Growth of Helium Bubbles in Tungsten under Realistic Rates

June 23, 2015

Luis Sandoval, Danny Perez, Blas P. Uberuaga and Arthur F. Voter

Nuclear fusion

Advantages of fusion power:

- No carbon emissions.
- Abundant fuels.
- Energy efficiency.
- Significantly less radioactive waste.
- Safety.

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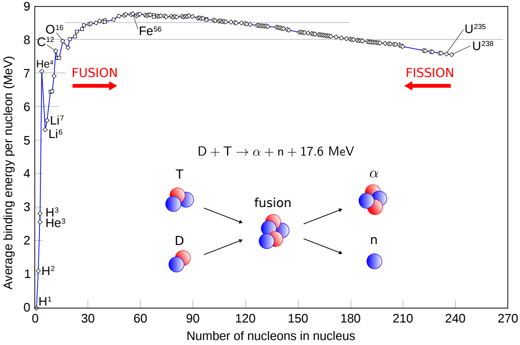
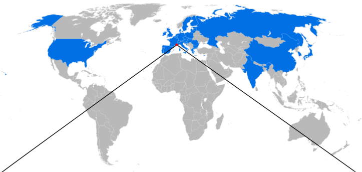


Most promising reaction (deuterium-tritium):

$$^{2}_{1}H + ^{3}_{1}H \rightarrow ^{4}_{2}He(3.5\,\text{MeV}) + ^{1}_{0}n(14.1\,\text{MeV})$$

ITER: International Thermonuclear Experimental Reactor

Participating nations



Cadarache (France)

ITER: (Latin) journey, march, path, road, ...

Participating nations

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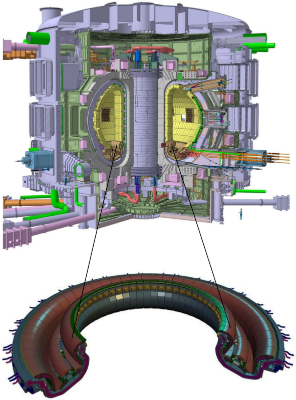
Participating nations

Cadarache (France)

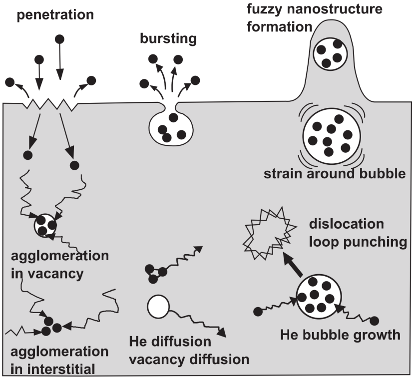
Tokamak

(**To**roidal **cha**mber with **ma**gnetic **c**oils)



Divertor

Motivation: Helium induced morphology in tungsten



From Ito et al. (2015).

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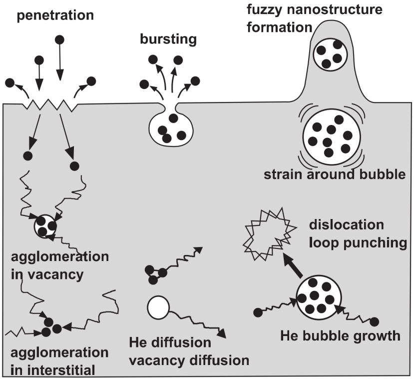

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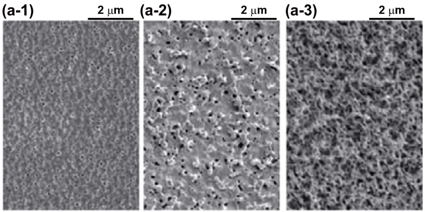

From Kajita et al.(2015).

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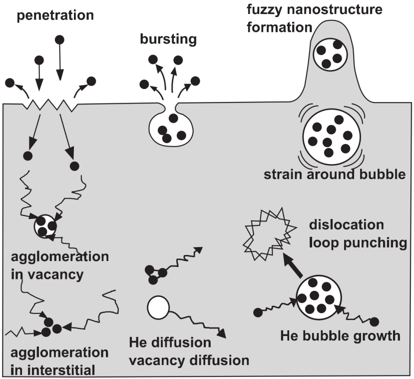

