SAND2019-2266C

Large-Scale Atomistic Simulations of Materials using SNAP Potentials

Aidan Thompson

Mitchell Wood

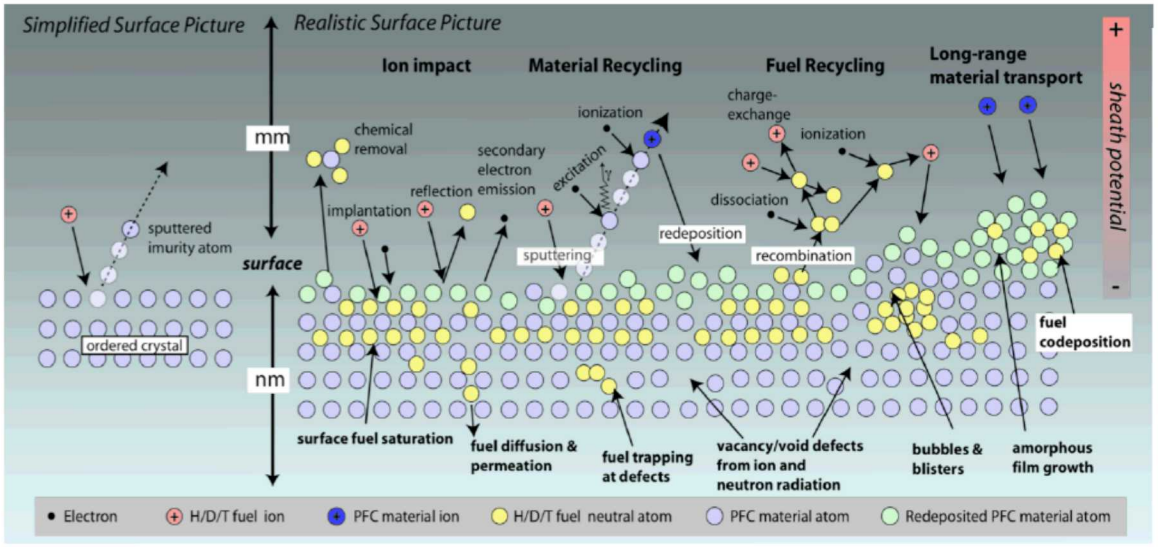
Mary Alice Cusentino

Center for Computing Research, Sandia National Laboratories

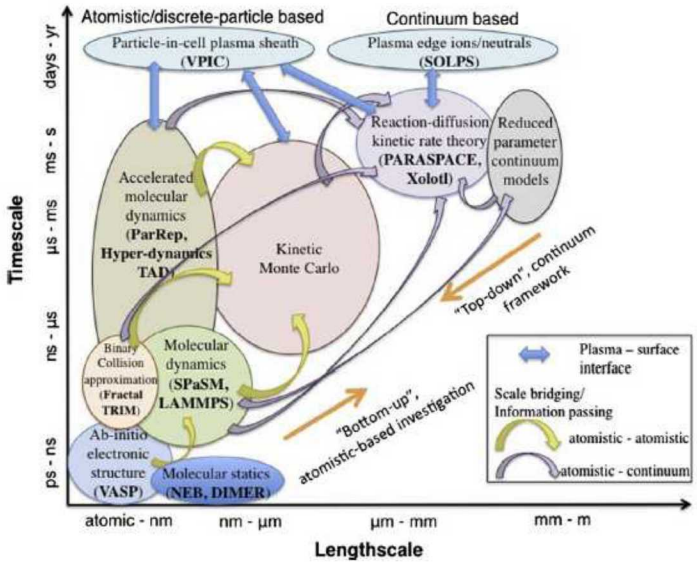
This work has been supported by the U. S. Department of Energy, Office of Science, Office of Fusion Energy Sciences, Office of Advanced Scientific Computing Research through the Scientific Discovery through Advanced Computing (SciDAC) project on Plasma-Surface Interactions.

This research used resources of the Oak Ridge Leadership Computing Facility at the Oak Ridge National Laboratory, which is supported by the Office of Science of the U.S. Department of Energy under Contract No. DE-AC05-00OR22725.

