

Code Validation Experiments

Dwaipayan Dasgupta (DD)
University of Tennessee, Knoxville

2nd MPEX User Research Forum
September 13, 2021

Contributors:

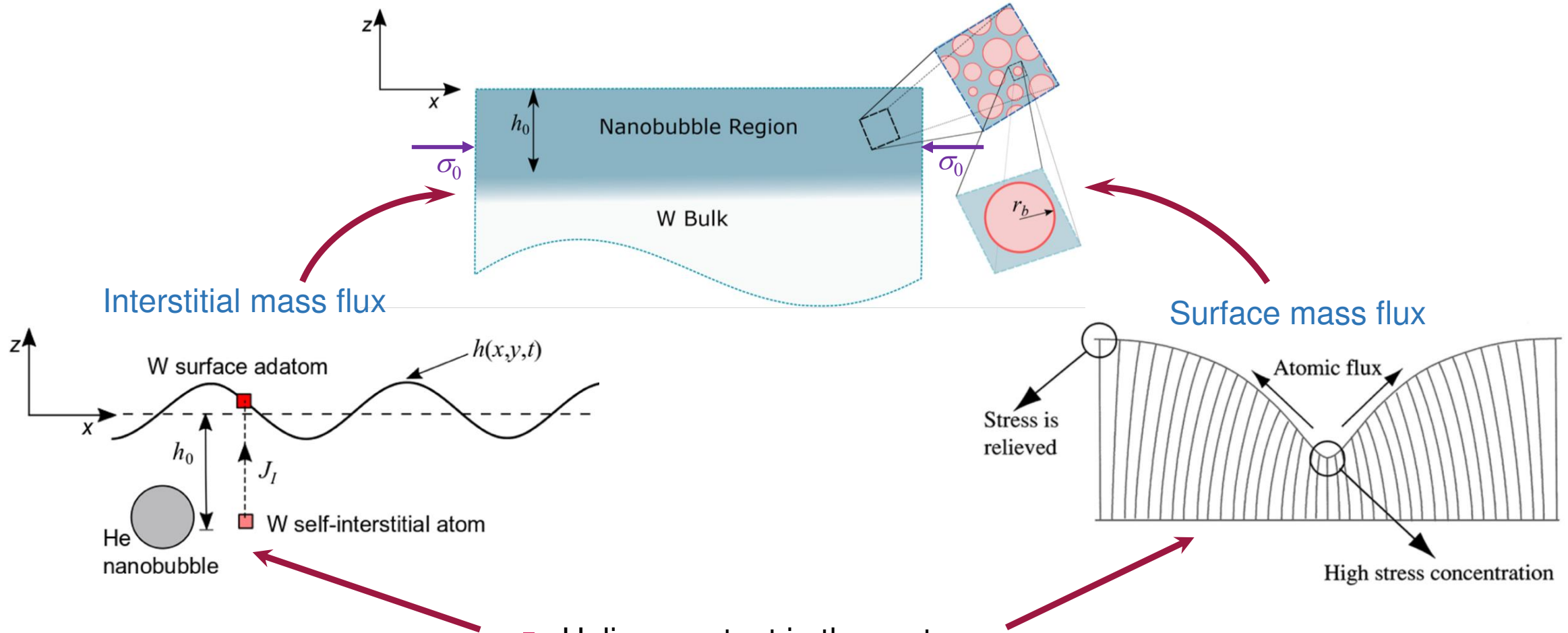
Chao-Shou Chen, Asanka Weerasinghe, and Dimitrios Maroudas
University of Massachusetts, Amherst

Sophie Blondel and Brian D. Wirth
University of Tennessee, Knoxville

Robert D. Kolasinski
Sandia National Laboratories-Livermore

Karl D. Hammond
University of Missouri

Surface Morphological Evolution Model (< 100 eV He⁺)

