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Sandia National Laboratories

Molecular Dynamics Simulations of Hydrogen and Nitrogen Implantation in Tungsten

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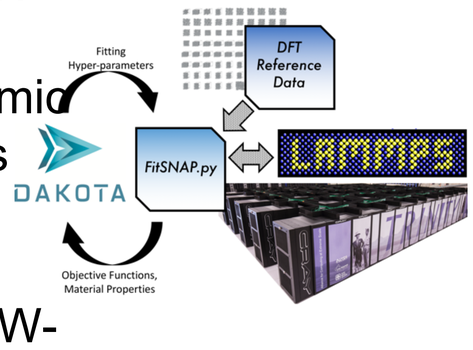
Motivation

- Divertor component will be subject to high fluxes of mixed ion species including hydrogen and nitrogen
- Hydrogen retention in reactor components is a concern and better understanding of trapping mechanisms is needed
- Experiments of nitrogen implantation in tungsten has resulted in tungsten nitride formation which increases hydrogen retention[1]
- Critical to understand how tungsten nitrides form and increase hydrogen retention

SNAP Potential Development

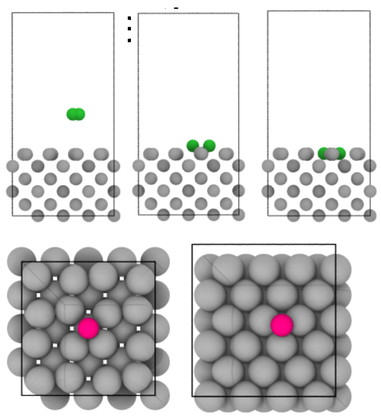
- Few existing potentials for W-H and W-N with limited accuracy
- SNAP[2] is a machine learned interatomic potential trained to DFT data and has improved accuracy[3] compared to traditional potentials
- Extension of W[4,5] SNAP to W-H and W-N



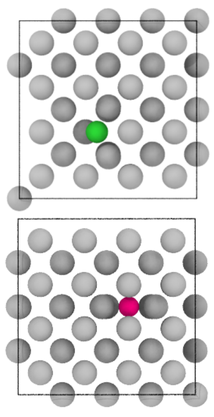
DFT Training Data

W: Grey H: Green N: Pink

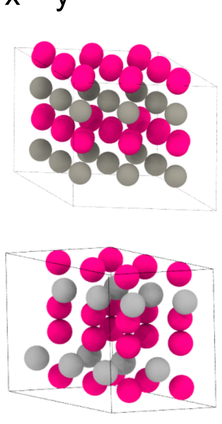
Surface



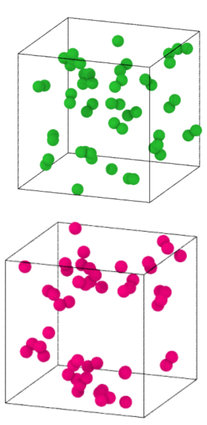
Bulk Defects



W_xN_y Structures



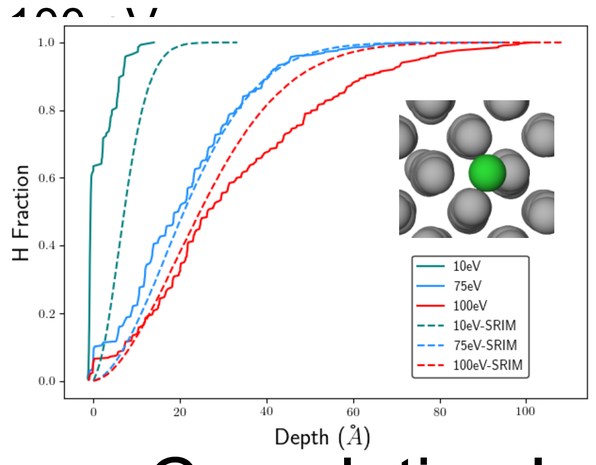
Gas



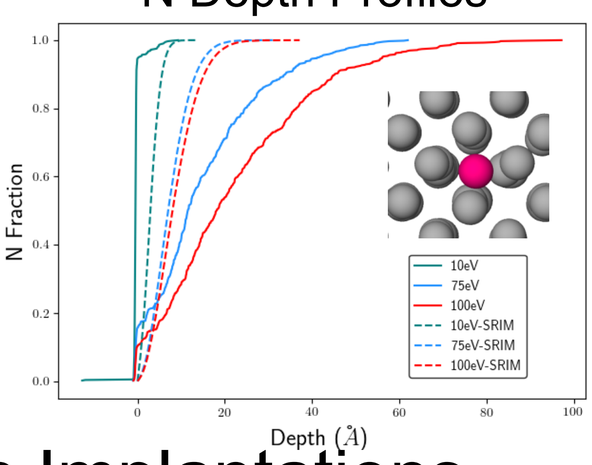
Single Ion Implantations

- Performed series of single ion implantations to assess depth profile for H and N including comparison with SRIM
- Simulations performed at 1000 K for 10 eV, 75, eV and 100 eV

