Machine Learned Interatomic Potentials for Modeling Plasma Material Interactions

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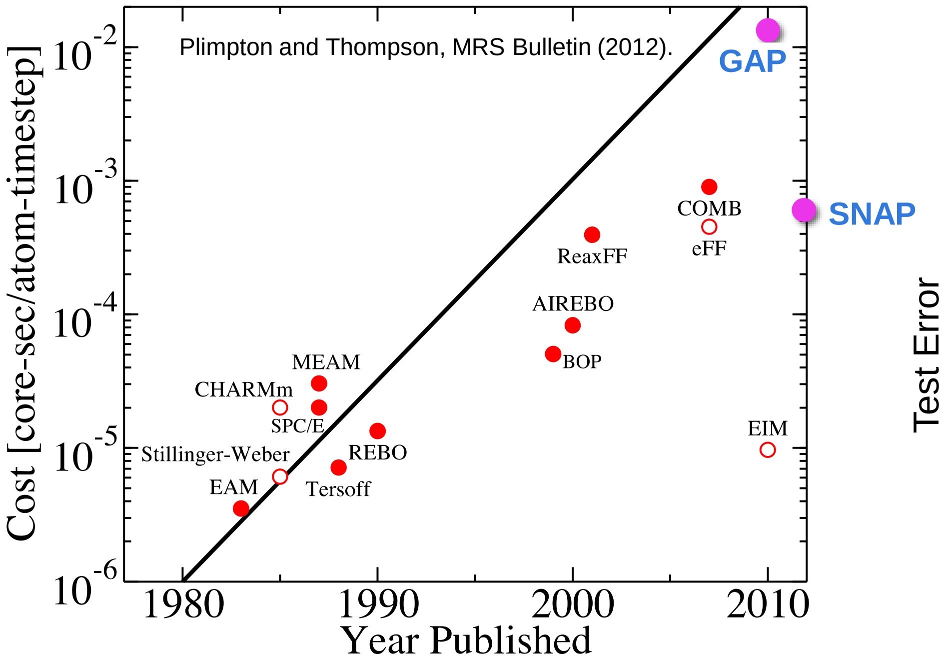
Evolution of Interatomic Potentials

Twobody (B.C.)
Lennard-Jones, Hard Sphere, Coulomb, Bonded

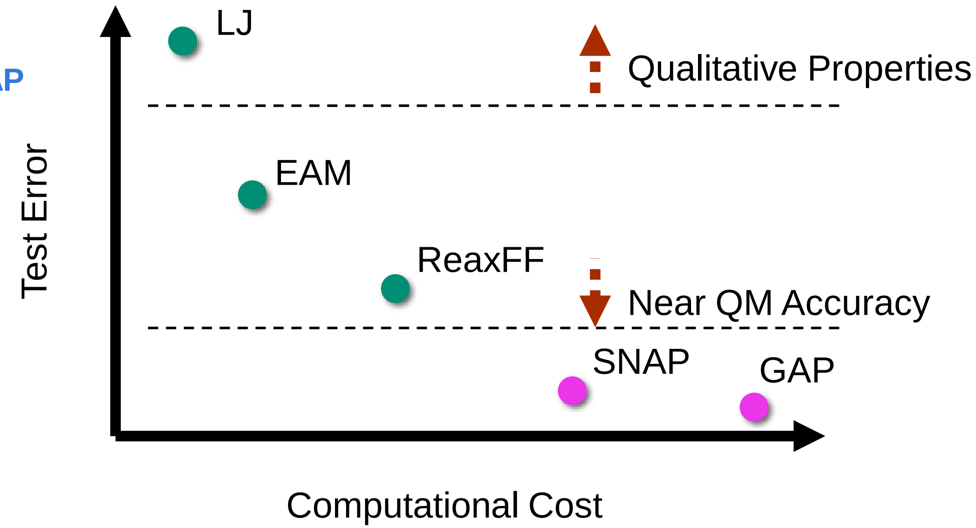
Manybody (1980s)
Stillinger-Weber, Tersoff, Embedded Atom Method

Advanced (90s-2000s)
REBO, BOP, COMB, ReaxFF

Machine Learning (2010s)
NNP, GAP, SNAP, ChIMES, MTP, Deep NNs…



- **Resources are limited, which is your best choice?**



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)

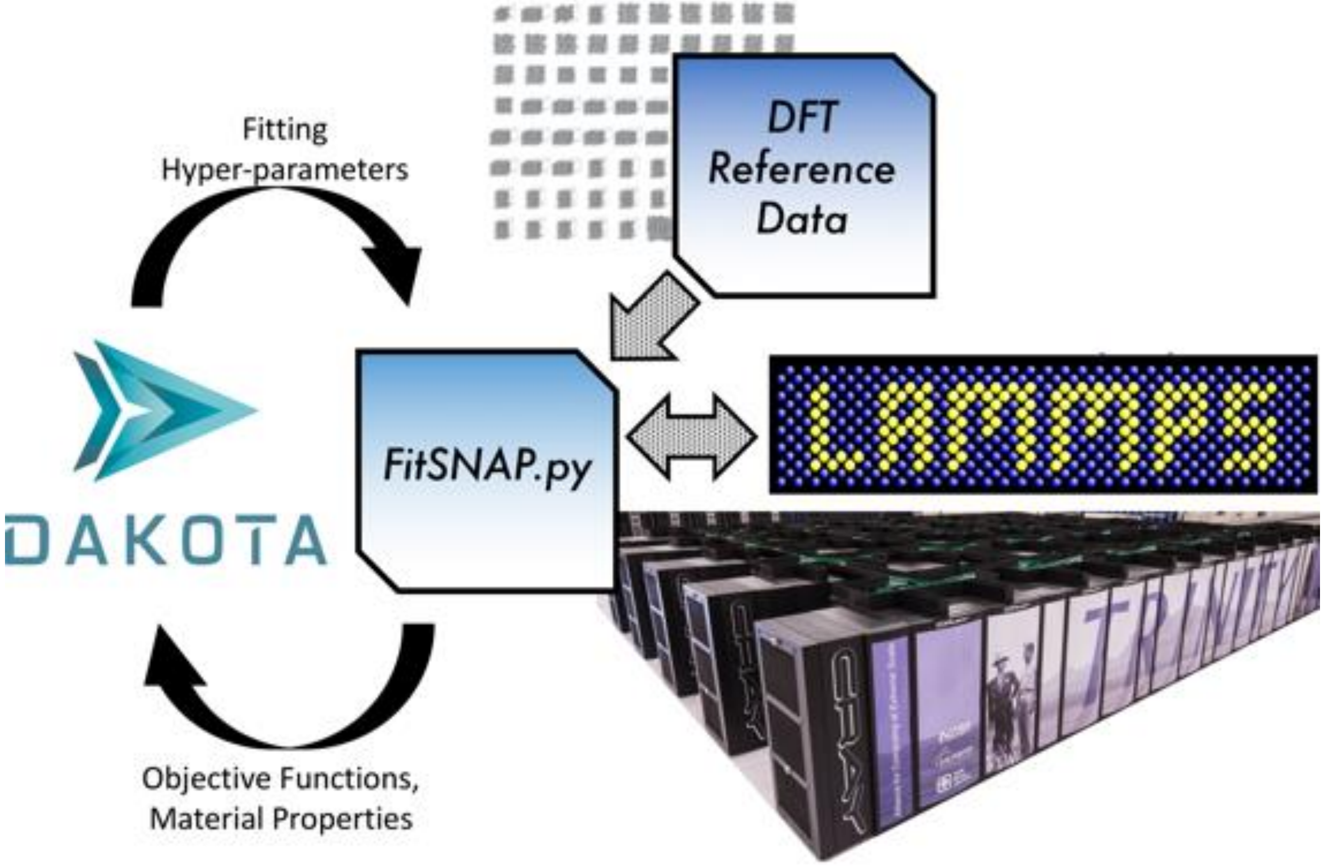
$$E^i_{SNAP} = \beta_0 + \sum_{k=1}^{K} \beta_k (B_k^i - B_{k0}^i)$$

