Sandia National Laboratories

SAND2019-15078D

Machine Learned Interatomic Potentials for Studying Plasma Material Interactions

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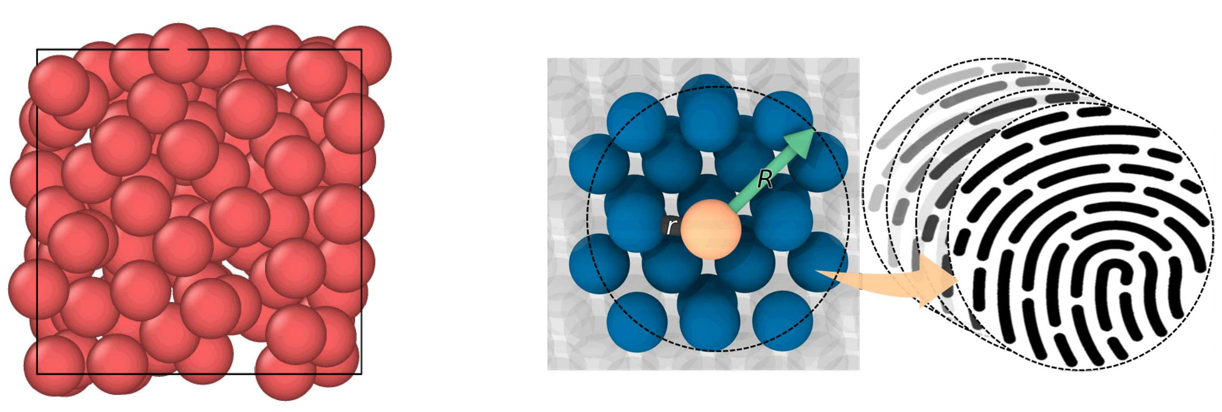
Modeling of Plasma Material Interactions

- Many complex interactions occurring at the interface between fusion reactor components (W, Be) and plasma (H, He, Be, N) leading to microstructural changes of material components
- Molecular Dynamics (MD) provides insight into atomistic processes and mechanisms not accessible by experiments but accuracy is limited by interatomic potential
- Machine learned interatomic potentials (ML-IAP) have shown increased accuracy compared to traditional physics based potentials
- W-Be is a good candidate material for ML-IAP development due to current lack of interatomic potentials to study W-Be plasma material interactions

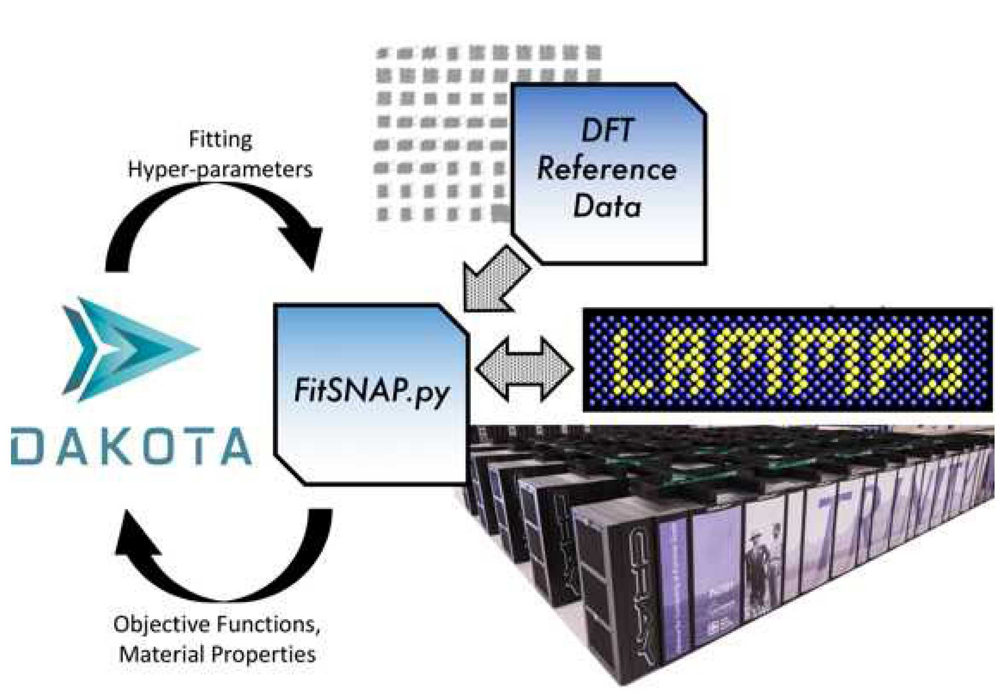
Spectral Neighbor Analysis Potential (SNAP)



$$E^{SNAP} = \sum_{i=1}^{N} E_i^{SNAP} + \sum_{j<i}^{N} \phi_{ij}^{rep}(r_{ij})$$

$$E_i^{SNAP} = \beta_0 + \sum_{k \in \{J<J_{max}\}} \beta_k B_k^i$$

Quantum accurate data for energy/forces and atomic positions → Geometric descriptors of atomic environments → Energy as a function of geometric descriptors