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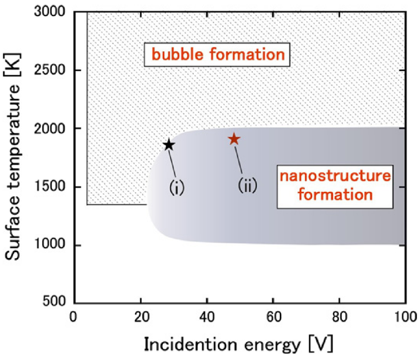
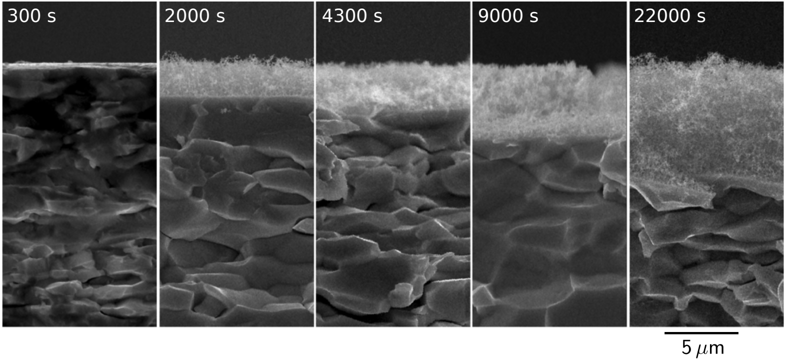


From Yamagiwa et al.(2011).

Motivation: Helium induced morphology in tungsten

The fuzzlike nanostructure increases the nucleation of He bubbles, the retention of H isotopes, and the production of high-Z dust.

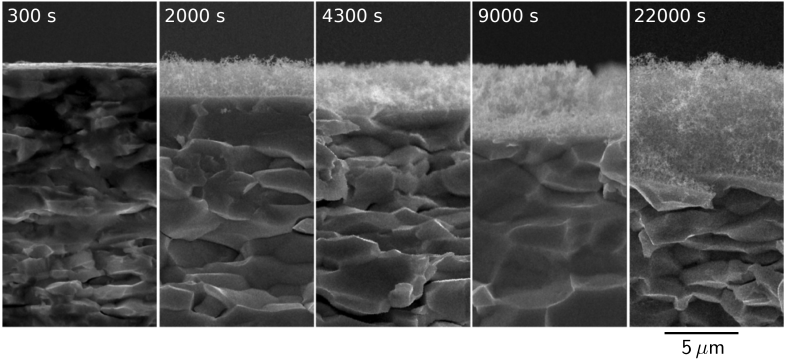


Cross-sectional SEM images of W targets exposed to He plasma. T = 1120 K, $\Gamma_{He_+} \sim 5 \times 10^{22} m^2 s^{-1}$, $\langle E_{ions} \rangle \sim 60$ eV. [1]

[1] Baldwin, M. J. and Doerner, R. P. *Nucl. Fusion* **48**, 035001 (2008).

Motivation: Helium induced morphology in tungsten

The fuzzlike nanostructure is potentially detrimental for the material and plasma performance.