Regression Method

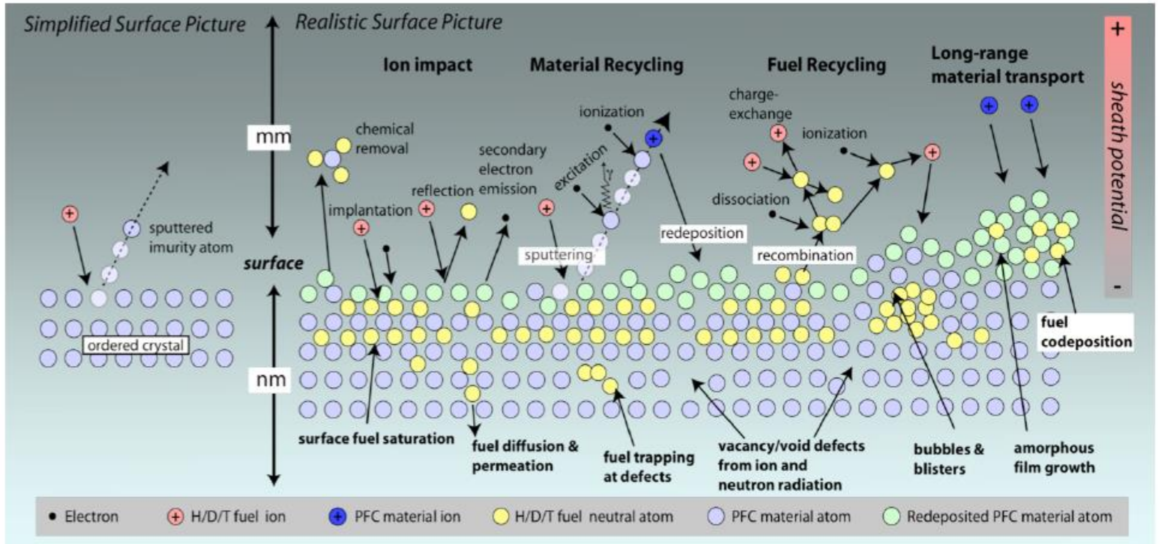
- β vector fully describes a SNAP potential
- Decouples MD speed from training set size

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

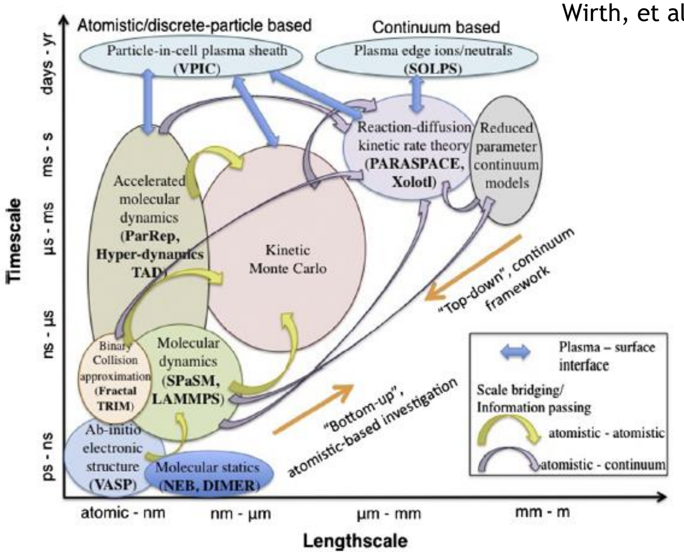
Weights   Set of Descriptors   DFT Training



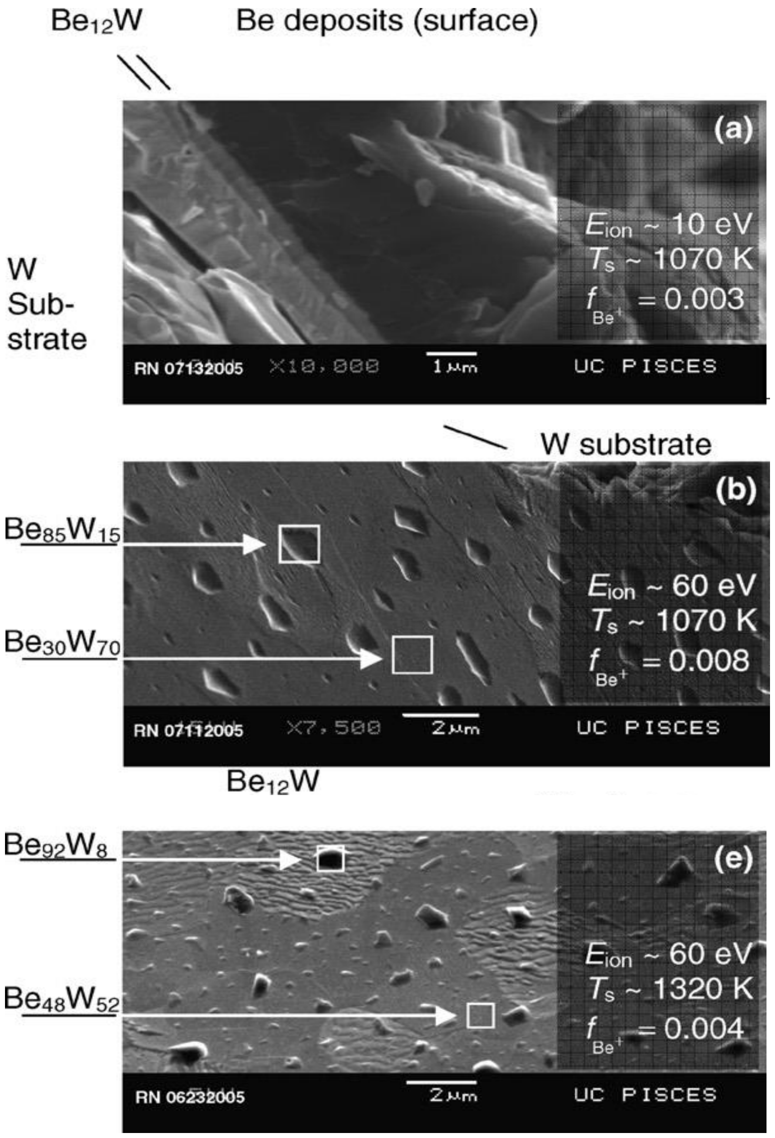
Role of Atomistic Modeling in Studying Plasma Material Interactions



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



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



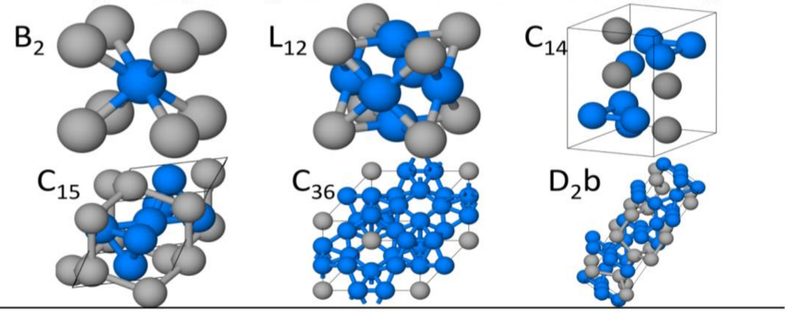
Baldwin, et. al. J. Nucl. Mater. 363-365 (2007) 1179-1183