H Depth Profiles



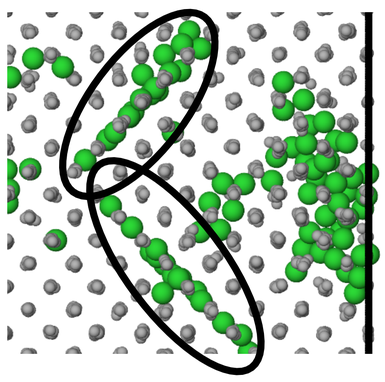
N Depth Profiles

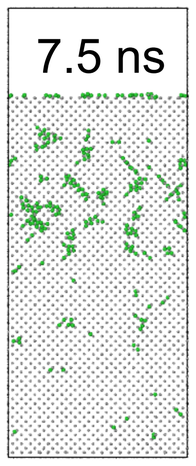


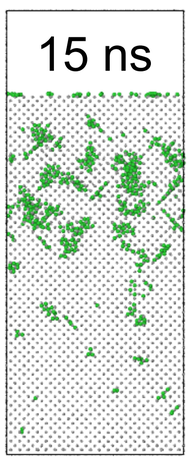
Cumulative Ion Implantations

- Performed cumulative ion implantations at 1000 K for 75 eV ion energies where ions are implanted every 10 ps

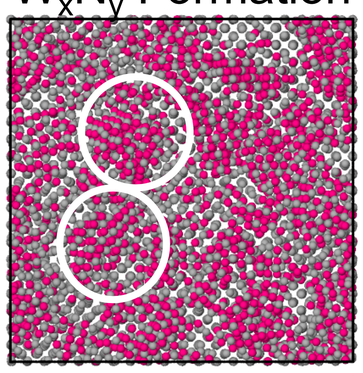
H Oriented Clusters

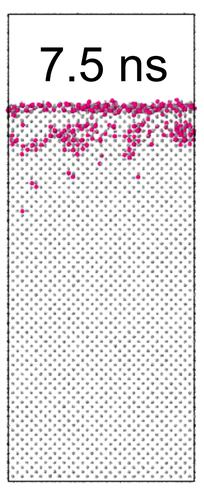


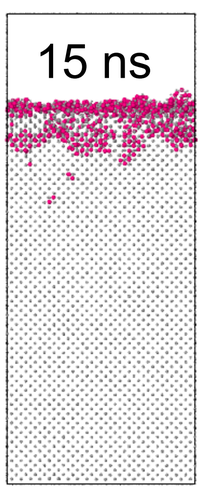




W_xN_y Formation







Fitted Properties

- SNAP can reproduce both gas-phase and condensed-phase chemical interactions
- One set of descriptors for very different atomic species

Formation Energies

H Defects	DFT (eV)	SNAP (eV)
E_f^{Tet}	0.88	2.50
E_f^{Oct}	1.26	3.24
E_f^{Sub}	4.08	5.38
E_f^{H2}	-4.74	-4.75

N Defects	DFT (eV)	SNAP (eV)
E_f^{Tet}	1.85	1.89
E_f^{Oct}	1.11	1.09
E_f^{Sub}	4.72	2.90
E_f^{N2}	-9.79	-9.47

* units in eV	P62mmc (WN_2)	P6m2 (WN_2)	NiAs (WN)	WC (WN)	$MoSi_2$ (W_2N)
DFT	-1.82	-0.91	-0.84	-0.23	-0.03
SNAP	-2.13	-1.45	-0.46	-1.16	0.36

Surface Adsorption Energies

H Ads.	DFT (eV)	SNAP (eV)
(100) Ads. Site	Bridge	Bridge
(100) Ads. Energy	-0.96	-1.57
(100) H_2 Ads. Energy	-0.80	-0.76
(110) Ads. Site	Hollow	Hollow
(110) Ads. Energy	-0.75	-0.69
(111) Ads. Site	Bridge	Bridge
(111) Ads. Energy	-0.59	-1.42

N Ads.	DFT (eV)	SNAP (eV)
(100) Ads. Site	Hollow	Hollow
(100) Ads. Energy	-3.52	-4.33
(100) N_2 Ads. Energy	-2.94	-8.63
(110) Ads. Site	Hollow	Bridge
(110) Ads. Energy	-3.59	-2.58
(111) Ads. Site	Bridge	Hollow
(111) Ads. Energy	-3.08	-3.44

- Nitrogen defects and W_xN_y energies well reproduced
- H surface properties well reproduced but tradeoff in defect energies
- N surface energetics good but wrong site predicted for some surfaces

[1] Kreter, et al. Nucl. Fus. 59, 086029 (2019)
[2] Thompson, et al. J. Comp. Phys. 285, 316-330 (2015)
[3] Zuo, et al. J. Phys. Chem. A 124, 731-745 (2020)
[4] Wood and Thompson, J. Chem. Phys. 148, 241721 (2018)
[5] Wood, et al. Phys. Rev. B 99, 184305 (2019)

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