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SciDAC PSI Team

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	GA/DIII-D	Phil Snyder (snyder@fusion.gat.com)	Rui Ding, Houyang Guo, Adam McLean (LLNL on assignment at DIII-D) *Emeriti:* Vincent Chan
	LANL	Xianzhu Tang (xtang@lanl.gov)	Jim Ahrens, Sham Bhat, David Higdon, Li-Ta "Ollie" Lo, Danny Perez, Luis Sandoval, Arthur Voter, Blas Uberuaga
	ORNL*	**Brian D. Wirth* (wirthbd@ornl.gov)**	Alexander "Sasha" Barashev, David E. Bernholdt, Sophie Blondel, John Canik, Ane Lasa, Jeremy Meredith, Philip C. Roth, Roger Stoller *Alumni:* Stanislav Golubov, Crystal Jernigan *Emeriti:* Jay Jay Billings
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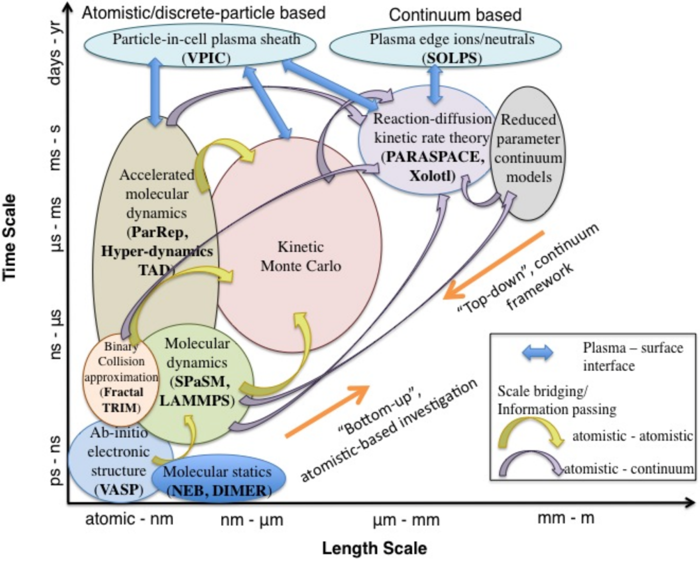
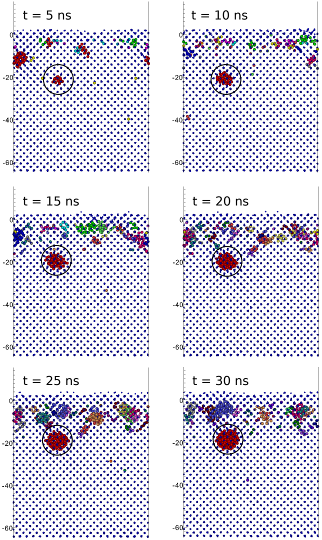
	U Tennessee - Knoxville		Mary Alice Cusentino, Tim Younkin *Additional UTK collaborators are supported through the Plasma Surface Interactions (PSI) Science Center.*

* Lead Institution and Lead Principal Investigator.

SciDAC PSI Approach



Motivation: time limitations of direct MD simulations



- Impact of He atoms on W at a rate of 0.2 He /ps. The kinetic energy per He atom is 60 eV, and the temperature of the system is 1000 K.

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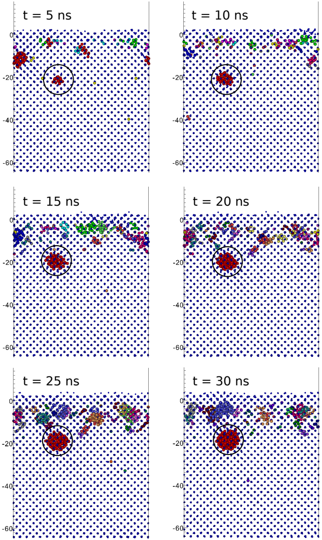

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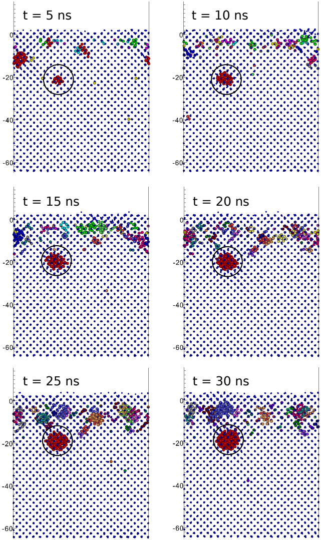

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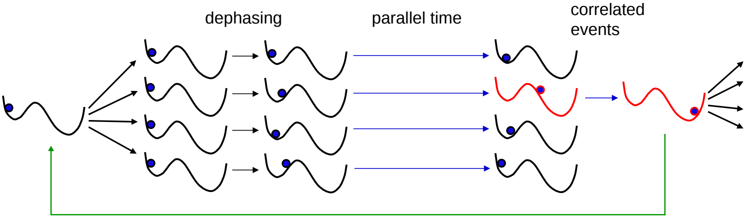
- For the simulation box used, this impact rate corresponds to a flux of 5×10^{27} He m /s ($\sim$ 4 orders of magnitude higher than the one expected in the ITER divertor).
- A study at slower impact (and growth) rates, comparable to experiments, is needed.