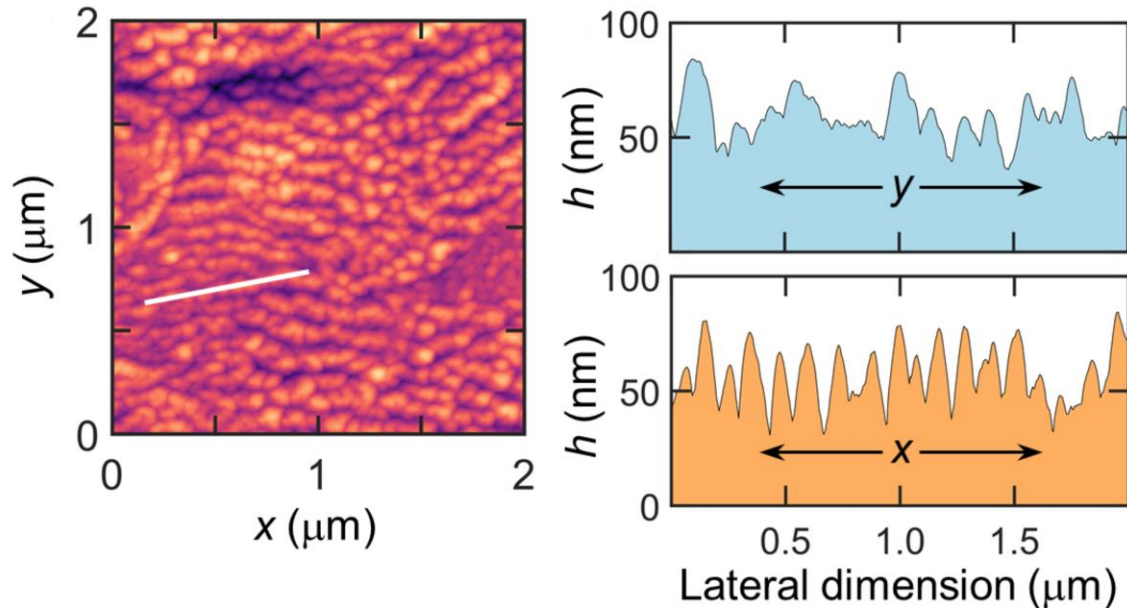


- Helium content in the system
- Average helium bubble size
- Thermomechanical properties

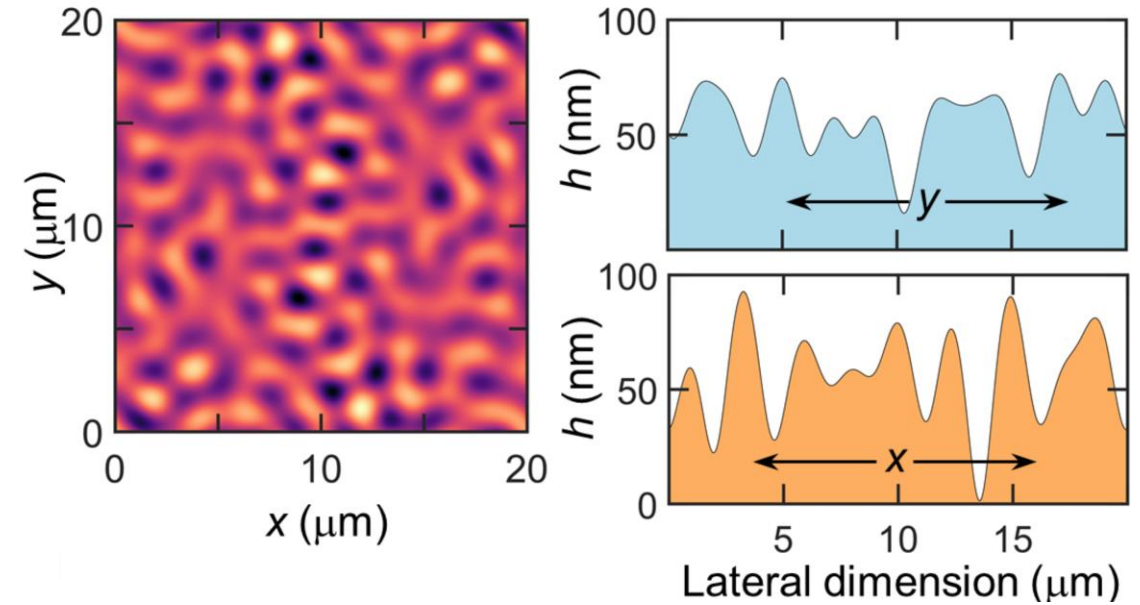
Simulation Predictions and Experimental Measurements: Comparisons

- **Experiment:** RF plasma source (2.7×10^{20} He $\text{m}^{-2} \text{s}^{-1}$); 75 eV He; ITER-grade W at 840°C

Experiment:



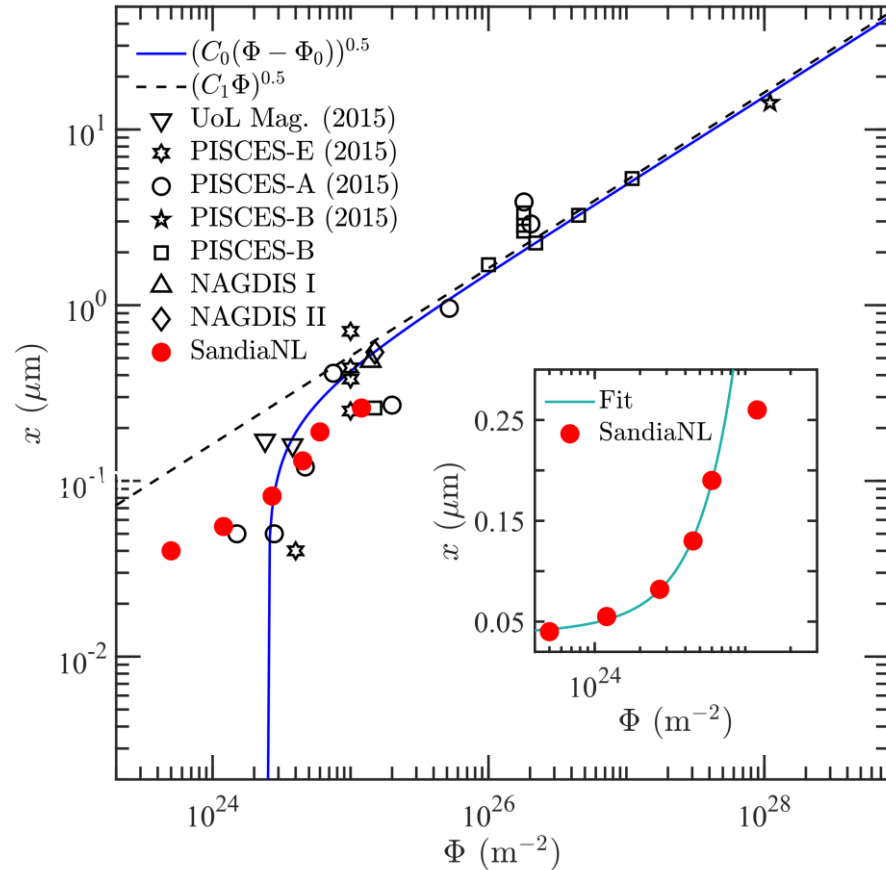
Simulation:



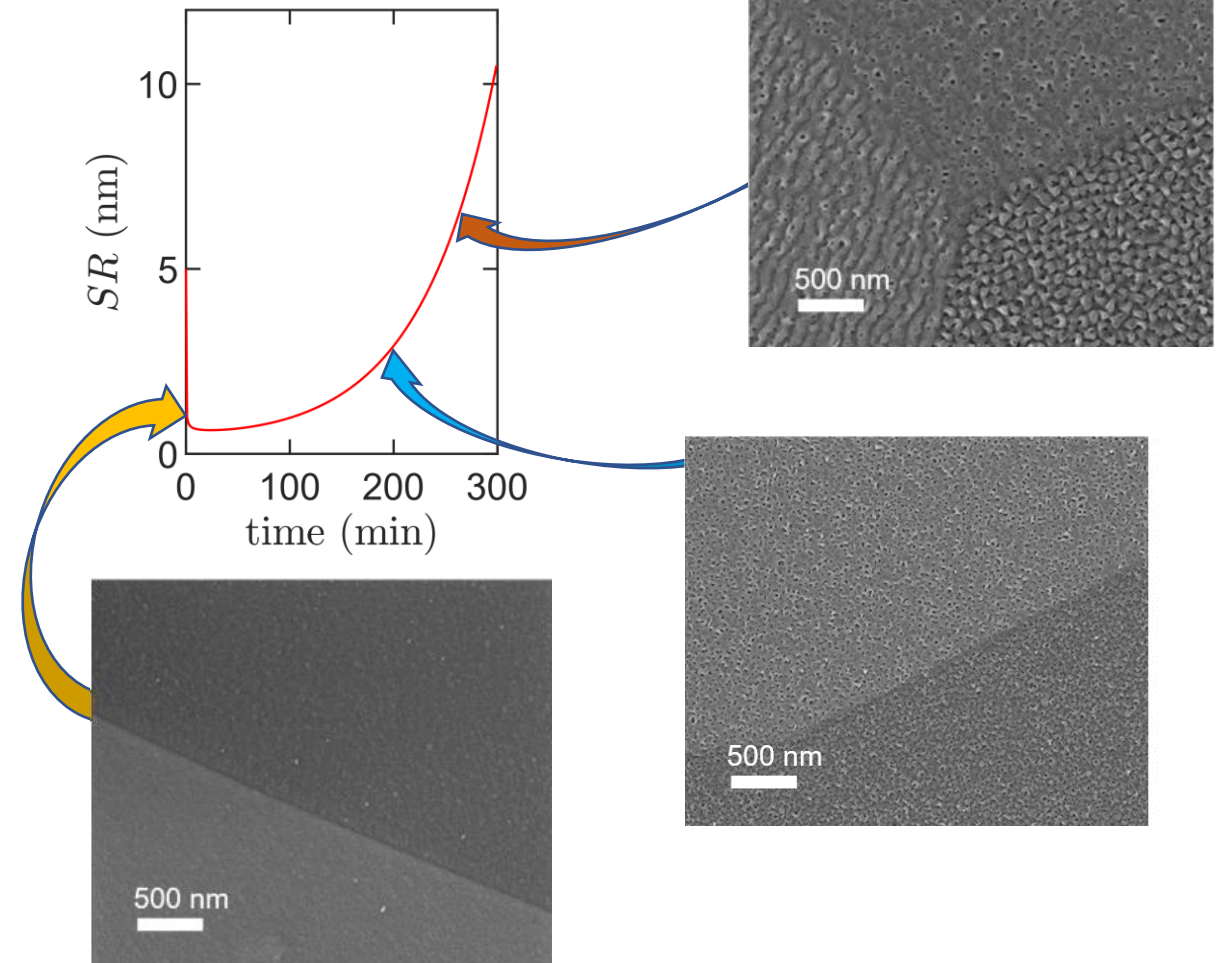
- The model can capture nanotendrils formation at high temperature and gives good predictions of the nanotendrils growth rate
- The predictions of the nanotendrils width and separation are off by a factor of 5 - 8.

