Large Scale Simulations of Plasma Facing Component Boronization

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Overview

- Project Background and Motivation
- Simulation Details
- Results
- Conclusions

Background

PFC Boronization Introduction

- Plasma facing components (PFCs) have an important role in containing and maintaining fusion plasmas.
- During plasma material interactions (PMIs), a variety of extreme conditions can be imposed on PFCs:
  - High temperatures
  - Energetic particle fluxes
  - Fluctuating pressures
- To maintain proper operation of fusion devices, PFCs need to limit:
  - Sputtering
  - Recycling of PFC materials or plasma ions back into main plasma
  - Failures due to vacancies and/or complex stress states
- Boron coatings of PFCs (i.e. graphite) have been found to reduce these undesirable behaviors

Prior Work and Motivations

- Prior simulations' methodologies[1]:
  - Number of atoms: ~500
  - C/B/O mixed before deuterium bombardment
  - Randomized positions for all atoms, with relative amounts informed by experimental measurements.
- Resulting Limitations:
  - PFC panels typically made from graphite, which has a defined crystal structure.
  - Experimentally found boron carbides/amorphous boron films not necessarily captured via random generation
  - Small simulation size may limit capturing full D trajectories
- Necessitates large, first principles simulation of boronization process to accurately represent PFC graphite

Current Work

Classical Molecular Dynamics (CMD)

- Applies Newton's Laws to a system of N particles through the following set of equations:

$$\frac{d\,\vec{r_i}}{dt} = \vec{v_i},\ \vec{r}_i\,(t=0) = \vec{r_i^0}$$

$$\frac{d\,\vec{v_i}}{dt} = \vec{a_i} = \frac{\vec{f}_{net,i}}{m_i},\ \vec{v}_i\,(t=0) = \vec{v_i^0}$$

$$\vec{f}_{net,i} = -\vec{\nabla}_{r,i}U, 1 \le i \le N$$

- CMD boasts relatively high computational speed.
  - Allows for large simulations with relatively quick results
  - Current simulations: ~1300 atoms for 50 ps – 1 day of runtime on 16 processors
- Accuracy of CMD simulations highly dependent on choice of interatomic potential *U.*
  - Choice of *U* dependent on state of system being analyzed, inclusion of certain attractive/dispersive effects, etc.
  - Reactive Force Field (ReaxFF) potential used in this study for its high fidelity[2]
- Large Scale Atomic/Molecular Massively Parallel Simulator (LAMMPS), developed by Sandia Lab[3], used to run simulations

Simulation Details

- Graphite Layers (10 total):
  - Frozen layer (1) – Prevents z-motion during bombardment
  - Thermostat layers (2-6) – Simulates wall cooling at 300K and “catches” energetic species
  - Free layers (7-10) – Allows for reaction dynamics to happen without initial thermostat damping
    - Thermostat at 300K 0.5 ps after B impact to dissipate excess energy
- Boron:
  - 1.0eV bombarding energy, normal to surface
  - Random x-y position 20Å above surface
  - Deposited every 2 ps