Tungsten-Beryllium SNAP Fitting

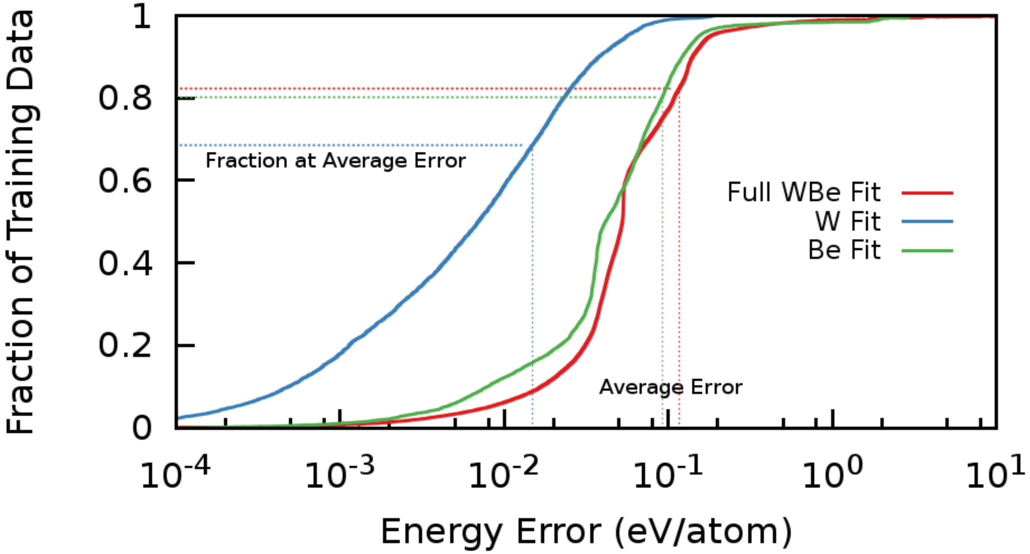
- Initially fit SNAP potential for pure elements
- Making a multi-element SNAP potential does sacrifice some accuracy from either pure component fit.
- Training set includes W-Be intermetallic structures

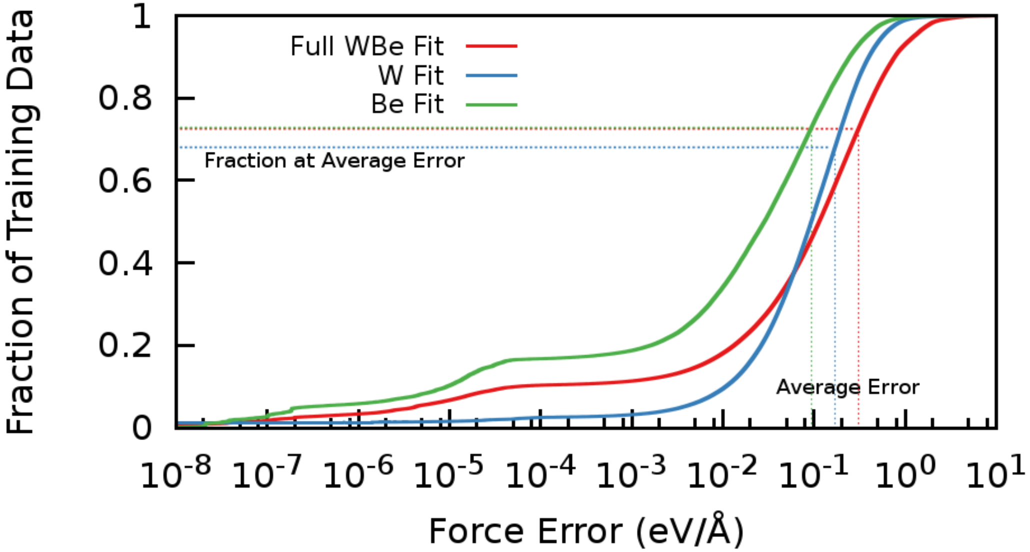
Description	N_E	N_F	σ_E	σ_F
W-Be:				
Elastic Deform†	3946	68040	$\mathbf{3 \cdot 10^5}$	$2 \cdot 10^3$
Equation of State†	1113	39627	$2 \cdot 10^5$	$4 \cdot 10^4$
DFT-MD†	3360	497124	$7 \cdot 10^4$	$6 \cdot 10^2$
Surface Adhesion	381	112527	$2 \cdot 10^4$	$\mathbf{9 \cdot 10^4}$

† Multiple crystal phases included in this group:



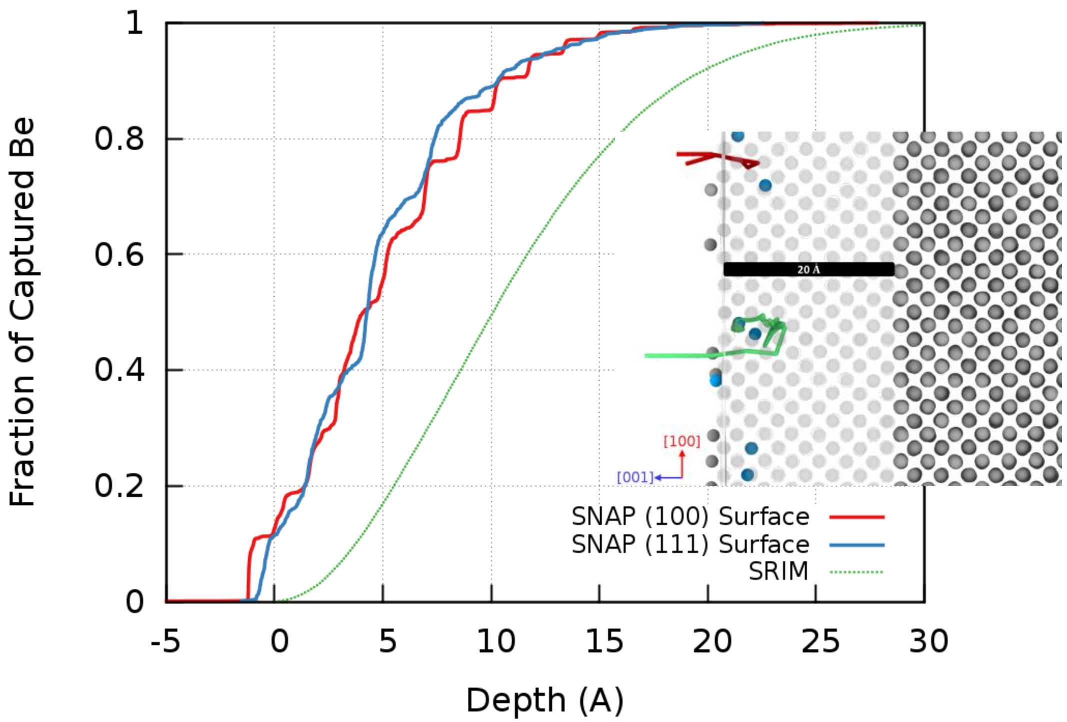
M. A. Wood, et al., Phys. Rev. B 99, 184305





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	Percent of Implanted Be (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 statistics match formation energies