Representative Simulation Results: Incubation Time

- **Irradiation conditions:** 2.7×10^{20} He $\text{m}^{-2} \text{s}^{-1}$; 75 eV He; ITER-grade W

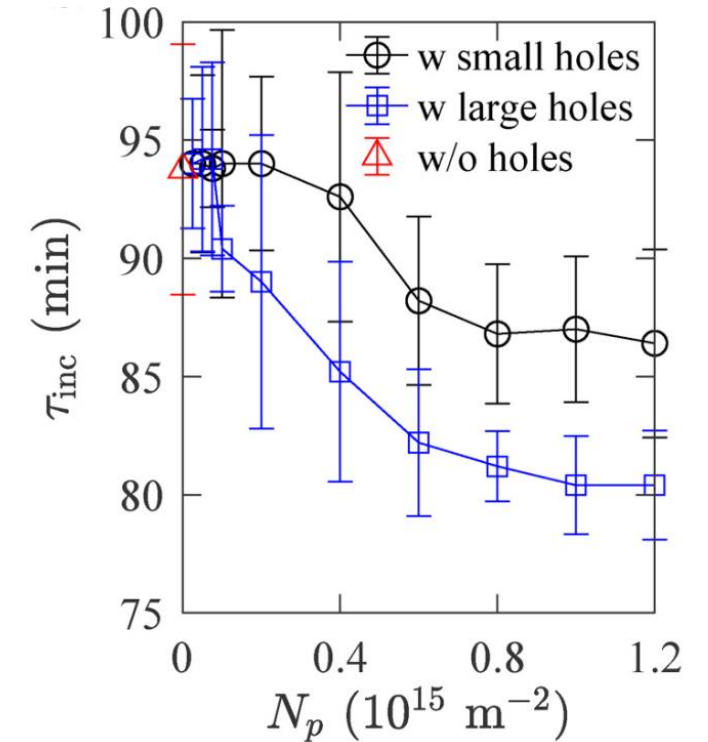
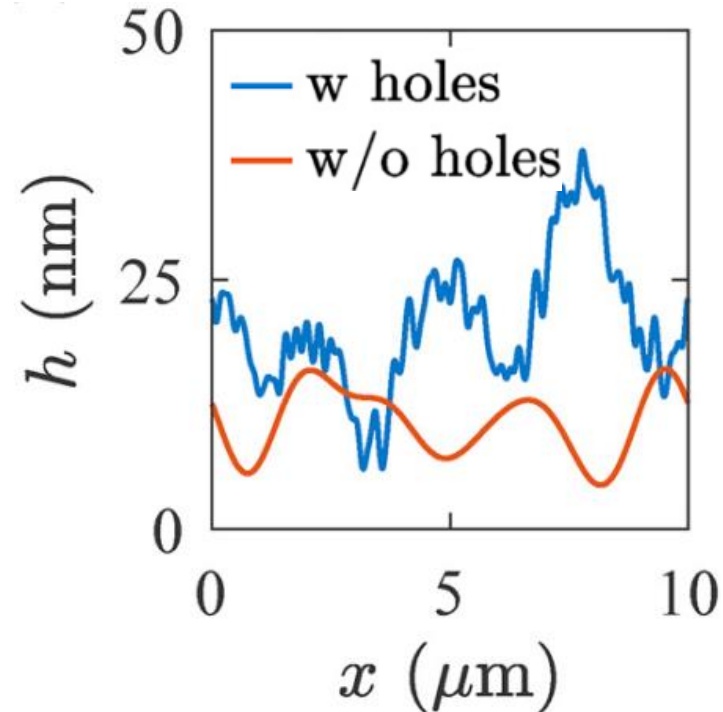
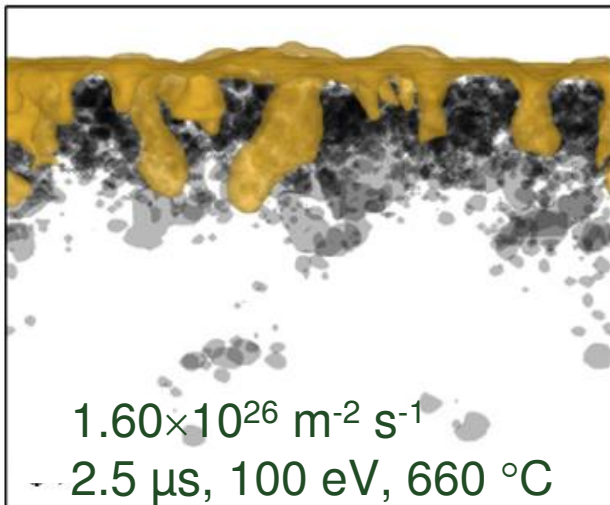
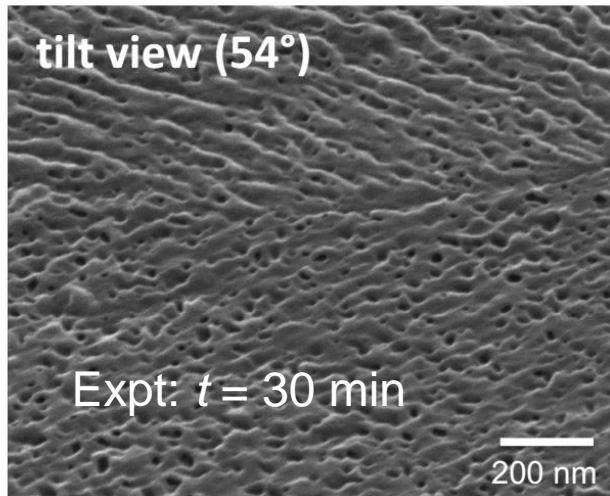