- Generate DFT training set
- FitSNAP generates bispectrum components using LAMMPS and performs linear regression to solve for β coefficients
- DAKOTA performs genetic algorithm to select hyper parameters and group weights

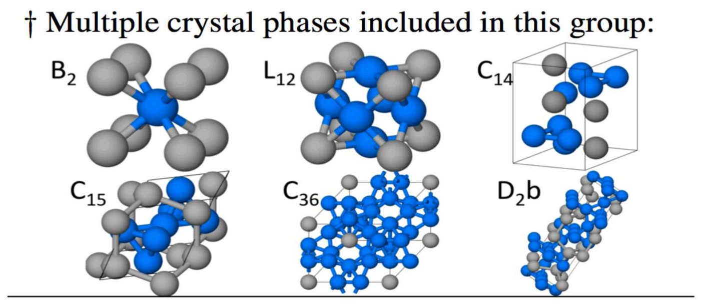
W-Be Fitting

- ~25,000 W, Be, and W-Be configurations
- Average energy and force errors of 0.12 eV/atom and 0.31 eV/Å respectively
- Potential well reproduces W and Be properties like elastic constants and self-interstitial defect formation energies

W-Be Intermetallic Training Data

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:



Beryllium Implantation in Tungsten

- MD simulations of Be 75 eV implantation and athermal deposition to study formation of W-Be intermetallics observed in experiments

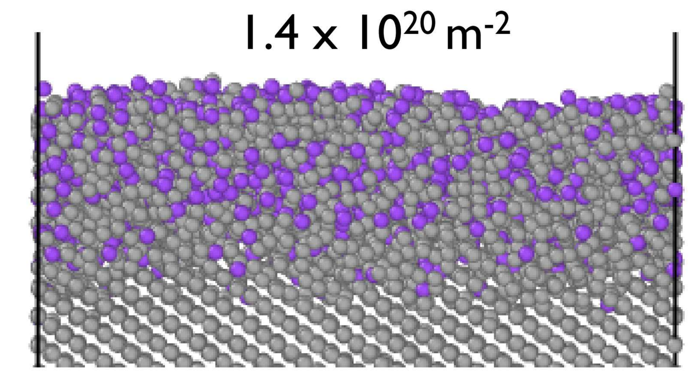
(1) Formation of mixed W-Be amorphous layer