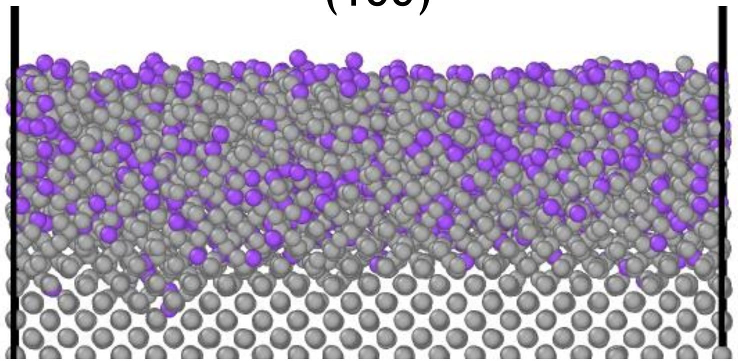
Defect Type	Formation Energy (eV) DFT	SNAP	BOP
[111] Dumbbell	4.30	3.66	0.67
Substitution	3.11	3.29	-2.00
[100] Surf. Hollow Site	-1.05	-1.39	-3.52
Tetrahedral Interstitial	4.13	4.20	-0.28
[110] Dumbbell	4.86	4.29	-0.03
Octahedral Interstitial	3.00	5.11	0.34
[100] Surf. Bridge Site	1.01	0.44	-1.30

M. A. Wood, et al., Phys. Rev. B 99, 184305

Cumulative Energetic Be Implantation in W

5000 inserted Be atoms
50 ns
1.1 x 10^{20} m^{-2}

(100)



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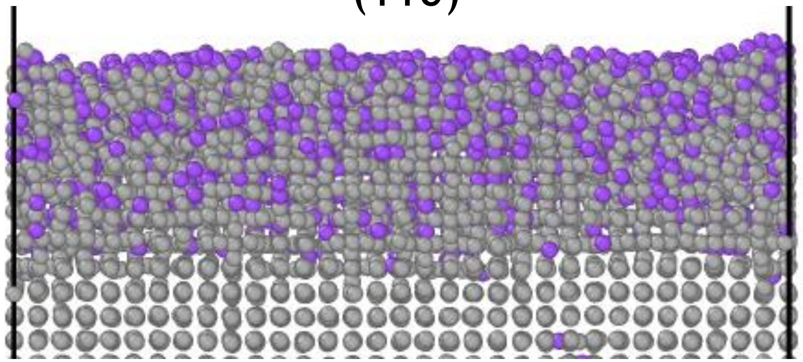

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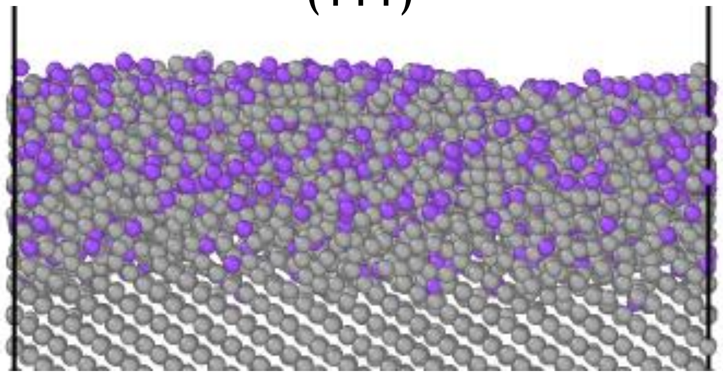
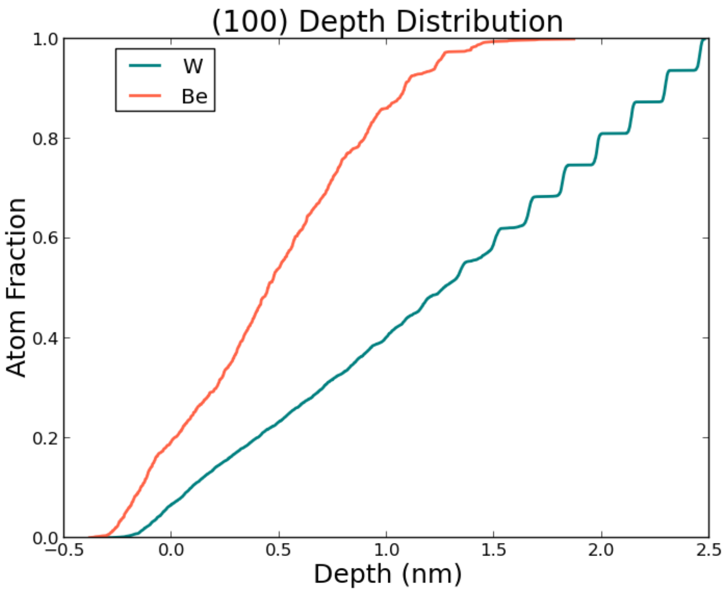
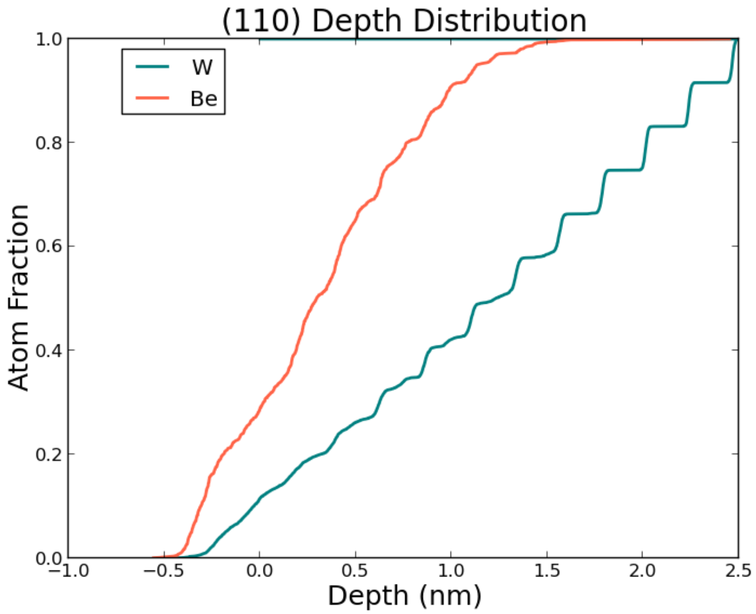
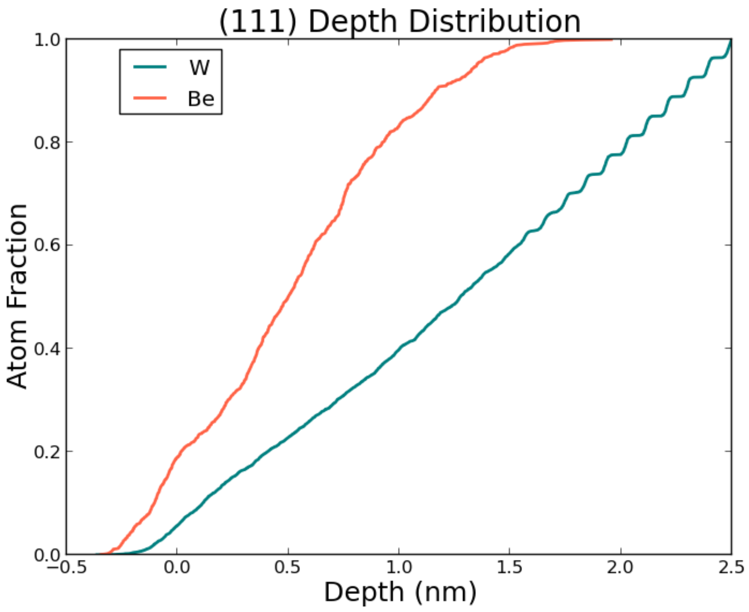