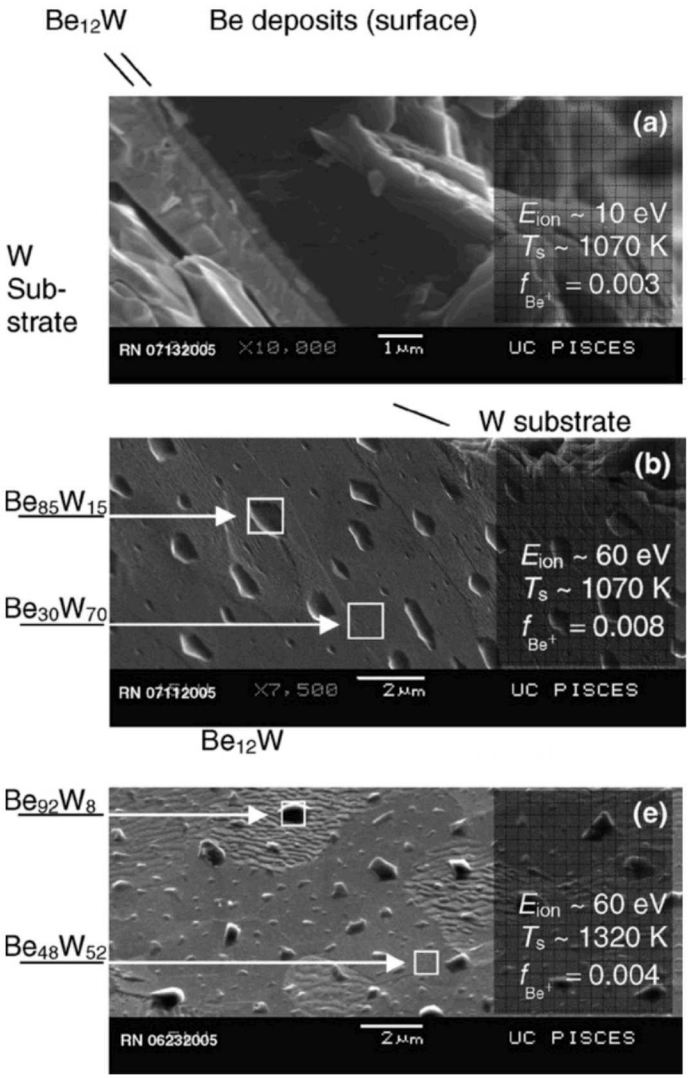
Role of Atomistic Modeling in Studying Plasma Material Interactions



Wirth, et al. MRS Bulletin 36 (2011) 216-222



Wirth, et. al. J. Nucl. Mater. 463 (2015) 30-38



Baldwin, et. al. J. Nucl. Mater. 363-365 (2007) 1179-1183

SNAP Definition and Work Flow

Model Form

- Energy of atom i expressed as a basis expansion over K components of the bispectrum (B_k^i)