Purple: Be Grey: W

5000 inserted Be atoms

50 ns

1.4×10^{20} m^{-2}

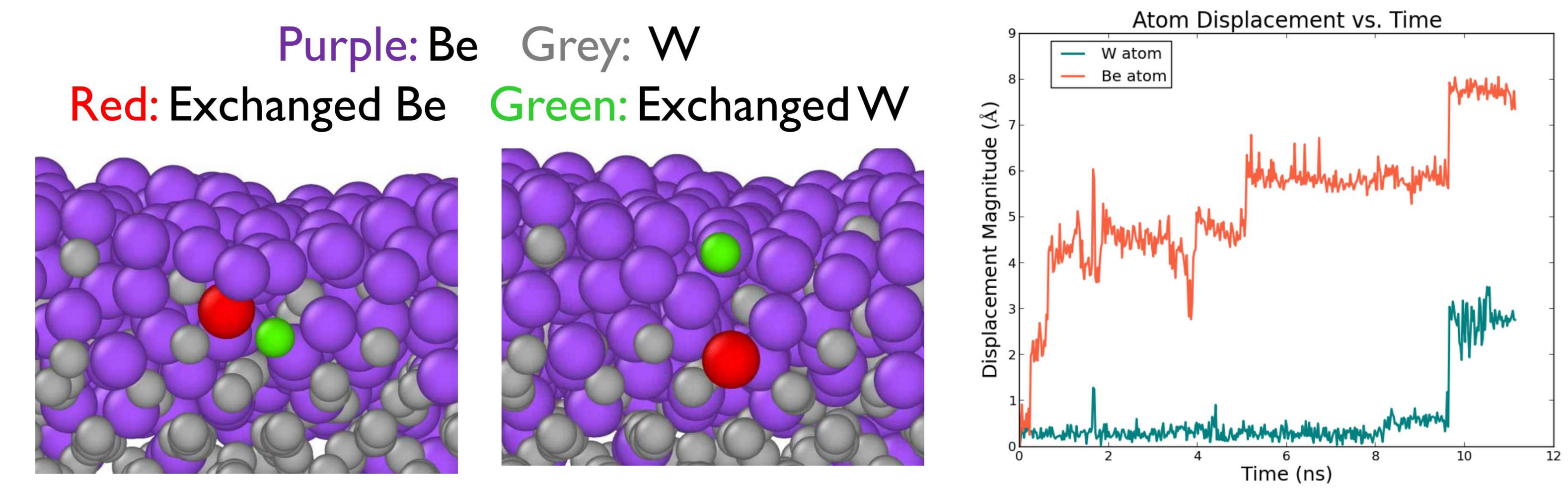


- Mixed layer forms that is limited to first 2 nm of surface
- No penetration of Be into W bulk

(2) Exchange Mechanism allows for intermixing

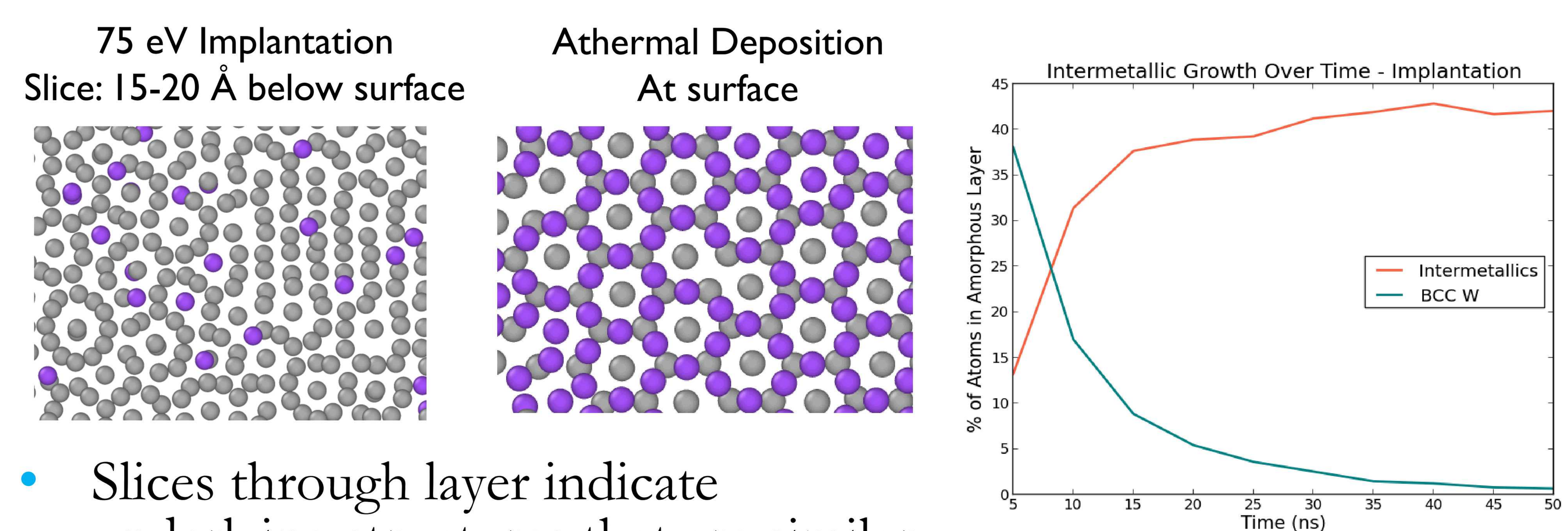
Purple: Be Grey: W

Red: Exchanged Be Green: Exchanged W



- Be exchanges with W to allow for both intermixing and W migration into mixed surface layer