Simulated RMS roughness evolution:



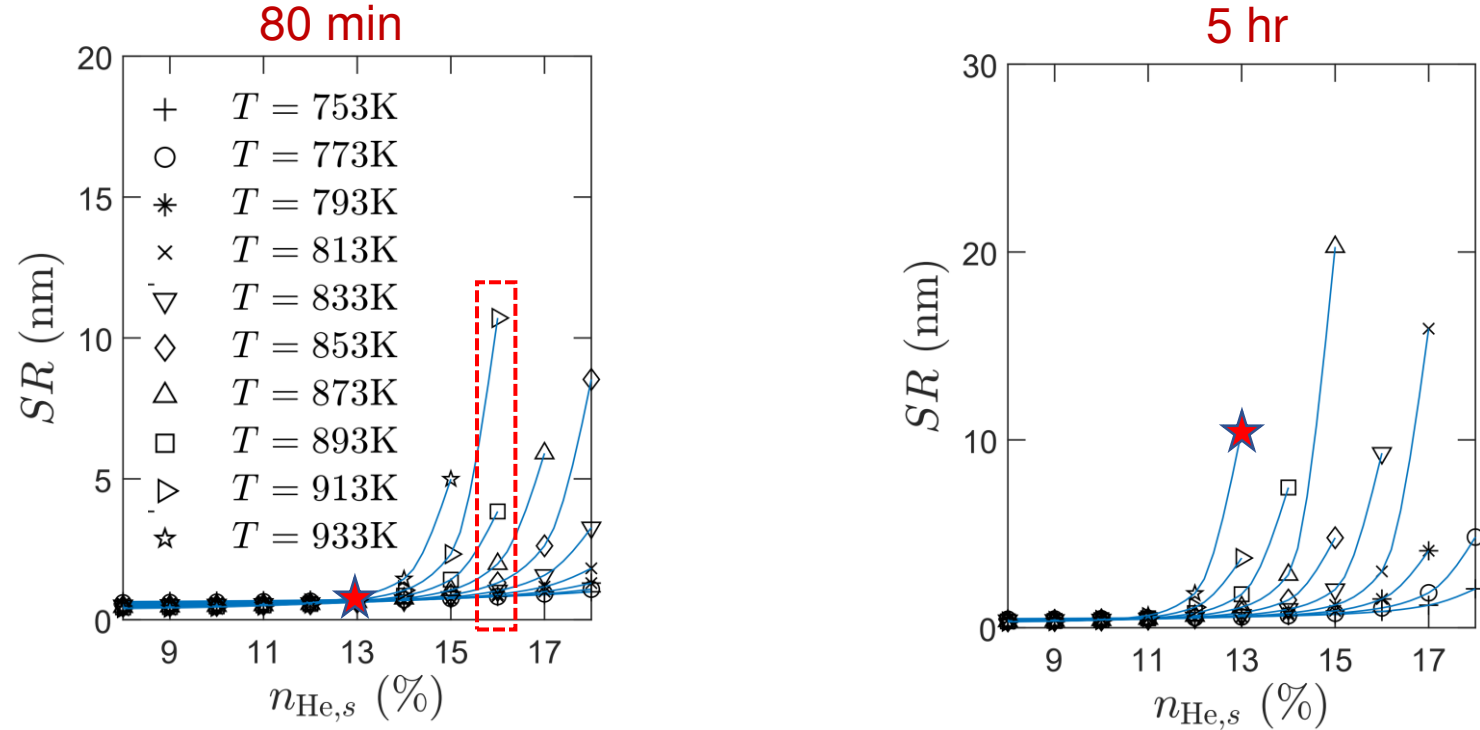
[T.J. Petty *et al.*, Nucl. Fusion **55**, 093033 (2015)]

Representative Simulation Results: Effect of Bubble Bursting



- RF plasma-exposed surface features depend weakly on nanobubble size at low fluence, but show a much stronger dependence at high He fluence
- Bubble bursting/pinhole formation plays an important role in surface morphological evolution

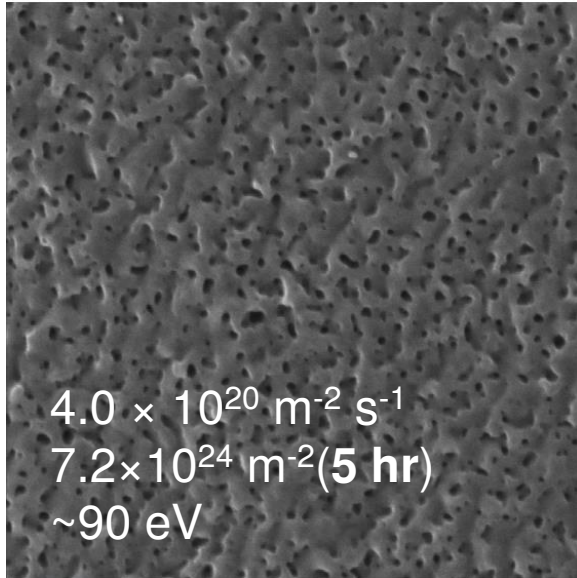
Representative Simulation Results: Effect of Temperature



