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Development of Machine Learned Interatomic Potentials for Modeling the Effect of Mixed Material Layers on Hydrogen Retention

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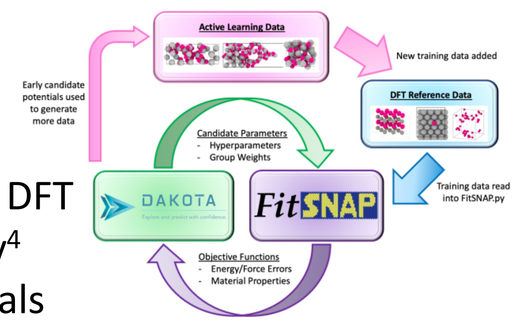
Motivation

- Divertor component will be subject to high fluxes of mixed ion species including hydrogen, helium, beryllium, and nitrogen
- Hydrogen retention in reactor components is a concern
- Experiments have shown that implantation of other plasma species in the divertor greatly affects H retention[1]
- Critical to understand how these mixed materials layers form and their effect on hydrogen diffusion, trapping, and retention

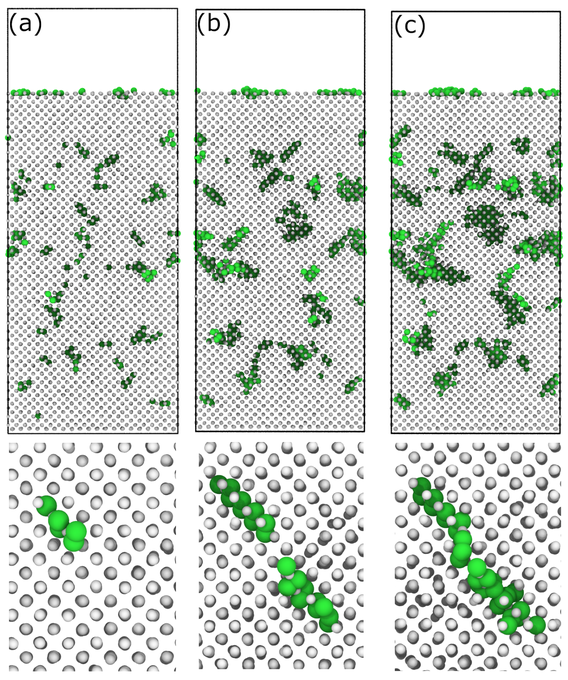
SNAP Potential Development

- Need new potentials that can capture complex chemistry at plasma-material interface
- SNAP[2,3] is a machine learned interatomic potential trained to DFT data and has improved accuracy[4] compared to traditional potentials
- Extension of W-Be[5] SNAP for H and N



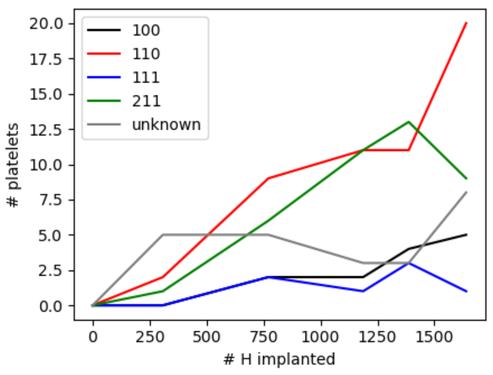
W-H

- 75 eV H implantation into (100) W at 1000 K
- SNAP predicts formation of 2D platelet structures primarily along the (110) direction

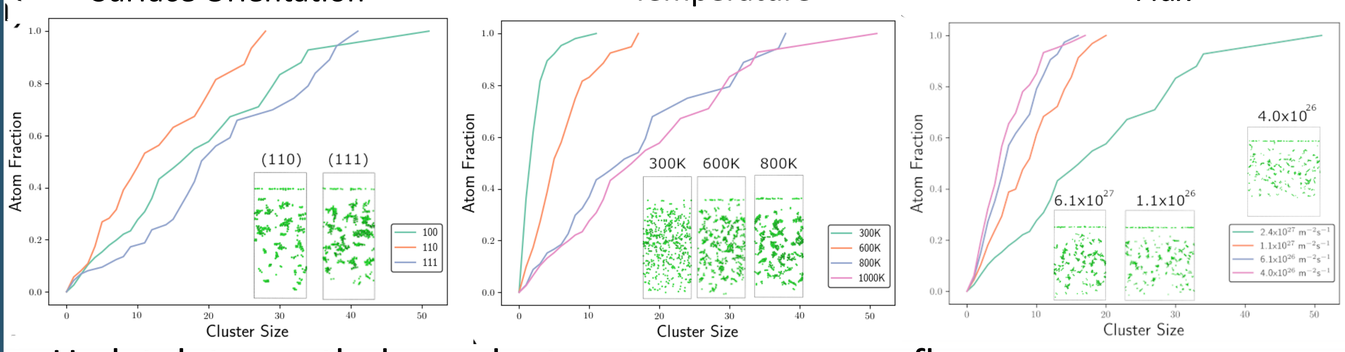


Atomistic snapshots of hydrogen (green) implantation in tungsten (grey) at (a) 5 ns, (b) 10 ns, and (c) 15 ns. Bottom images depict the growth of one platelet in the simulation.