Parallel Replica Dynamics[2] (ParRep)

True infrequent events have an exponential first-passage time distribution:

$$p(t) = k \exp(-kt)\,. \tag{1}$$

We can exploit properties of exponential to parallelize time, by having many processors seek the first escape event:

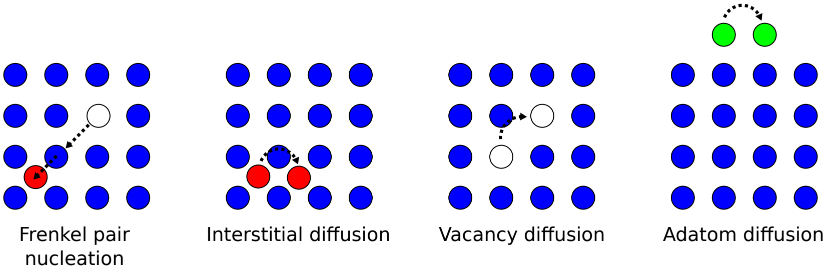


Arbitrary accurate dynamics if implemented carefully.

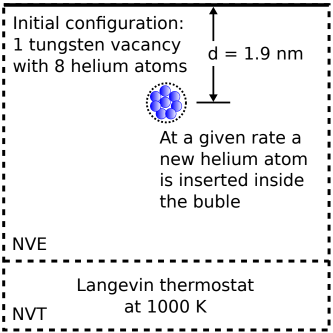
[2]Voter, A. F. *Phys. Rev. B* **57**, 13985 (1998).

Parallel Replica Dynamics

- In our study, ParRep transitions are defined as changes in atomic positions where at least one tungsten atom has moved a distance greater than 0.25 nm, slightly lower than $\langle 111 \rangle / 2$, the Burgers vector of prismatic $\langle 111 \rangle$ dislocation loops.



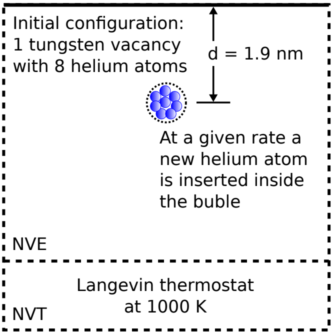
Single He Bubble Growth in a perfect W lattice



Simulation setup.

- The growth of a single He bubble is controlled by directly inserting He atoms into the bubble at constant time intervals.

Single He Bubble Growth in a perfect W lattice

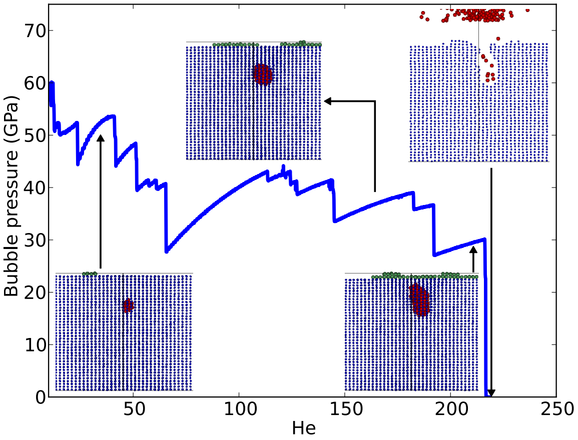


Simulation setup.

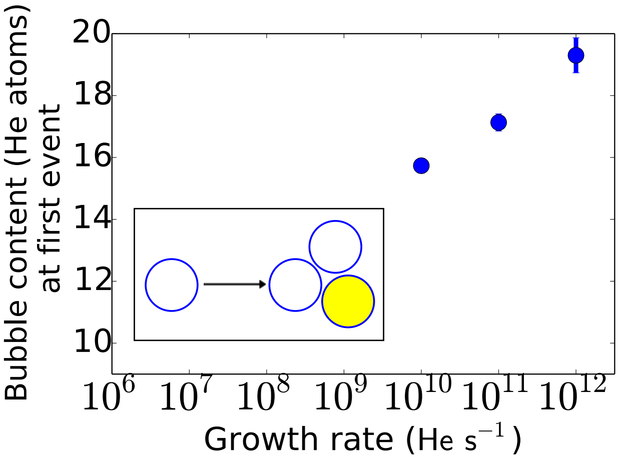
- The growth of a single He bubble is controlled by directly inserting He atoms into the bubble at constant time intervals.
- In reality, this process would occur following the absorption of isolated He atoms or small He clusters that encounter the bubble as they diffuse in the W bulk.

Single He Bubble Growth in a perfect W lattice

For all the simulations, we tracked the evolution of the pressure experienced by the helium bubble.