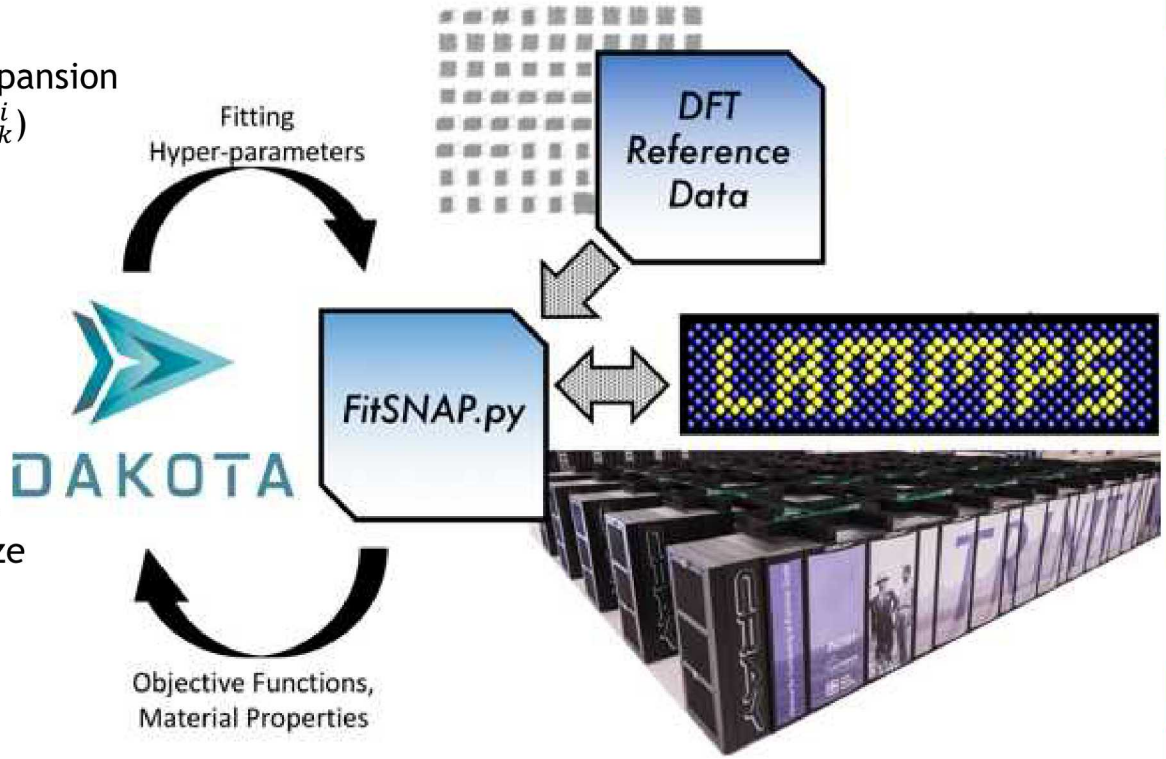
$$E_{SNAP}^i = \beta_0 + \sum_{k=1}^{K} \beta_k (B_k^i - B_{k0}^i)$$

Regression Method

- β vector fully describes a SNAP potential
- Decouples MD speed from training set size

$$\min(||\mathbf{w} \cdot D\boldsymbol{\beta} - T||^2 - \gamma_n \, ||\boldsymbol{\beta}||^n)$$