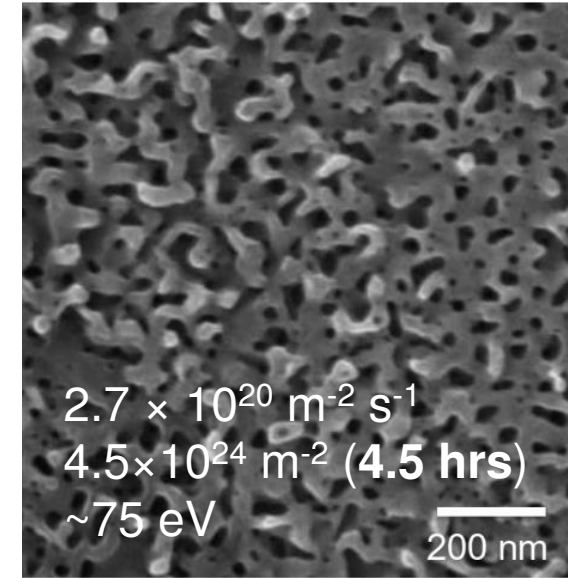
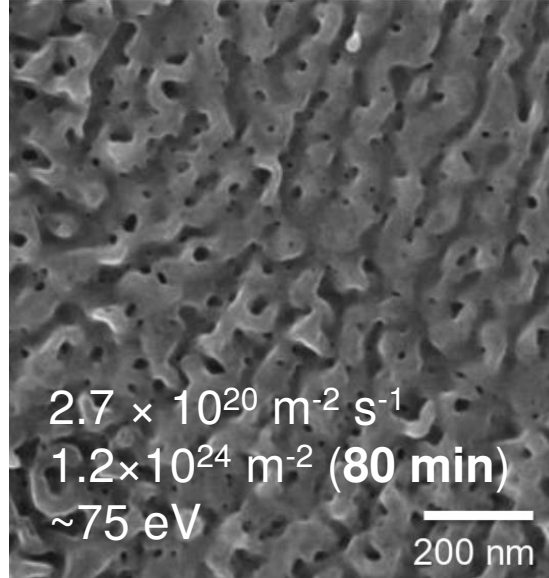
- Plasma exposure duration is critical as opposed to the implanted helium fluence
- Fuzz can grow at temperatures lower than those reported in the literature
- Elastic softening – *thermal* and due to *helium loading* - leads to higher growth rate of nanotendrils
- The average helium bubble size and steady state helium content are the important factors which affect fuzz formation