Growth rate effects



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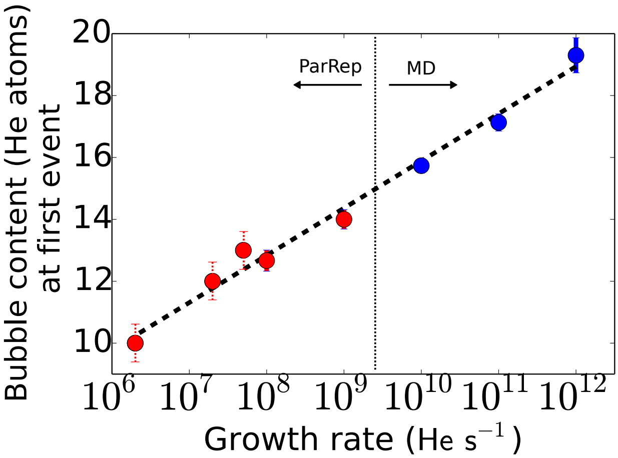

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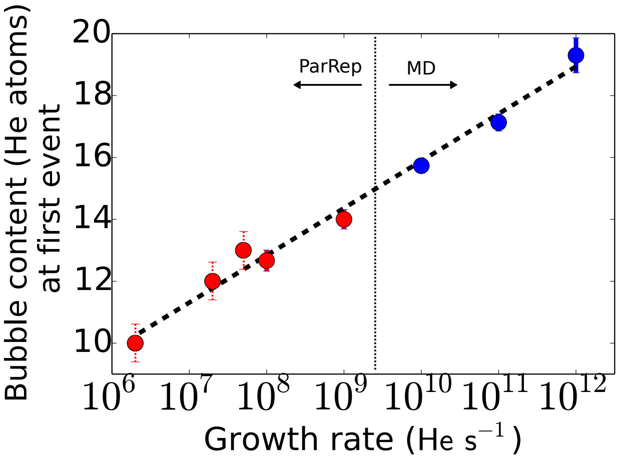

As the growth rate is lowered, the probability of creating a new Frenkel pair increases, leading to smaller He-to-vacancy ratios.

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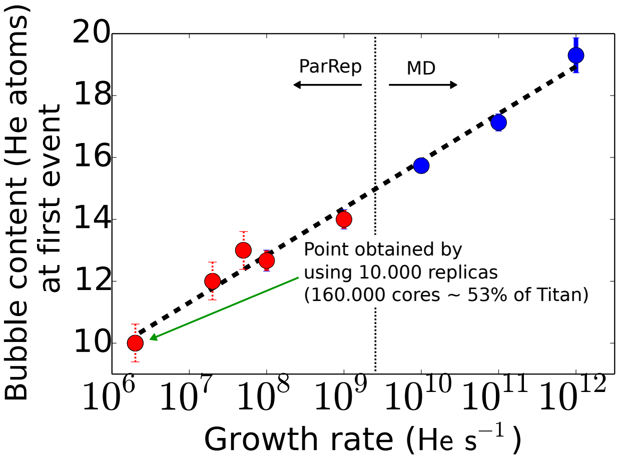

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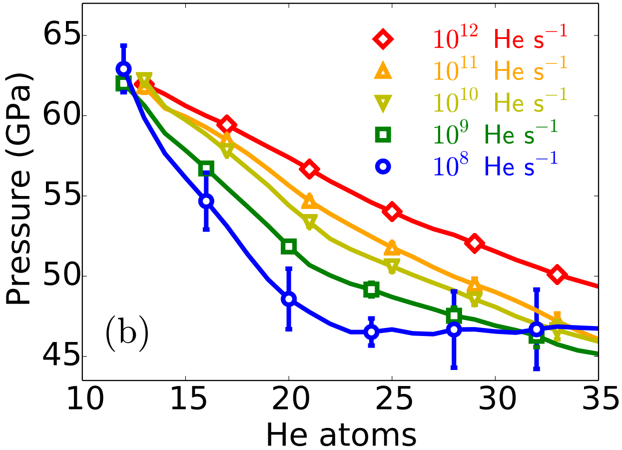
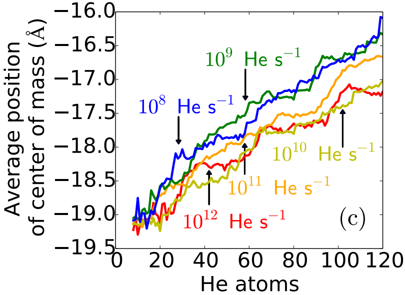
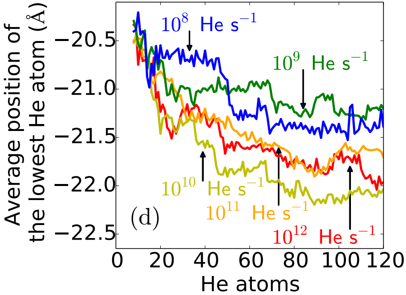


As the growth rate is lowered, the probability of creating a new Frenkel pair increases, leading to smaller He-to-vacancy ratios, and hence lower pressures.