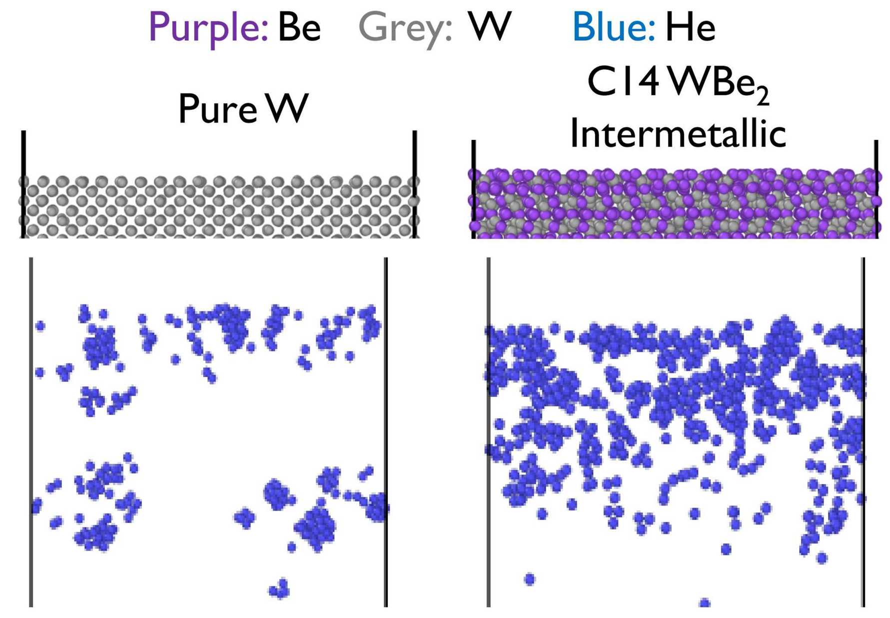
(3) Intermetallics observed within amorphous layer



- Slices through layer indicate underlying structures that are similar to expected intermetallics