Weights Set of Descriptors DFT Training

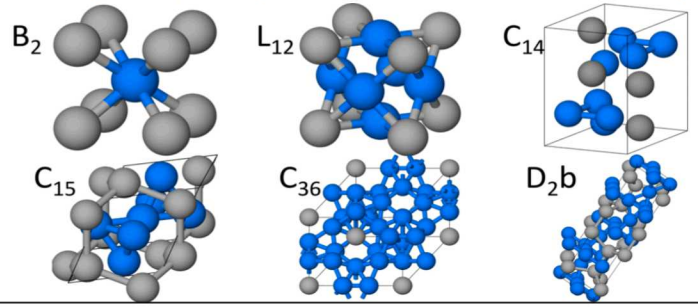


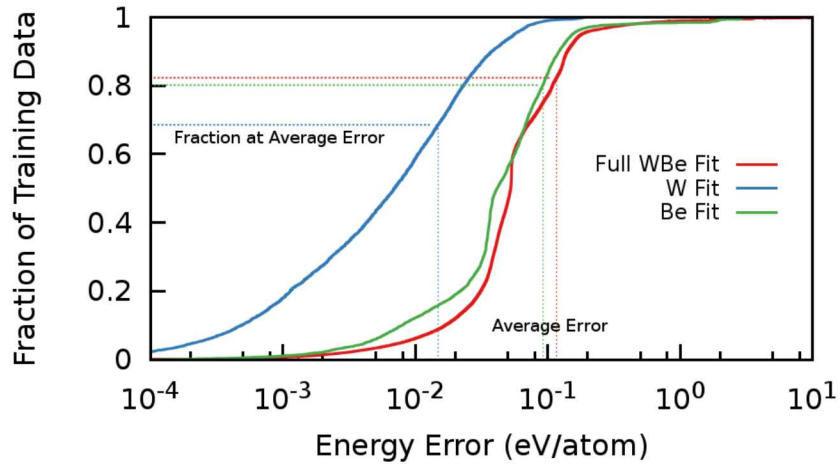
Tungsten-Beryllium SNAP Fitting

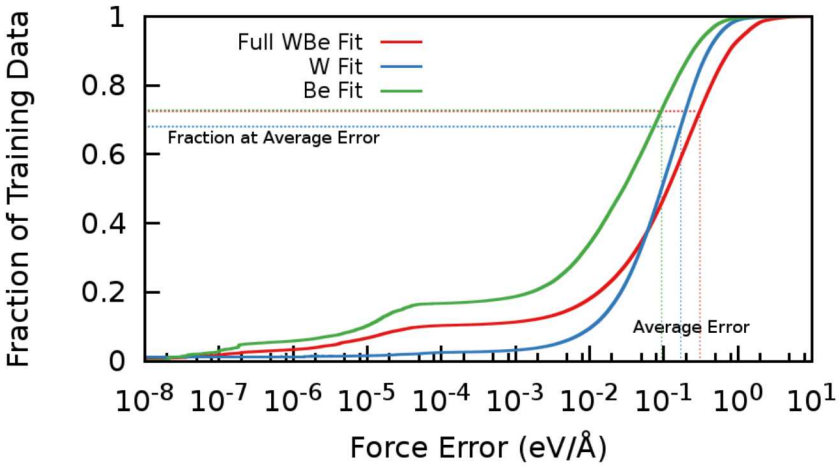
- Initially fit SNAP potential for pure elements
- Making a multi-element SNAP potential does sacrifice some accuracy from either pure component fit.
- Training set includes W-Be intermetallic structures

Description	N_E	N_F	σ_E	σ_F
W-Be:				
Elastic Deform†	3946	68040	$\mathbf{3 \cdot 10^5}$	$2 \cdot 10^3$
Equation of State†	1113	39627	$2 \cdot 10^5$	$4 \cdot 10^4$
DFT-MD†	3360	497124	$7 \cdot 10^4$	$6 \cdot 10^2$
Surface Adhesion	381	112527	$2 \cdot 10^4$	$\mathbf{9 \cdot 10^4}$

† Multiple crystal phases included in this group:

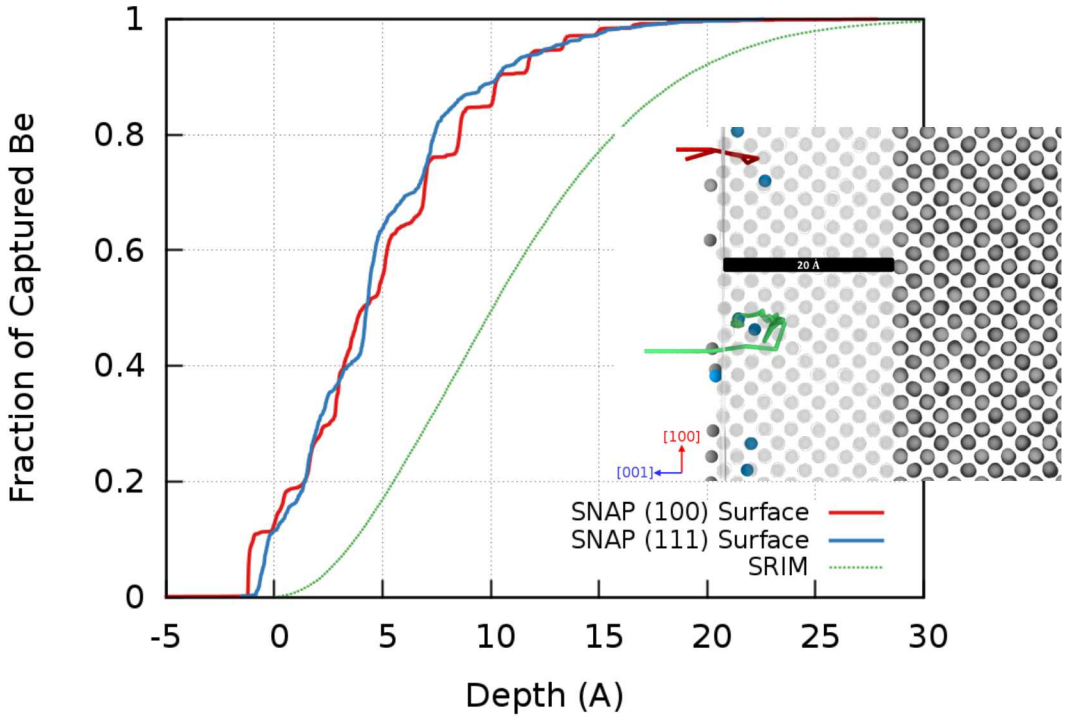






Extrapolation Testing – Single Implantation Simulations

- Single implantations of 75 eV Be in W
- MD depth profile is more shallow than binary collision models predict
- Capture rate is lower than BC model at 40% (versus 60%)
- Improvement in defect formation energies