Growth rate effects

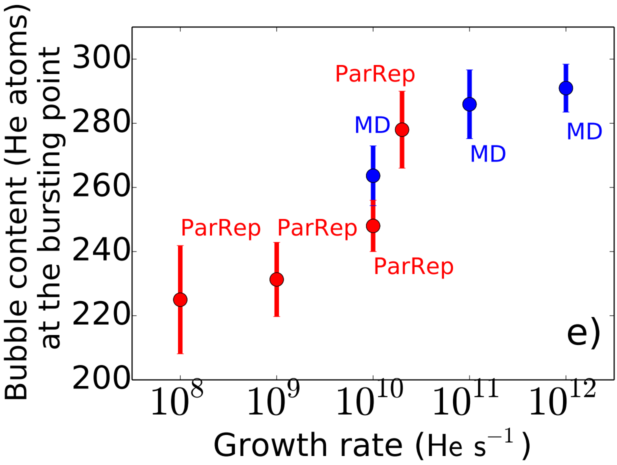
Slow growth rates favor growth that is more directed towards the surface compared to fast growth rates.





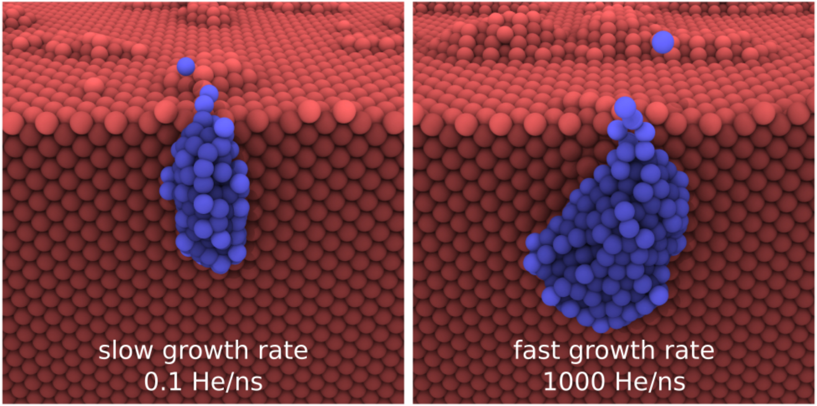
Growth rate effects

This behavior leads to bursting of the bubble at smaller size and lower He content.



Growth rate effects

Representative snapshots.

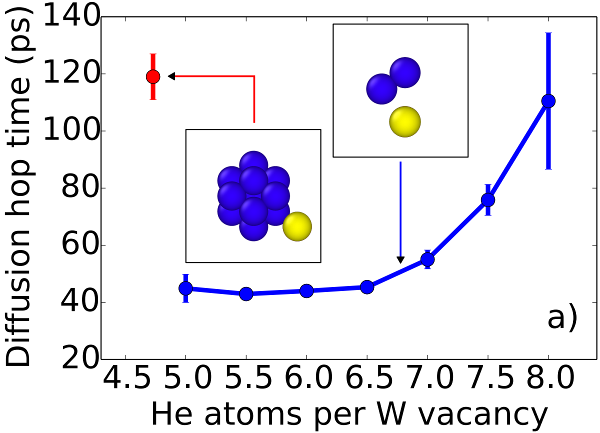


Origin of the growth rate effects

To understand the origin of the growth rate effects, we studied the behavior of interstitials and vacancies nucleated around the He bubble.

Interstitial diffusion and adatom formation

We find that at the slowest growth rates considered in this work, the W interstitials are able to diffuse around the surface of the bubble.