Platelet Growth Over Time

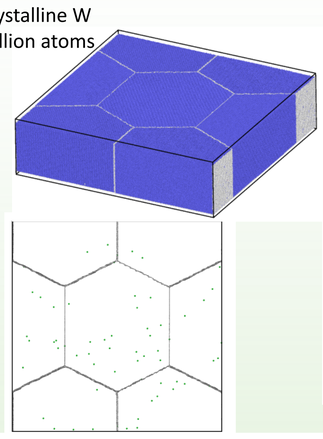


Surface Orientation | Temperature | Flux

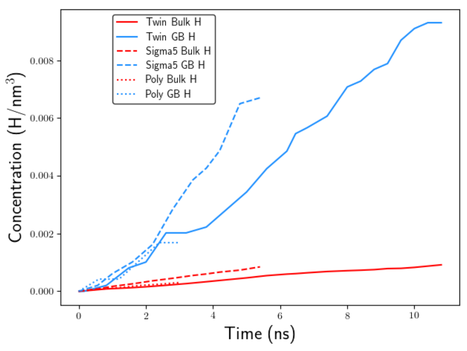


- H platelet growth dependent on temperature on flux
- Requires temperatures higher than 600 K

Polycrystalline W
~16 million atoms



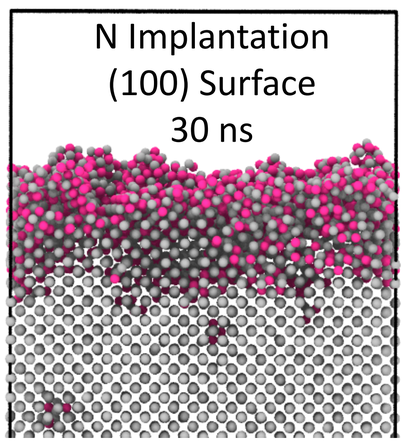
GB vs. Bulk H Concentration



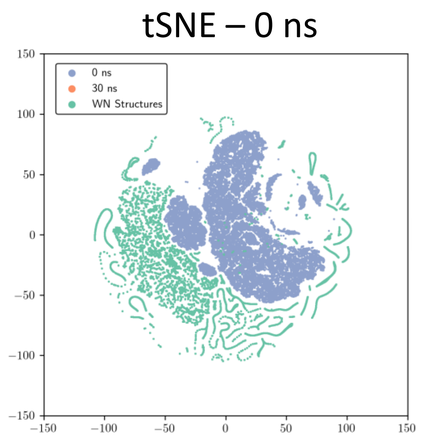
- Grain boundaries remain a strong trapping site even compared to platelets
- Higher concentrations of H found at GB compared to bulk
- Similar observations at higher H concentrations

W-N

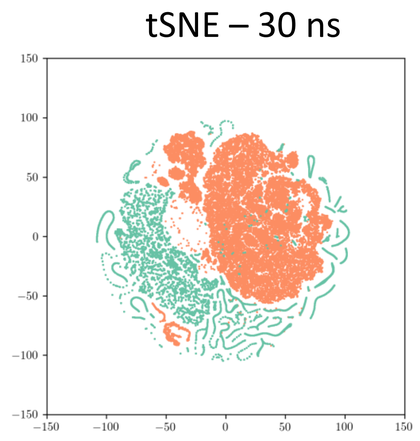
- 75 eV N implantation into (100) W surface at 1000 K
- Nitrogen remains near surface and forms a ~2 nm mixed layer
- tSNE analysis indicates shift in descriptors between 0 ns and 30 ns to more closely align with W-N structures in the training data



tSNE – 0 ns



tSNE – 30 ns

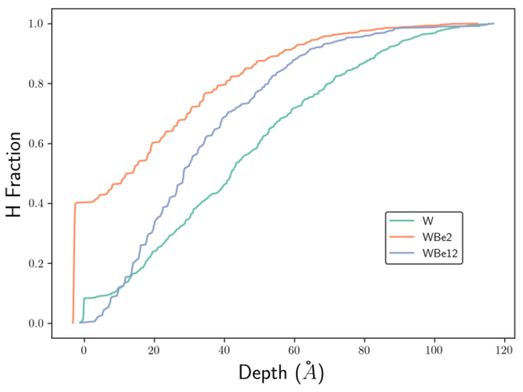


W-Be-H

- Single 60 eV H implantation in WBe_2 and WBe_{12} at 1000 K indicated high H retention and comparable, but shallower, H depth profiles