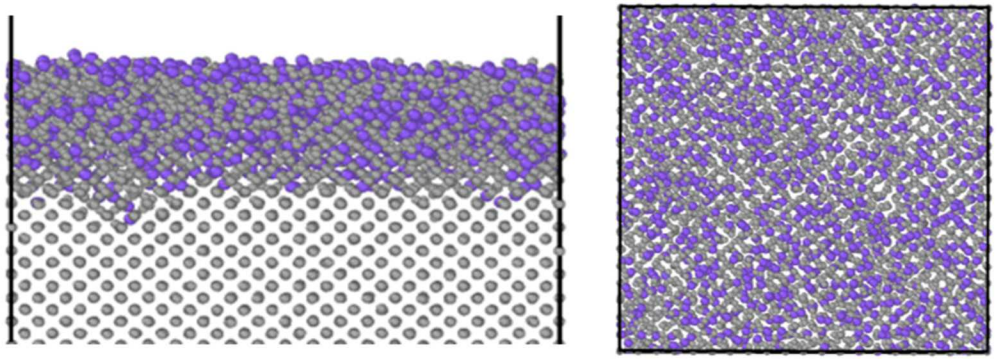


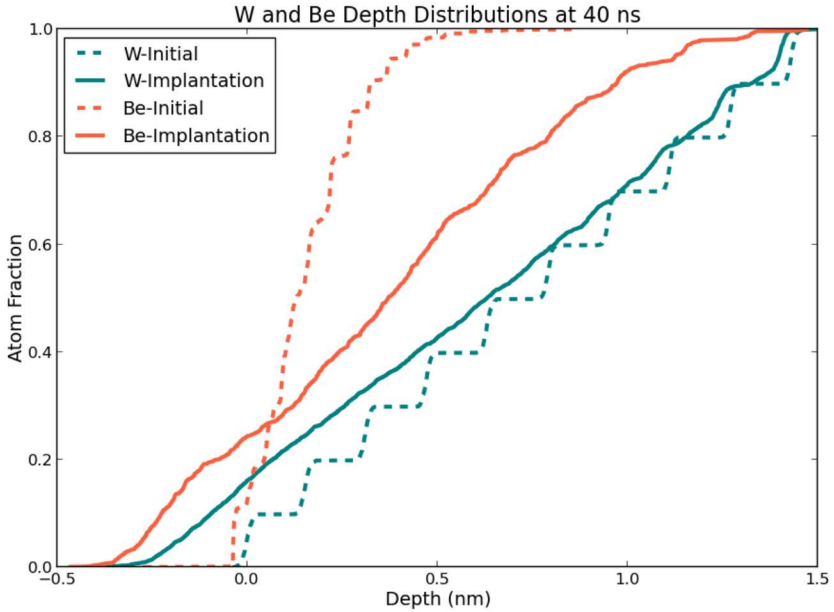
Defect Type	Percent of Implanted Be (100) Surface	(111) Surface
[111] Dumbbell	41.2	23.9
Substitution	22.2	34.6
[100] Surf. Hollow Site	12.3	8.3
Tetrahedral Interstitial	10.4	12.4
[110] Dumbbell	8.4	11.3
Octahedral Interstitial	5.3	4.1
Other	0.4	2.8
Surf. Bridge Site	0.03	2.6

Defect Type	Formation Energy (eV) DFT	SNAP	BOP
[111] Dumbbell	4.30	3.66	0.67
Substitution	3.11	3.29	-2.00
[100] Surf. Hollow Site	-1.05	-1.39	-3.52
Tetrahedral Interstitial	4.13	4.20	-0.28
[110] Dumbbell	4.86	4.29	-0.03
Octahedral Interstitial	3.00	5.11	0.34
[100] Surf. Bridge Site	1.01	0.44	-1.30