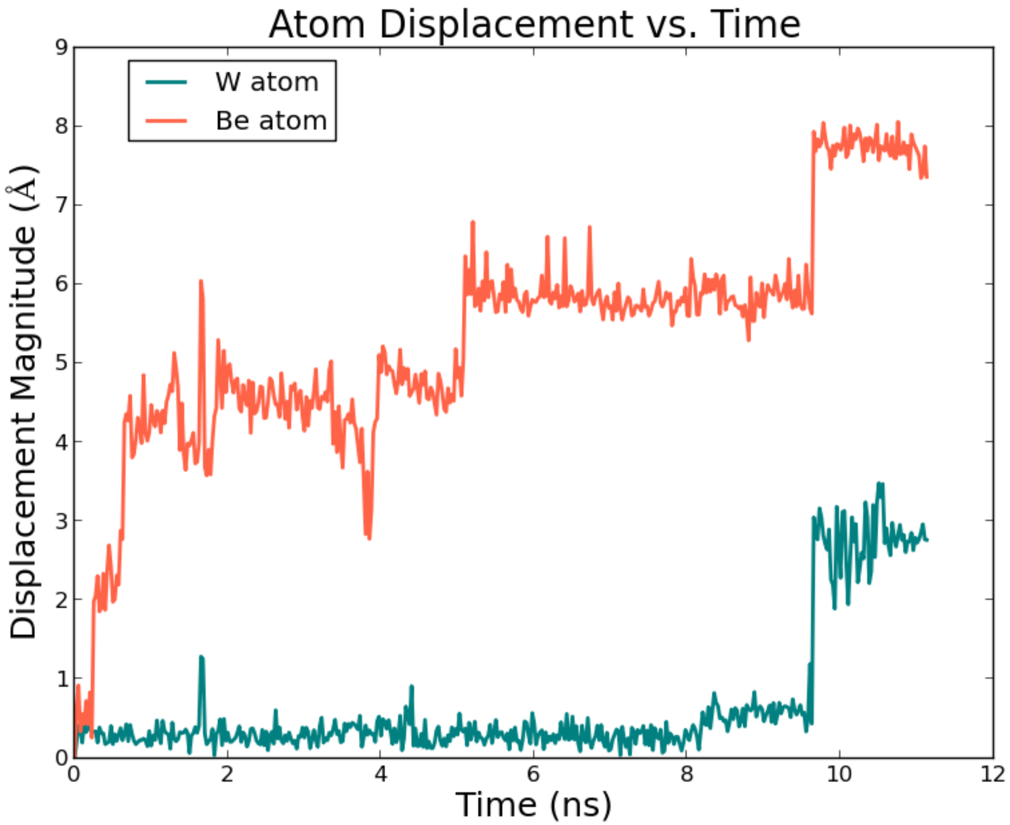


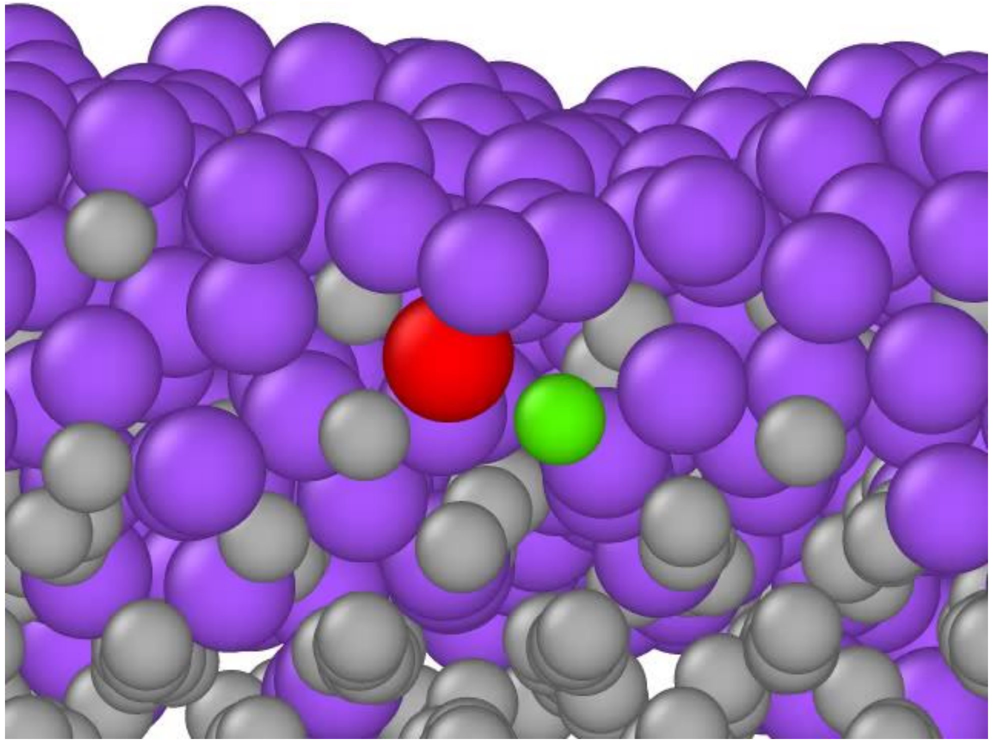




Exchange Mechanism with Beryllium

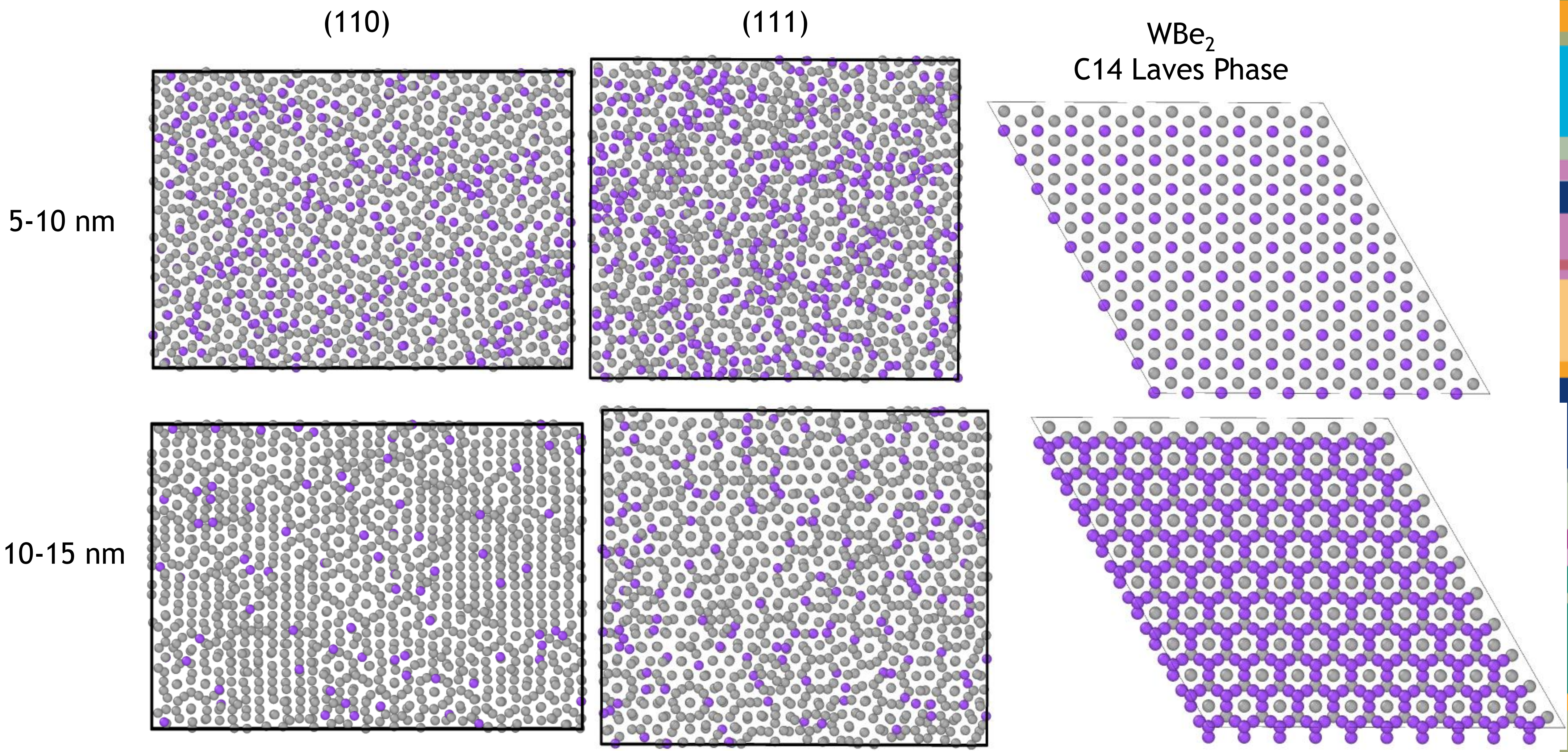
Red: Be Exchanged
Green: W Exchanged
Purple: Be
Gray: W





