Modeling of Fuzz Formation on Helium-Ion-Irradiated Tungsten Surfaces

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Motivation: Fusion Materials

- Plasma facing materials (PFMs): Tungsten
  - Low hydrogen solubility, low sputtering yield, high melting point, and high thermal conductivity
  - He irradiation modifies near surface microstructure: Increase in retention of tritium, fuzz-like nanostructure
  - Divertor of ITER: Nucleation of bubbles, retention of hydrogen isotopes, and production of high-Z dust
- ‘Fuzz’: Temperature (1000-2300K), He energy (∼10eV), and He flux

State of Knowledge in the Field

- Bubble density in nanobubble layer and bubble diameter depend on the surface temperature and fluence
- The bubbles grow via trap mutation reaction. Bubbles are favorable to grow for bubble concentration ~10^{-40}/ W
- Surface diffusion, loop punching, and bubble bursting leads to pinholes, dips, and protrusion formation on the surface
- Subsurface bubble growth further propagates the surface morphological evolution; the edge becomes sharper and the dip becomes deeper in this process.


State of Knowledge in the Field


- Large scale MD simulations: Successfully predicted subsurface He bubble dynamics but maximum timescale captured so far is $O(10^3\text{ns})$ while onset of fuzz-formation happens $O(10^3\text{s})$. For a typical MD run time on ANL Mira ($O(2 \times 10^7 \text{atoms})$ simulation on $O(2 \times 10^4 \text{cores})$), to reach onset of fuzz formation requires $O(300 \text{ Million years})$ wallclock time. [K. D. Hammond et al., Fusion Sci. Technol. 71(1), 7-21 (2017).]

- KMC simulations†: KMC extended the MD results from $\text{ns-Å}$ to $\text{s-μm}$ scale, but unable to reach the experimental $\text{hr-mm}$ range.

- MD and MC hybrid simulations: Semi-2D MD and MC hybrid simulations have captured the fuzz formation.

Continuum domain model is based on following assumptions:

- Nanobubble region is a homogeneous layer of spherical bubbles with uniform size and number density;
- Nanobubble region is under constant stress due to overpressurized bubble;
- Subsurface bubble dynamics is not included in the current model.

Model parameterization relies on material and thermophysical properties obtained through either atomic-scale simulations or experimental results available in the literature [Ref: K. D. Hammond et al., Acta Materialia (Article in press); S. E. Donnelly, Radiat. Eff. 90, 1-47(1985) ]
Model

- Continuity equation:
  \[
  \partial_t h = \frac{H'\delta_s}{k_B T} \nabla_s \cdot J_s + \Omega J_I - \Omega J_{sp}
  \]

- Surface mass flux \((J_s)\):
  \[
  J_s = \Omega D_s \nabla_s (-\gamma / \kappa + \epsilon)
  \]

- Young-Laplace equation for overpressurized bubble
- Average microscopic stress:
  \[
  \bar{\sigma}_b = \left( p - \frac{2\gamma'}{r_b} \right) \frac{A_b}{1 - A_b}
  \]

- Sputtering loss \((J_{sp})\):
  \[
  J_{sp} = \Gamma_{He} Y_{sp}
  \]
  \[
  Y_{sp} = Y_\infty \left[ 1 - d_E \left( \frac{\beta}{\alpha} \right)^2 \kappa \right]
  \]

- Interstitial mass flux \((J_I)\):
- Thermodynamic driving force:
  \[
  -\nabla_z \mu' = -\frac{\Delta \mu'}{\Delta z} = -\frac{\mu - \mu_I}{0 - (-l_D)}
  \]
- Mass-flux:
  \[
  J_I = \frac{D_IC_{I,0}}{k_B T h_0} \left[ \Omega \gamma / \kappa - \Omega \epsilon \right] + \text{const.}
  \]
Results: Benchmarked against Experiments

- **Experiment:** A medium-flux RF plasma source (2.7×10^{20} He m^{-2} s^{-1}) was used to expose ITER-grade W specimens to ion fluences ranging between 5×10^{23} – 1.2×10^{25} He m^{-2} (corresponding to exposure times ranging between 30 min. to 12 hrs.). For each test, the sample temperature (840 °C) and incident ion energy (75 eV) were identical.

- **Simulation:** The W surface morphology was perturbed with small amplitude normal wave random perturbations (with an rms value, 10^{-4}, much lower than polished W surface). The sample temperature and incident ion energy were identical with experiments. Helium retention was assumed to be ~1%.
Results: Benchmarked against Experiments

Expt: $t = 30$ min

Sim: $t = 60$ min

Expt: $t = 80$ min

Sim: $t = 80$ min

$f$ (μm$^{-1}$) vs. height (nm)

- Expt: $t = 30$ min
- Sim: $t = 60$ min
- Expt: $t = 80$ min
- Sim: $t = 80$ min
Results: Benchmarked against Experiments

- Helium concentration reaches saturation level with negative exponential growth (approximately in 1500 s)
- Bubble bursting/pinhole formation appears to play an important in surface morphological evolution

Summary & Future Work

- An atomistically-informed, continuous-domain model is developed to describe the initial stages of surface deformation, leading to fuzz formation in helium-ion-irradiated tungsten and the simulation results are benchmarked against experimental studies.

- A spectral collocation method and discrete fast Fourier transforms are used to compute spatial profile of the field-variables (curvature, stress, etc.). For time stepping, an operator splitting-based semi-implicit spectral method with adaptive time step size is used to carry out self-consistent dynamical simulations. For a typical simulation run time on HPC ($O(1 \mu m \times 1 \mu m)$ surface) simulation on single core), to reach onset of fuzz formation requires $O(10 \text{ hours})$ wallclock time.

- Continuum domain model can qualitatively capture nanotendril formation at high temperature; the model predicts the growth rate of nanotendrils reasonably well and nanotendril widths are quantitatively comparable ($\sim 200$ nm) with those observed in experimental studies.

- Subsurface bubble dynamics and bubble bursting, redeposition of sputtered W, etc. soon to be included in the model.

- Model will be benchmarked against measurements from carefully designed experiments at different temperature and gas implantation conditions.