Representative Simulation Results: Effect of Temperature

600°C

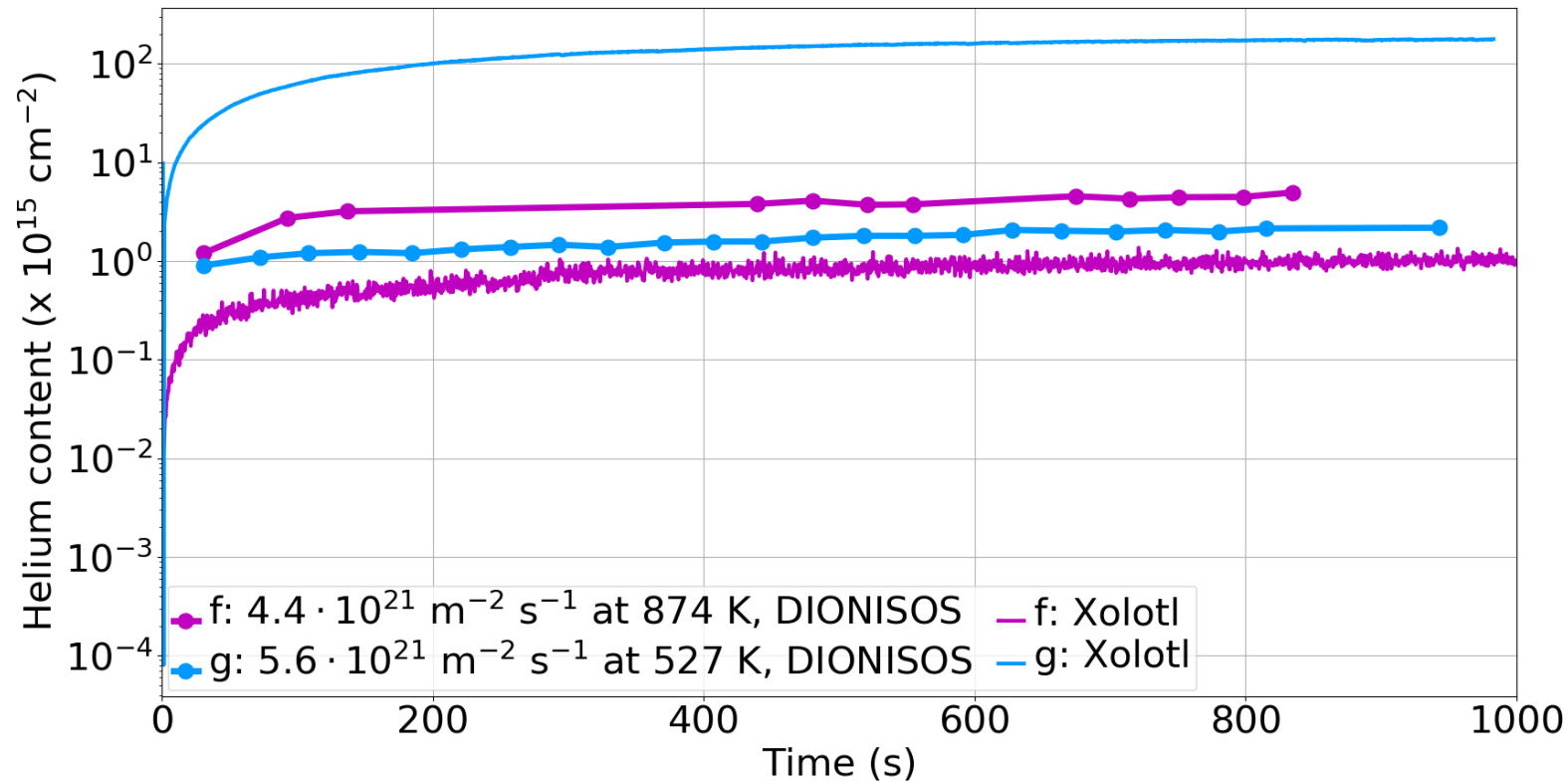


840°C



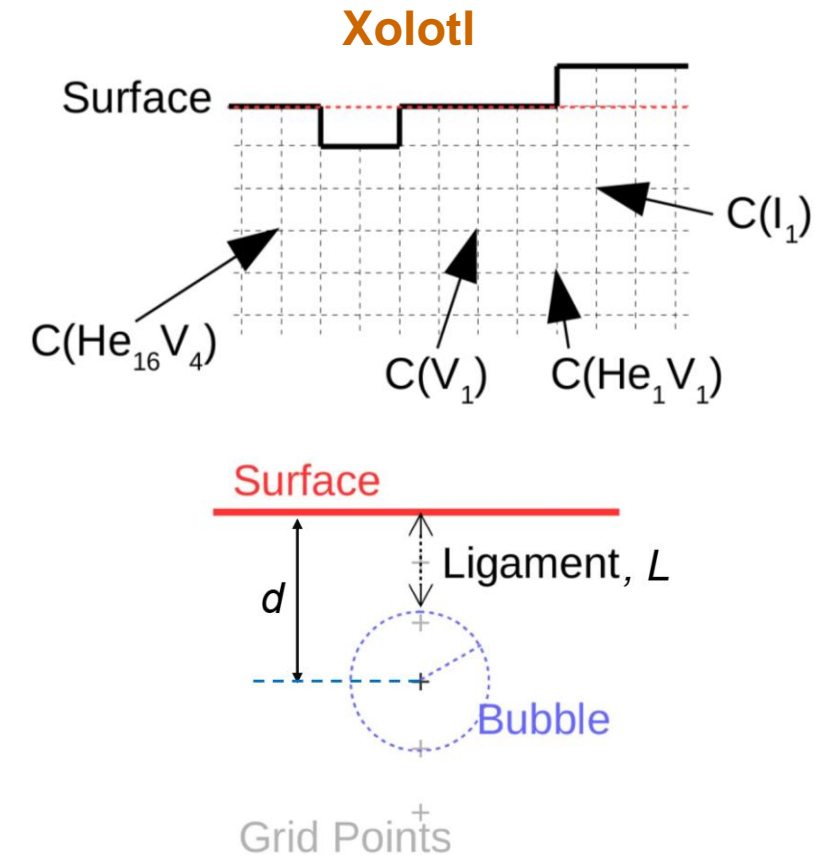
- Plasma exposure duration is critical as opposed to the implanted helium fluence
- Fuzz can grow at temperatures lower than those reported in the literature
- Elastic softening – *thermal* and due to *helium loading* - leads to higher growth rate of nanotendrils
- The average helium bubble size and steady state helium content are the important factors which affect fuzz formation