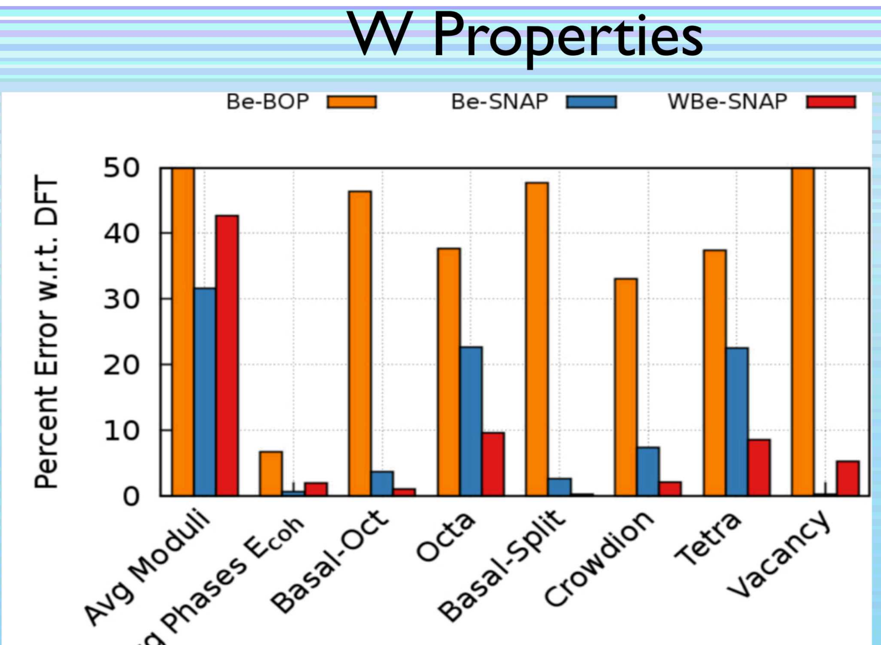
(4) Be modifies He bubble growth in W

Purple: Be Grey: W Blue: He

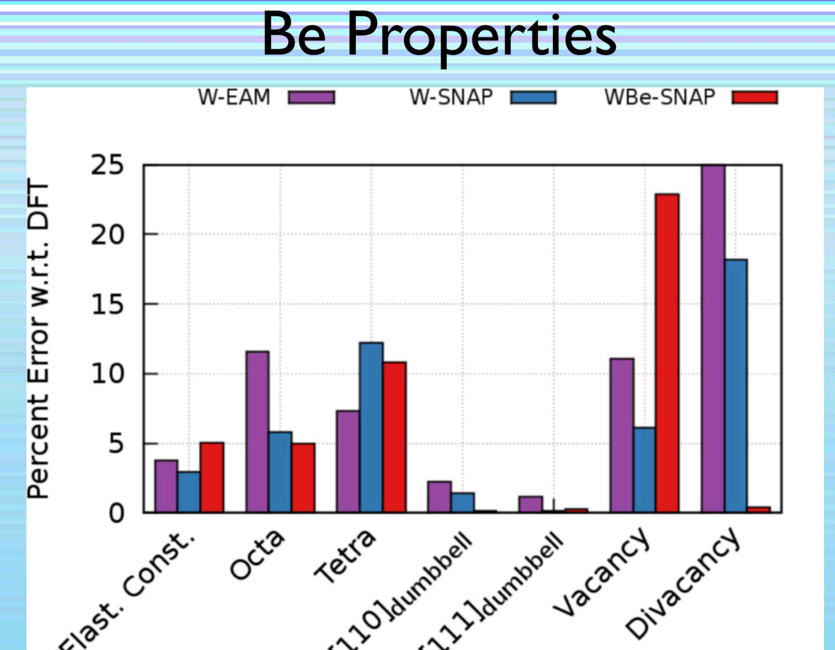


- Subsequent He implantation into W-Be samples
- Higher He retention, smaller He bubbles, and shallower He depth profile when Be is present
- Presence of Be may further affect He bubble growth process and possibly He fuzz growth

W Properties



Be Properties

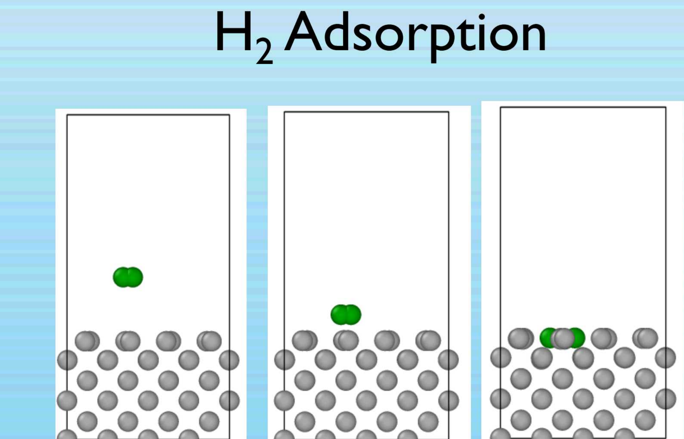


SNAP: M.A. Wood, et al., Phys. Rev. B 99 (2019) 184305
BOP: C. Bjorkas, et al., J. Phys.: Condens. Matter 22 (2010) 352206

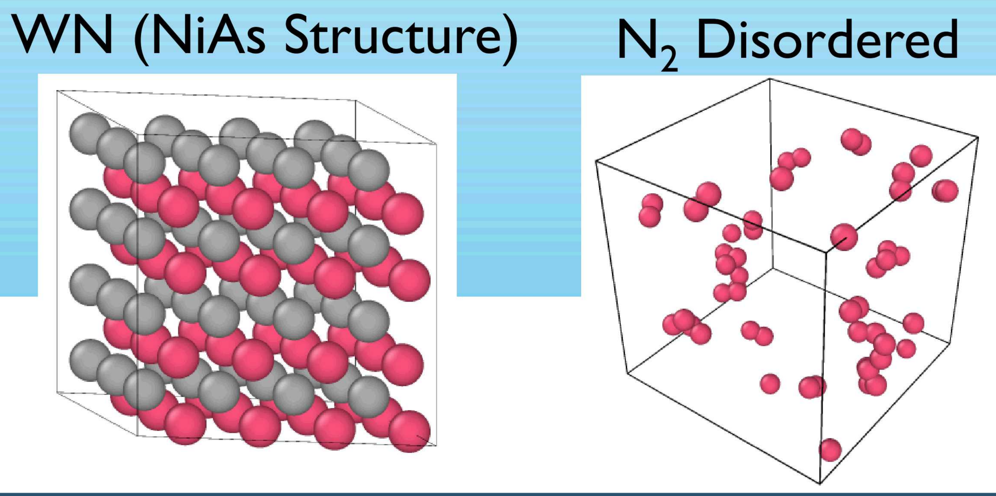
Extending SNAP to W-Be-H-N

- Interest in studying effects of Be and N on H retention
- Additional training data for new elements needed and fitting currently in progress

H_2 Adsorption



WN (NiAs Structure) N_2 Disordered



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EXASCALE COMPUTING PROJECT

SciDAC4-PSI2

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