- Clear jumps in tungsten displacement are exchanges with beryllium
- Low tungsten diffusion outside beryllium exchanges
- Exchange mechanisms occurs on the order of nanoseconds

Slices Through Amorphous Layer Indicate Structure



Extending the Potential for other Plasma Species - Helium

He Defect Formation Energies in Be

Defect	DFT (eV)	MD (eV)
Sub	2.20	2.90
Basal Split	5.46	5.41
Basal Tetrahedral	5.78	5.64
Basal Octahedral	5.81	5.60
Crowdion	6.11	5.72

- Extend potential to include helium
- Used form of existing W-He[1] pair potential for Be-He
- Fit to He defects in Be calculated using DFT
- Pair potential reproduces ordering of defects and formation energies are consistent with DFT

[1] N. Juslin and B.D. Wirth, Journal of Nuclear Materials 432 (2013) 61-66

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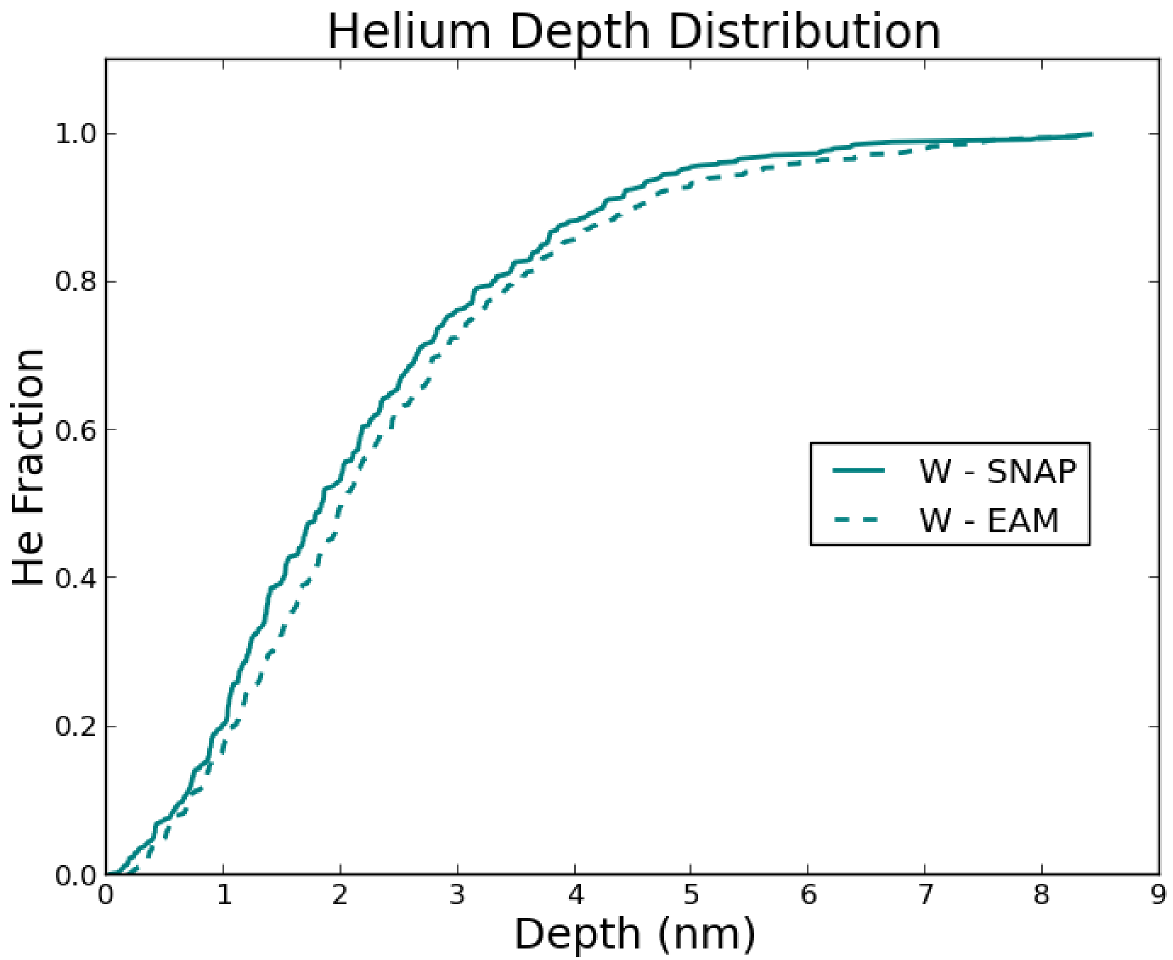
- In pure W, SNAP is consistent with existing EAM potential[1]