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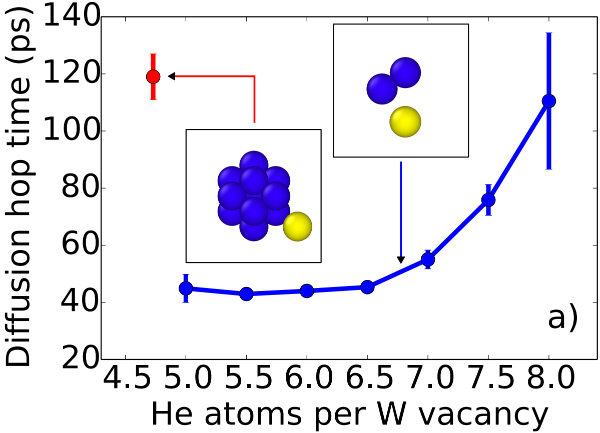


The time scale for interstitial hopping is $\sim$ 100 ps.

Interstitial diffusion and adatom formation

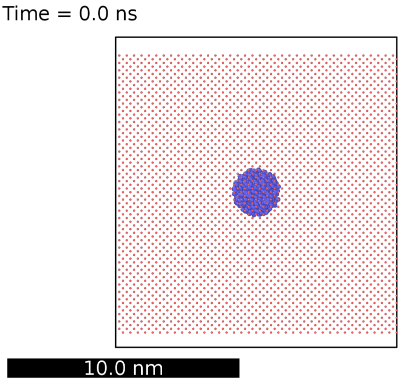
- In light of these results, we can define a criterion to separate the fast and slow growth rate regimes.
- For a given bubble size, if the growth rate allows for the free diffusion of interstitials around the bubble on the time scale of He insertion, this corresponds to a slow growth regime.
- In contrast, for fast growth, the insertion rate of He atoms into the bubble is faster than this diffusion rate, so that the crowdion clusters associated with the interstitial grow faster than they can diffuse.

Deeper He bubbles in W

- The previous slides showed results corresponding to shallow He bubbles (depth of 2 nm).
- The question now is how deeper He bubbles evolve.

Deeper He bubbles in W

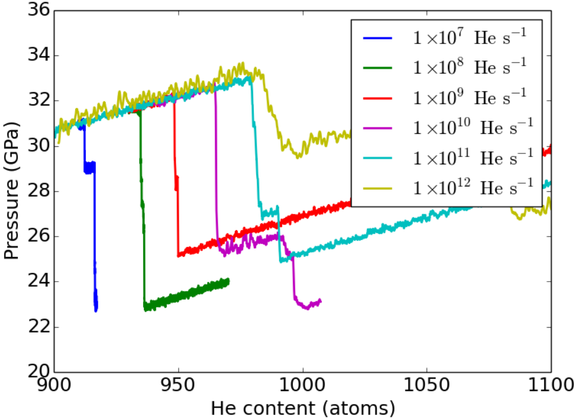
For this new set of simulations the He bubble is located at a depth of 6 nm.



- Single He bubble located in a spherical void of 277 W vacancies.
- The system temperature is kept at 1000 K.

Deeper He bubbles in W

As in the shallow bubble case, slower growth rates favour transitions with lower He content.



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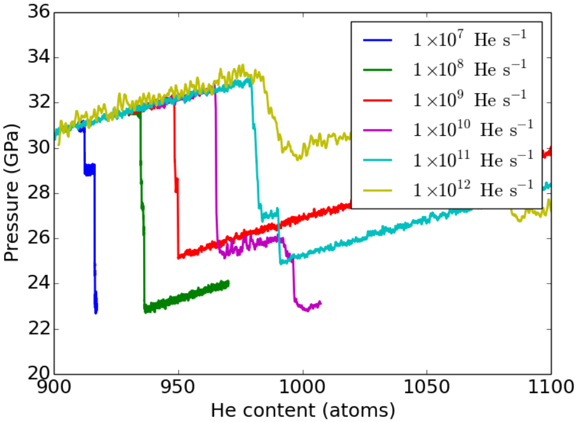
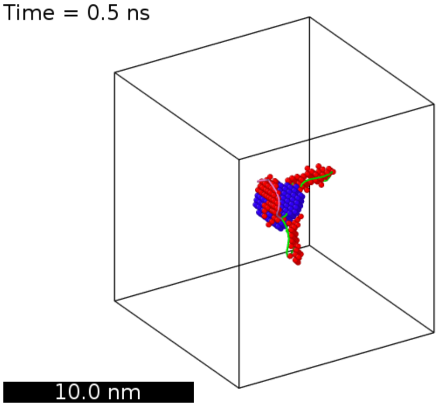


The slowest growth rates have required the use of 25%-50% of Titan, using up to 1M cpu-hours per run.