Representative Simulation Results: Steady-state He Content

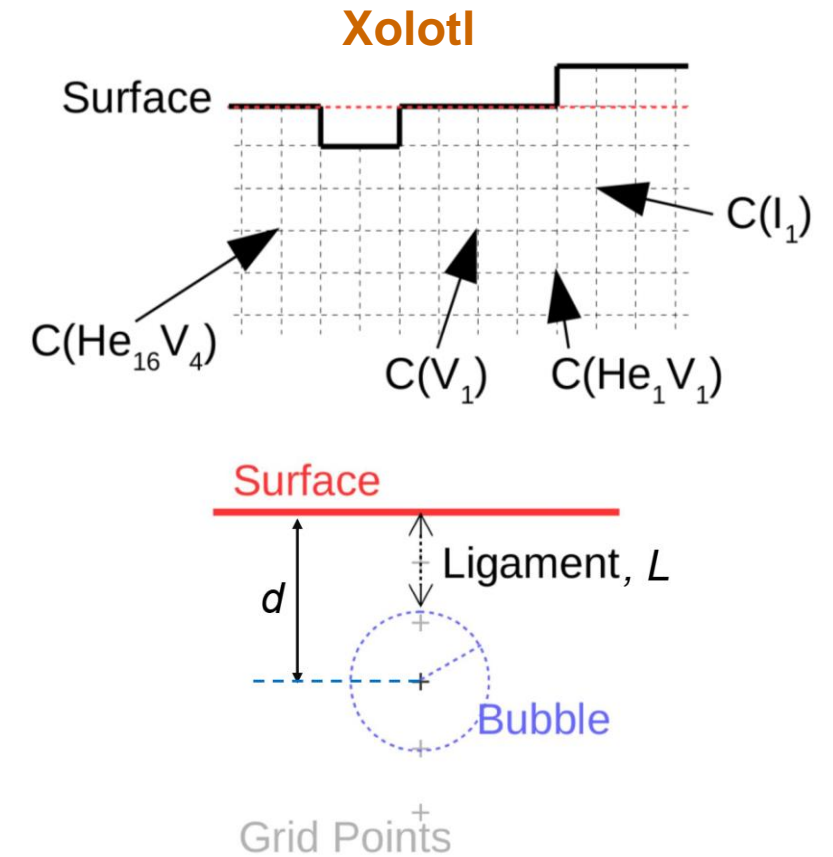
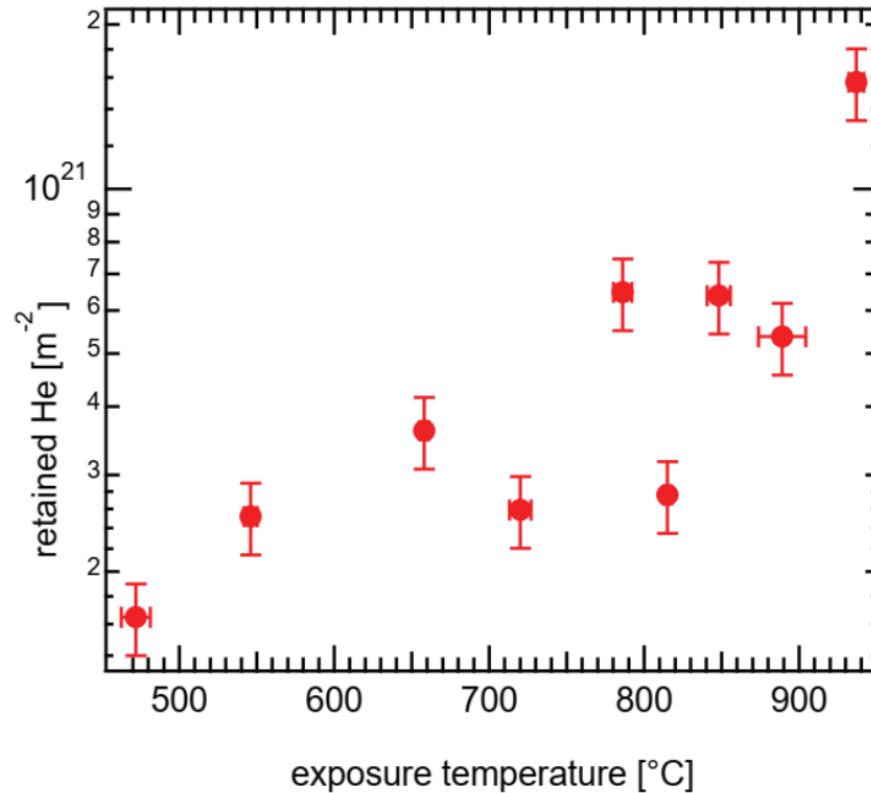


[Experimental Data: K.B. Woller *et al.*, J. Nucl. Mater. **463**, 289-293 (2015)]

- Xolotl simulations can predict He content at steady-state



Representative Simulation Results: Steady-state He Content









- Xolotl simulations can predict He content at steady-state but further studies and benchmarking are required to capture the trend with temperature

Data Needs and Summary of Published Work on Modeling Surface Evolution

- Low energy (below sputtering limit), low flux ($\sim 10^{20}$ - 10^{21} m⁻² s⁻¹) experiments under steady-state plasma:
 - *In situ* measurement of He content and surface (roughness) evolution
 - Surface characterization, He bubble size measurement, elastic moduli and stress state measurements for samples exposed to varying fluence and temperature
- Experiments under dynamic conditions – ELM-like

Questions & Comments?

Further reading:

- On surface morphological evolution model: D. Dasgupta *et al.*, Nucl. Fusion **59**, 086057 (2019). 
- Effect of temperature on surface morphology: D. Dasgupta *et al.*, Surf. Sci. **698**, 121614 (2020). 
- Effect of bubble bursting on surface morphology: C.-S. Chen *et al.*, J. Appl. Phys. **129**, 193302 (2021). 
- Effect of elastic softening on surface morphology: C.-S. Chen *et al.*, Nucl. Fusion **61**, 016016 (2021). 
- Elastic properties of He-implanted tungsten : A. Weerasinghe *et al.*, ACS Appl. Mater. Interfaces **12**, 22287-22297 (2020). 
- Steady-state He content prediction by Xolotl simulations: S. Blondel *et al.*, Nucl. Fusion **58**, 126034 (2018). 
- Large-scale MD simulations to study subsurface bubble growth: K. D. Hammond *et al.*, Nucl. Fusion **60**, 066035 (2020). 