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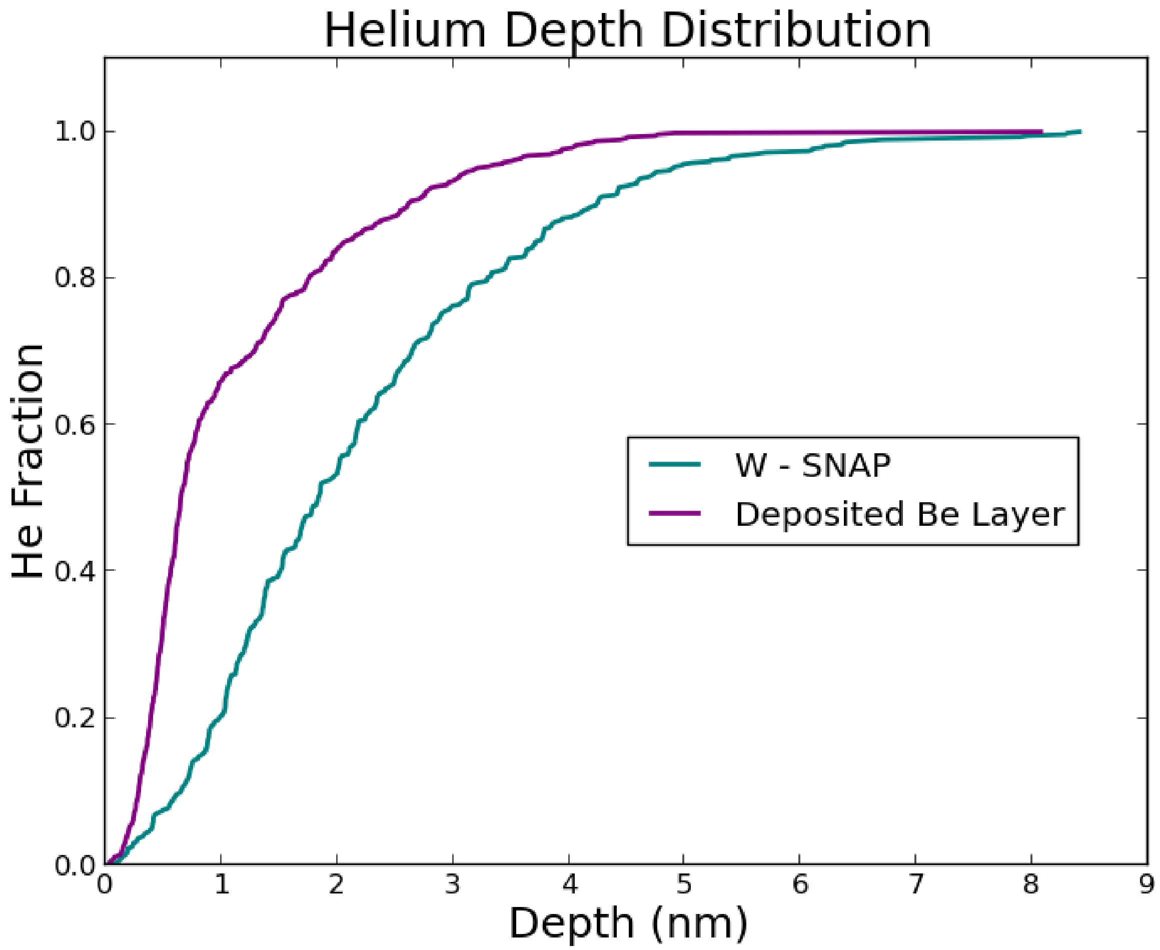

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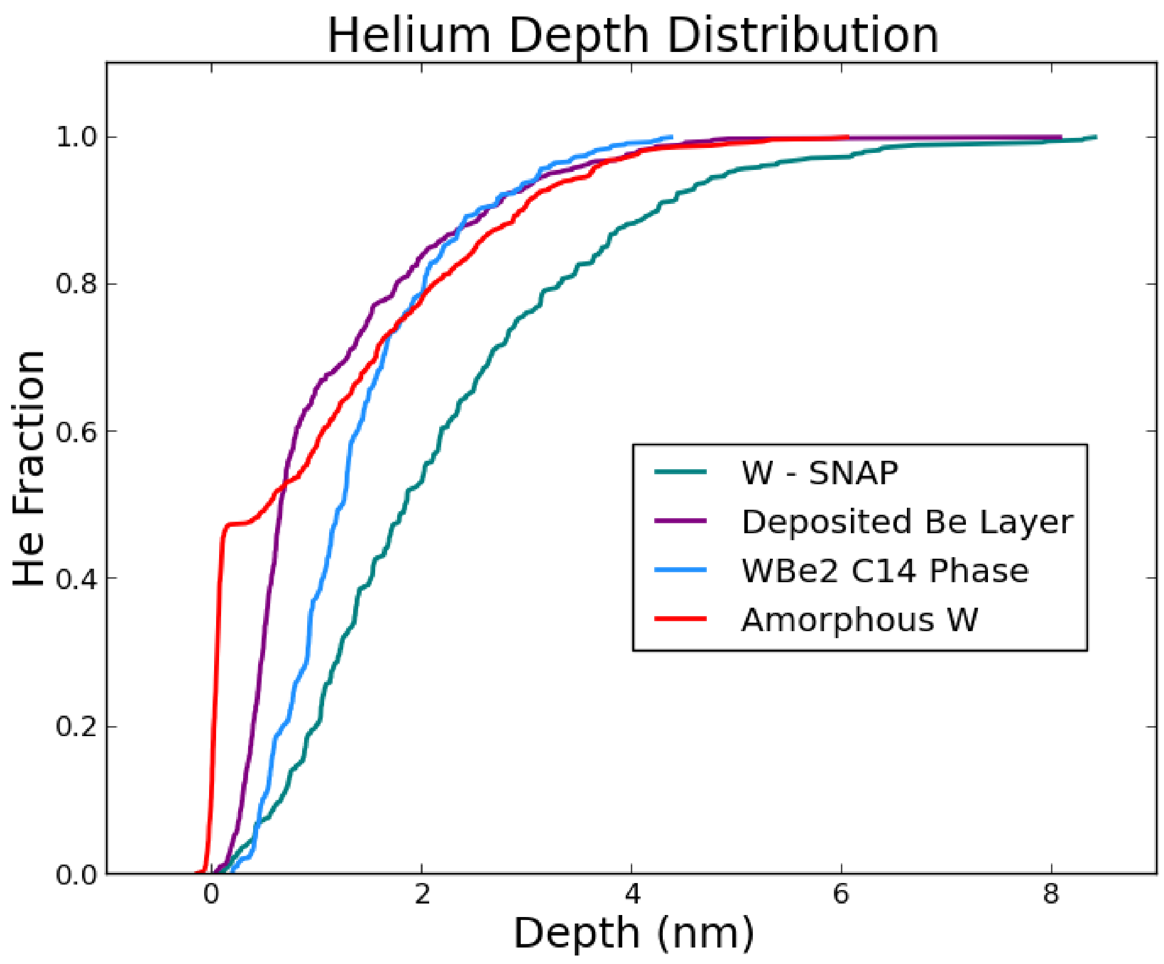
- He implantation in W-Be amorphous layer shifts depth profile
- Similar shift in WBe_2 structure and amorphous W



	W	Be Layer	C14	W Amorph
% Implanted	38.9	55.2	60.5	70.3

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Summary

- We have developed a machine learned SNAP potential for studying W-Be plasma material interactions and have extended it to include He
- 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 in tungsten
- An amorphous layer of mixed W-Be has been observed which may be a pre-cursor to intermetallic formation
- Structured layers similar to WBe_2 phases were observed
- An exchange mechanism allows tungsten to migrate into the surface amorphous layer
- Helium implantation and retention is modified when Be is present in W
- Physics observed in this work can be used to inform continuum codes
- This potential will be extended to include hydrogen and nitrogen and further MD simulations of mixed materials will be performed

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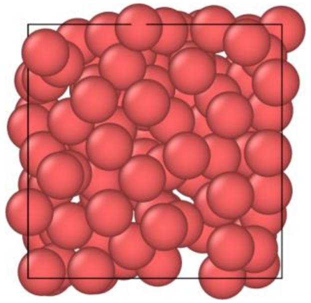
Backup Slides

SNAP: Spectral Neighbor Analysis Potentials

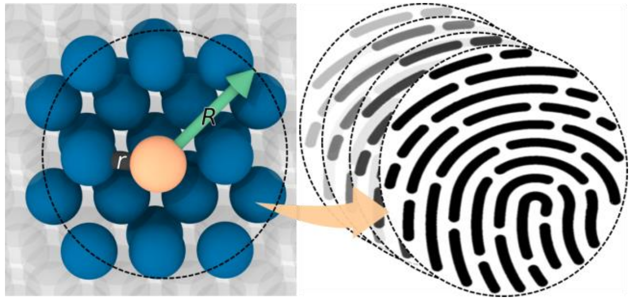


Geometric descriptors of atomic environments

Energy as a function of geometric descriptors

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

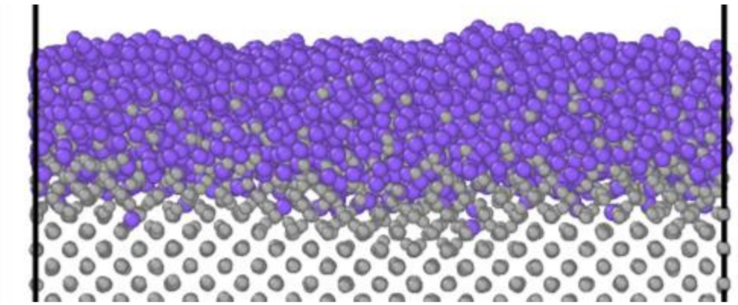
$$E_i^{SNAP} = b_0 + \sum_{k \in \{J<J_{max}\}} b_k B_k^i$$