Deeper He bubbles in W



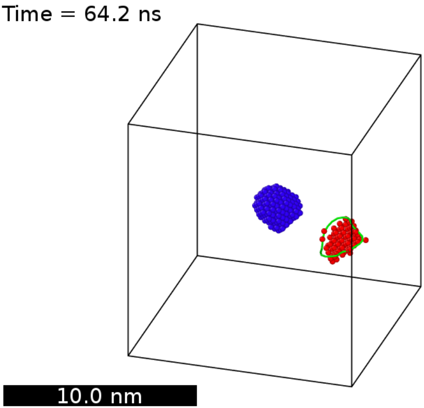
Fast regime: $1 \times 10^{12} \mathrm{He/s}$.

The growth rates accessible to direct MD simulation are too fast, potentially providing artificial phenomena, i.e. not seen at experimental time scales.

Deeper He bubbles in W

Slow regime: $1 \times 10^8 \mathrm{He/s}$.

Studying the growth process at slow (realistic) rates can exhibit new phenomena, hidden to MD, relevant to understand the multiscale process.

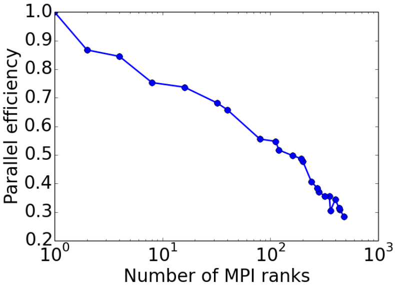


Technical aspects: computing performance

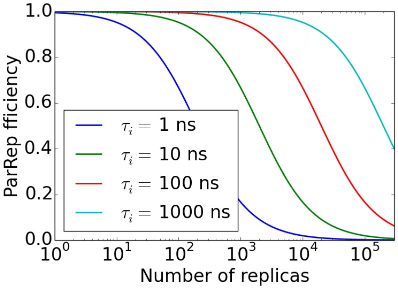
- Now I am going to discuss computational details about how ParRep performs, for this problem, on massively parallel computers.
- The following analysis is specific to this problem, as we have a temperature-independent growth rate, dictating time scales.

MD Efficiency

- System with 10^5 W atoms.
- Ackland-Thetford potential.
- LAMMPS.
- Benchmarking simulation on Titan.



ParRep Efficiency

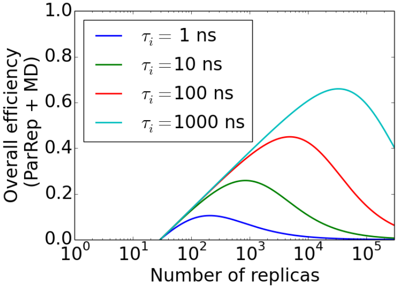


- At first approximation, the number of detected events corresponds to the number of He atoms inserted into the bubble.
- Given a He growth rate of $1/\tau_i$, a perfect ParRep efficiency would be equal to τ_i/N_r, with N_r denoting the number of replicas.
- Considering the dephasing period τ_d (5 ps), the real ParRep efficiency is given as

$$\text{ParRep}_{\text{eff}}(N_r, \tau_d) = \frac{\tau_i/N_r}{\tau_i/N_r + \tau_d}.$$

ParRep + MD Efficiency

- Let us consider an available number of cores $N_c = 3 \times 10^5$ cores ($\sim$ 100% Titan).
- The optimal number of replicas results from a competition between the decreasing spatial parallelization efficiency with increasing number of MPI ranks per replica, and the decreasing ParRep efficiency with increasing number of replicas.



$$\mathrm{ParRep}_{\mathrm{eff}}(N_r) \times MD_{eff}(N_c/N_r).$$

Conclusions

- For the slowest growth rates we considered, the system is able to efficiently explore the accessible state space, facilitating the occurrence of transitions involving fewer W atoms.
- Significant differences across time scales are observed, which include the pressure experienced by the He bubble, the number of W vacancies and He atoms in the bubble at bursting point, and the dynamics of Frenkel pair nucleation.
- Our main finding is 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.
- These findings highlight the importance of simulating materials under realistic conditions and the potential pitfalls of extrapolating from short timescale simulations alone.

Future directions

- Effects of surface orientations.
- Interaction of He bubbles with W dislocations.
- Behavior of He bubbles at grain boundaries.
- Bubble coalescence.
- Inclusion of H atoms into the system.

Acknowledgements I

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Acknowledgements II

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Thanks!