Cumulative Energetic Be Implantation in W

4000 inserted Be atoms, 1.1 x 10^{20} m^{-2}
35% Retention



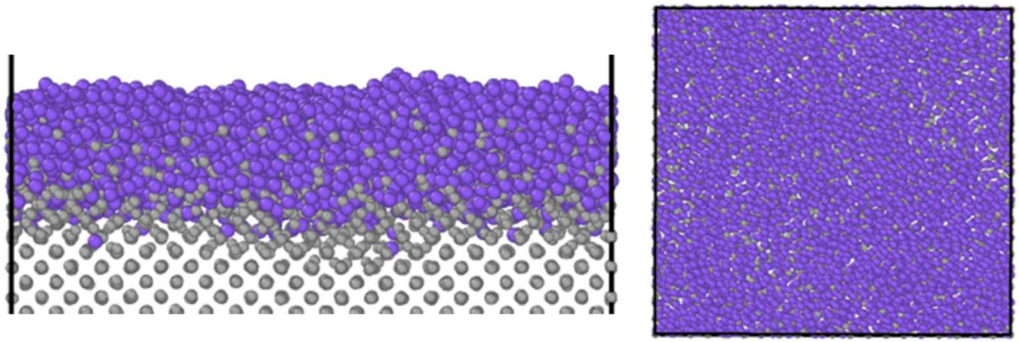


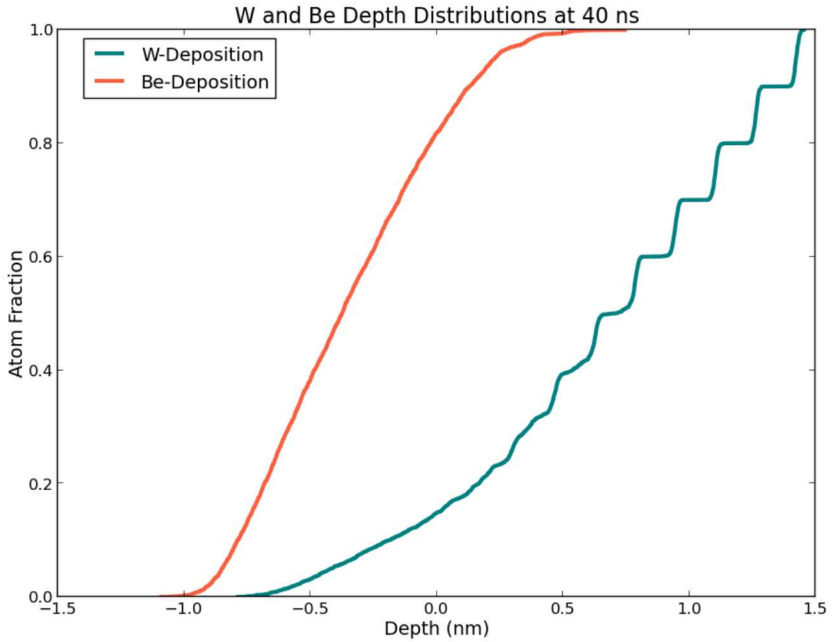
Purple: Beryllium
Gray: Tungsten

- 75 eV Be implanted every 10 ps
- 1000 K, (100) surface, 6 nm x 6 nm x 12 nm box
- Initially Be implants and resides in W as <111> dumbbell or substitutional defects
- Amorphous layer forms 1.5 nm into surface and 0.3 nm above surface
- W depth profile indicates loss of crystal structure at higher fluences
- Be depth profile is deeper than expected based on initial implantation depth