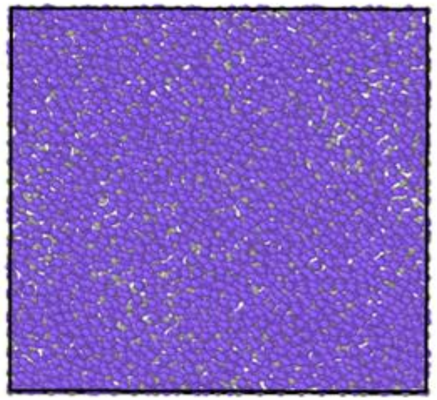


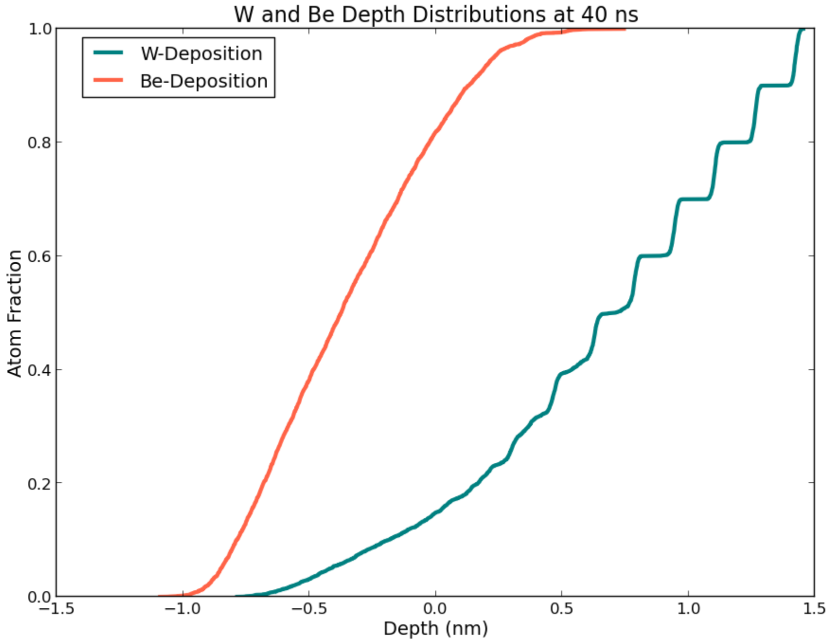
- **GAP (Gaussian Approximation Potential):** Bartok, Csanyi et al., *Phys. Rev. Lett, 2010.* Uses 3D neighbor density bispectrum and Gaussian process regression.
- **SNAP (Spectral Neighbor Analysis Potential):** Our SNAP approach uses GAP's neighbor bispectrum, but replaces Gaussian process with **linear regression**.
  - More robust
  - Lower computational cost (training and predicting)
  - Decouples MD speed from training set size
  - Enables large training data sets, more bispectrum coefficients
  - Straightforward sensitivity analysis

Cumulative Be Athermal Deposition on W Surface

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





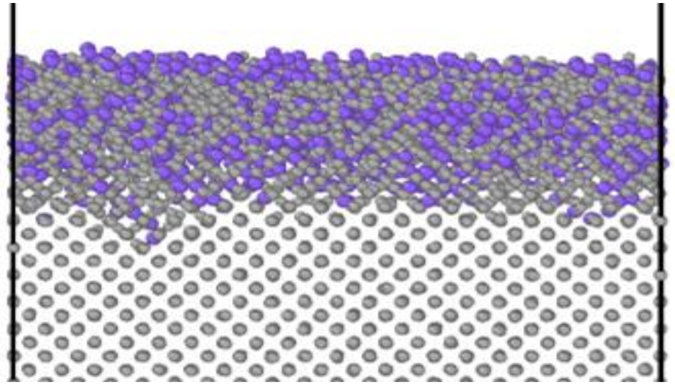


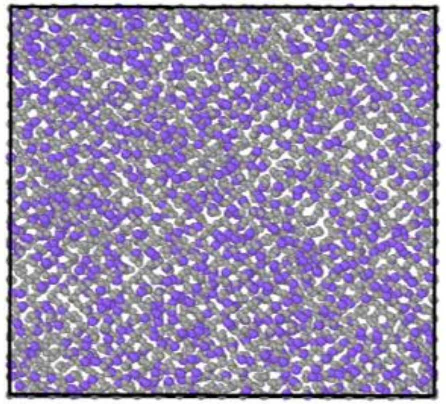
Purple: Beryllium
Gray: Tungsten

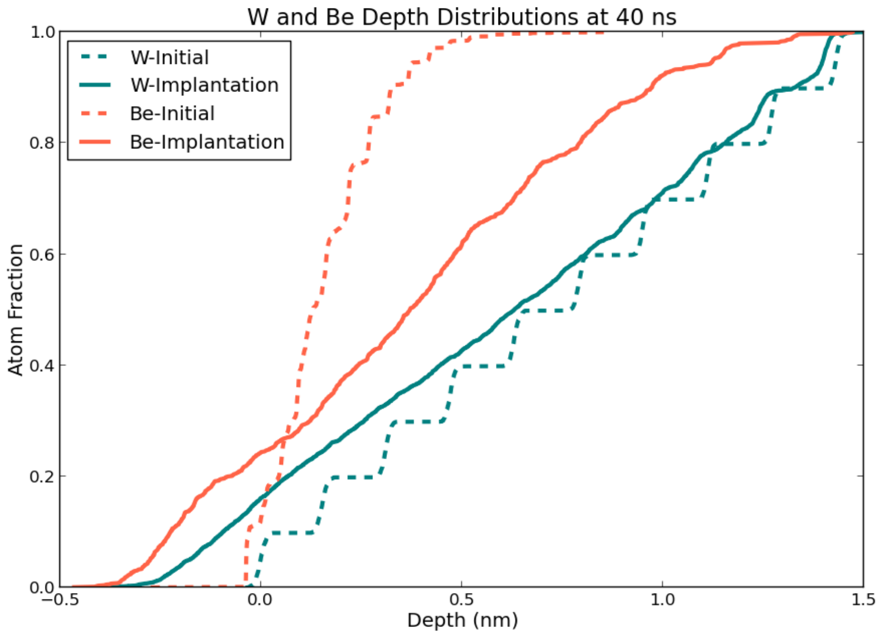
- Be randomly placed on surface every 10 ps with zero energy
- Initially Be resides at hollow sites
- Be begins to exchange with tungsten once hollow sites fill up
- Similar amorphous layer forms at higher fluences
- Thicker layer that extends from 0.5 nm below surface to 1 above surface
- Be remains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

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 that is 2 nm thick
- W depth profile indicates loss of crystal structure at higher fluences
- Be depth profile is deeper than expected based on initial implantation depth

Slices Through Amorphous Layer Indicate Structure