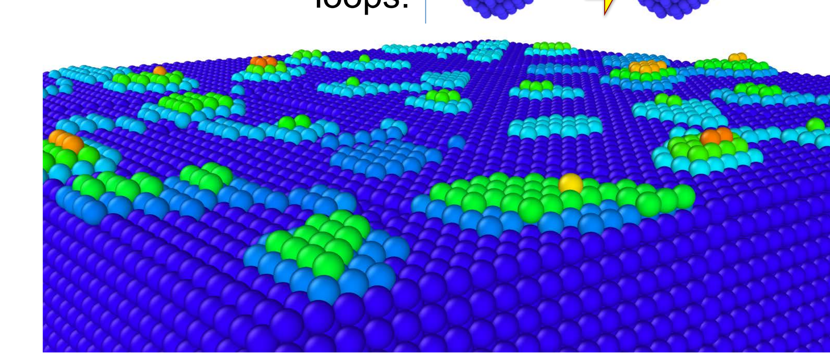
Thus, the size at which bubbles burst also decreases, as the bubble growth is more directed toward the surface.



Why? As the pressure increases, the mobility of W interstitials on the surface decreases → less ability to interact with the surface.

Process of adatom formation via the release of dislocation loops.





{100}-surface morphology, after bursting of 9 He bubbles grown slowly at a depth of 1.9 nm.

Key finding: the existence of two growth regimes, depending on whether the growth of the bubbles occur slower or faster than the diffusion of interstitials around it. At slower growth rates, the bubble "sees" the microstructure earlier and the morphology of both the bubble and surface is affected.