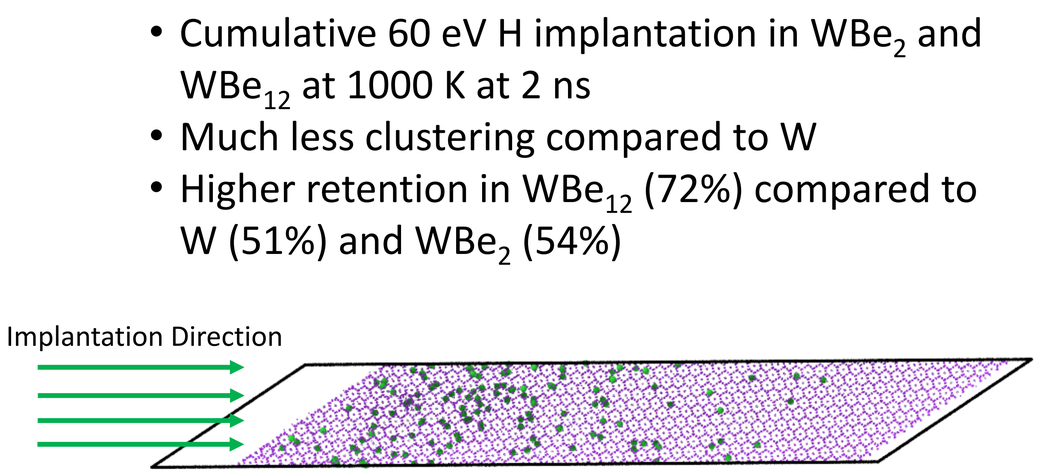
	Retention	W Sputt.	Be Sputt.
W – 60 eV	49.3	0	-
WBe_2 – 60 eV	96.1	0	0.038
WBe_{12} – 60 eV	99.1	0	0.017

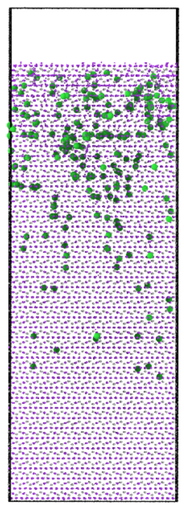
Single H Ion Implantation



- Cumulative 60 eV H implantation in WBe_2 and WBe_{12} at 1000 K at 2 ns
- Much less clustering compared to W
- Higher retention in WBe_{12} (72%) compared to W (51%) and WBe_2 (54%)

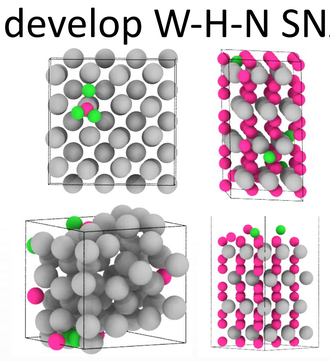
Implantation Direction





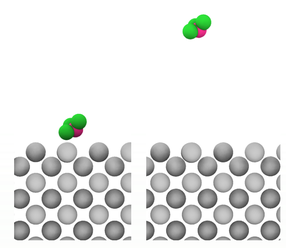
W-H-N

New efforts to develop W-H-N SNAP



Early candidate potentials predict NH_x surface binding energy

Surface Binding Energy	DFT (eV)	SNAP (eV)
NH_3	-1.05	-0.53
NH_2	-4.39	-1.44
NH	-6.6	-5.87



Conclusions

- Development of SNAP ML-IAPs for W, Be, H, and N
- SNAP predicts formation of H platelets after implantation
- N implantation results in a mixed materials layer that has structural similarities to tungsten nitrides
- W-Be intermetallics at the surface result in higher H retention particularly for WBe_{12}

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[1] Kreter, et al. Nucl. Fus.. 59, 086029 (2019)
[2] Thompson, et al. J. Comp. Phys. 285, 316-330 (2015)
[3] Rohskopf et al., Journal of Open Source Software, 8, 5118 (2023)
[4] Zuo, et al, J. Phys. Chem. A 124, 731-745 (2020)
[5] Wood, et al. Phys. Rev. B 99, 184305 (2019)