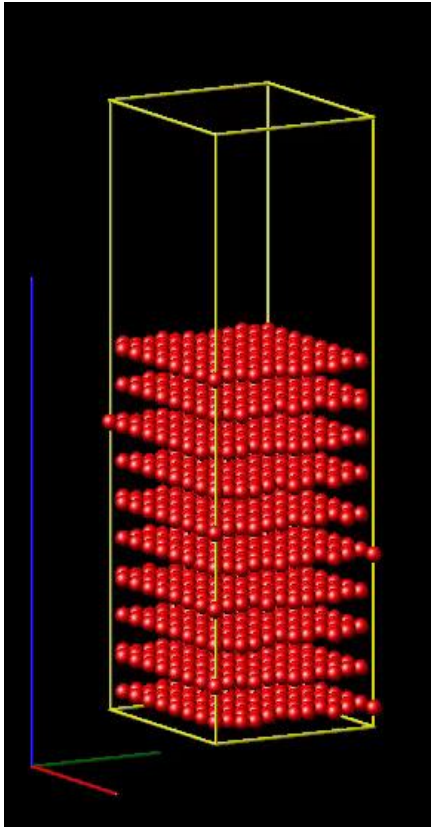

Fig 1. Video of bombardment process

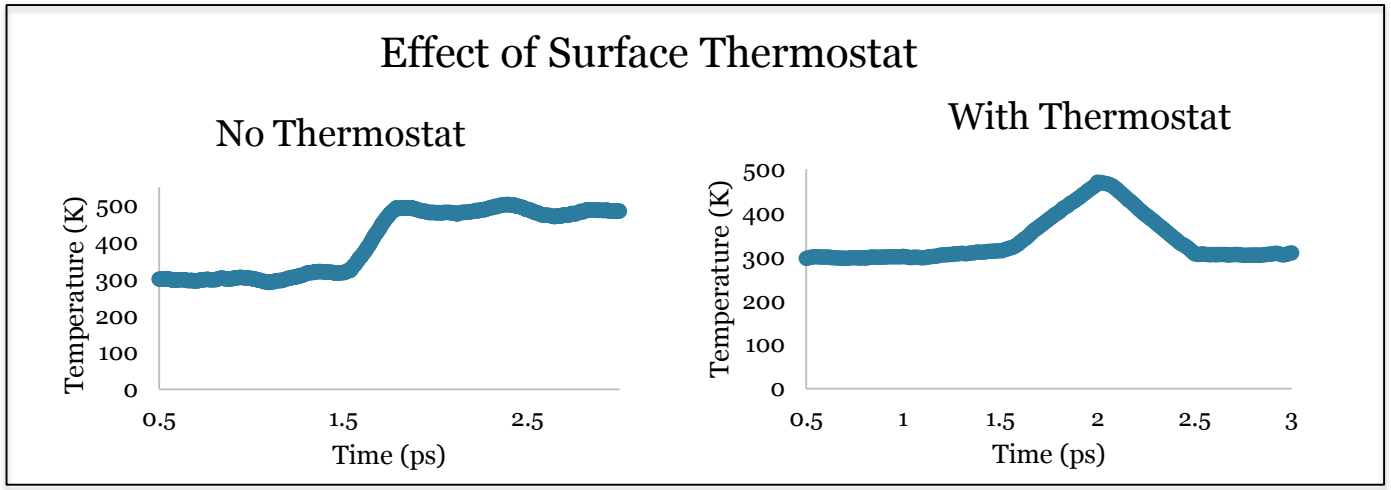

Fig 2. Comparison of the top layer temperature with (right) and without (left) a thermostat, showing how it dissipates energy.