Cumulative Be Athermal Deposition on W Surface

4000 inserted Be atoms, 1.1 x 10^{20} m^{-2}



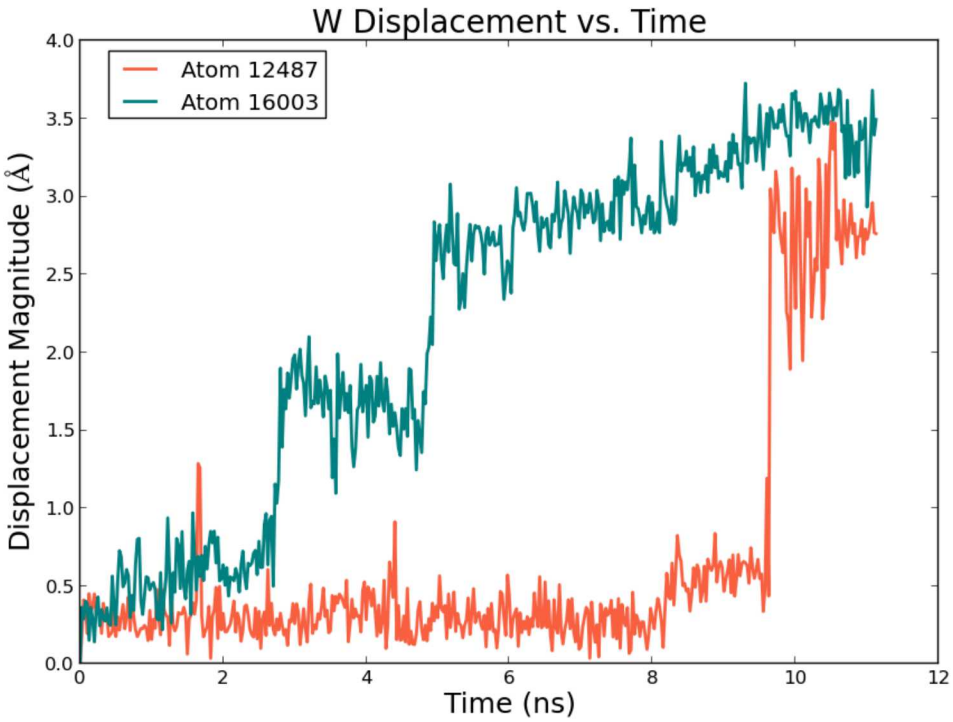


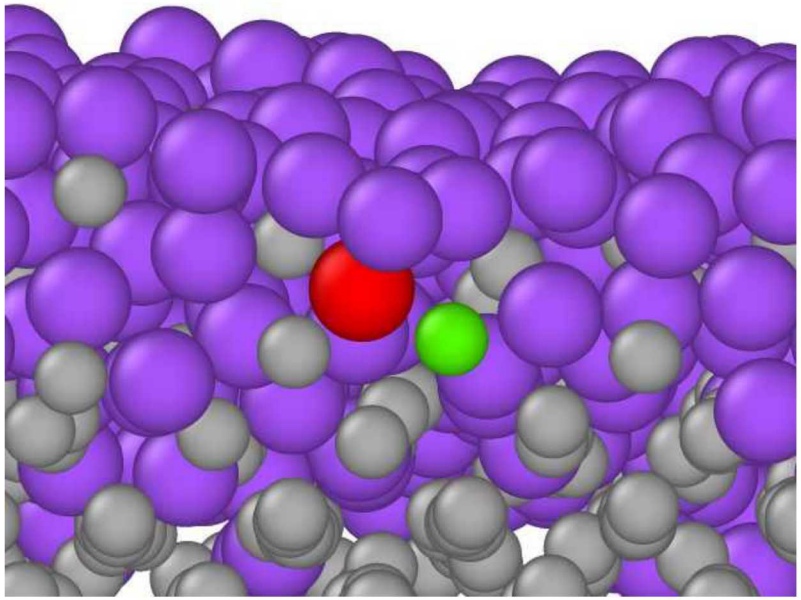
Purple: Beryllium
Gray: Tungsten

- Be randomly placed on surface every 10 ps with zero energy
- Initially Be resides at hollow sites
- Be begins to exchange with tungsten once hollow sites fill up
- Similar amorphous layer forms at higher fluences
- Thicker layer that extends from 0.5 nm below surface to 1 above surface
- Be remains near surface
- Almost 20% of W in the first 1.5 nm is now located above the original surface

Exchange Mechanism with Beryllium

Red: Be Exchanged
Green: W Exchanged
Purple: Be
Gray: W





- Clear jumps in tungsten displacement are exchanges with beryllium
- Low tungsten diffusion outside beryllium exchanges

Summary

- We have developed a machine learned SNAP potential for studying W-Be plasma material interactions
- The SNAP potential well reproduces both W and Be as well as W-Be intermetallic properties and improves upon existing potentials for parameters most relevant to radiation damage modeling
- We have performed large simulations of cumulative Be implantation or deposition on tungsten
- An amorphous layer of mixed W-Be has been observed which may be a pre-cursor to intermetallic formation
- An exchange mechanism allows tungsten to migrate into the surface amorphous layer
- This potential will be extending to include both hydrogen and helium