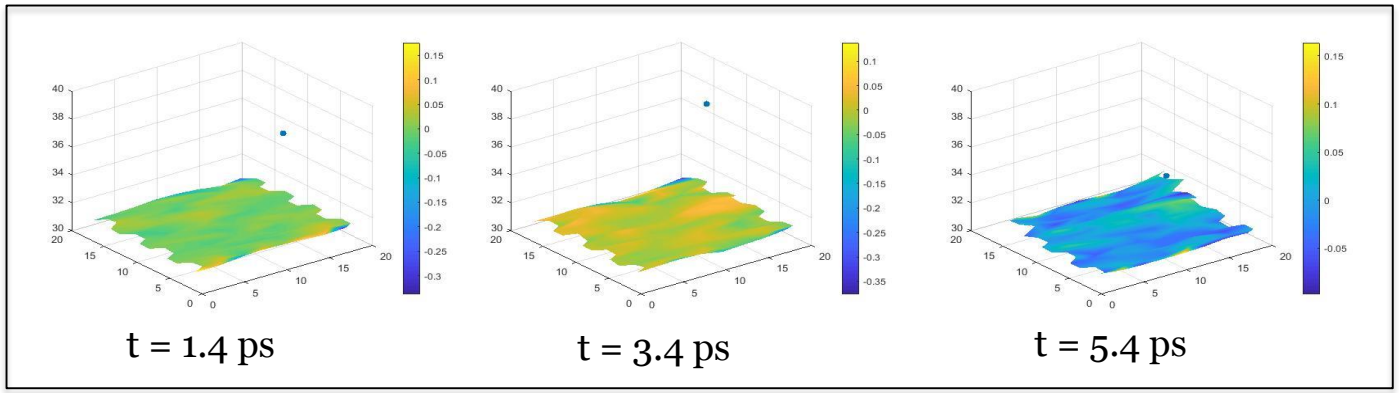

Fig 3. The evolution of the surface curvature in time due to impinging boron – three successive boron impacts are shown.

Results Cont.

- Potential barrier for boron adhering to carbon found via ReaxFF simulations
  - Barrier existence confirmed and magnitude measured using quantum chemistry (QC) methods
- QC shows barrier energy comes from altering planar sp^2 carbon atoms into non-planar sp^3 boron-carbon system
  - Corresponds to the large-scale curvature changes found using LAMMPS (Fig. 3).
- There is a threshold impact energy for boron to stick to graphite of ~ 0.5eV
- Only second barrier seen in CMD simulations – may be a result of ReaxFF parameterization

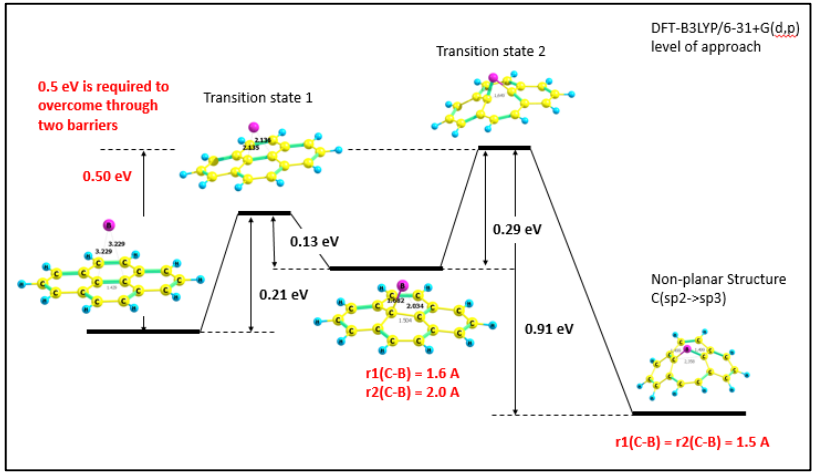

Fig 4. Diagram showing the different boron-graphene configurations with associated energy levels with each state.

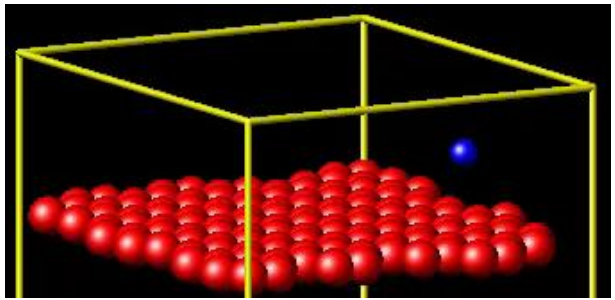

Fig 5. CMD simulation showing boron with 0.5eV boron being reflected from graphene sheet.

Conclusions and Future Work

Conclusions

- Layered substrate is important for accurately modeling surface interactions
- Surface-level thermostats needed to remove excess energy due to inefficient interlayer van der Waals interactions.
- Boron-carbon interactions influence surface topology through changes in curvature

Future Work

- Include oxygen to understand influence on boronization behavior
- Bombard boronized/oxidized graphite with D to observe sputtering/retention
- Repeat simulations with lithiumization
- Extend simulations to other PFC materials e.g. tungsten

Acknowledgement

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References

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