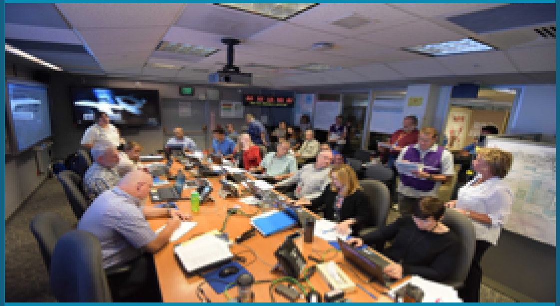
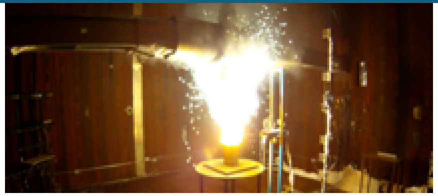
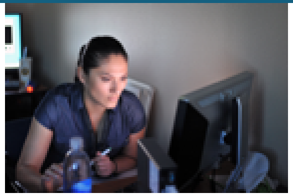
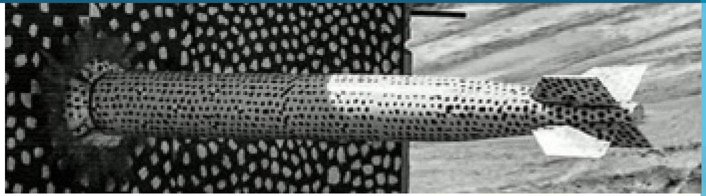
SAND2021-14043C

Atomistic Modeling of Beryllium and Helium Implantation in Tungsten Using Machine Learned Interatomic Potentials









Mary Alice Cusentino

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2021 APS-DPP

November 8, 2021

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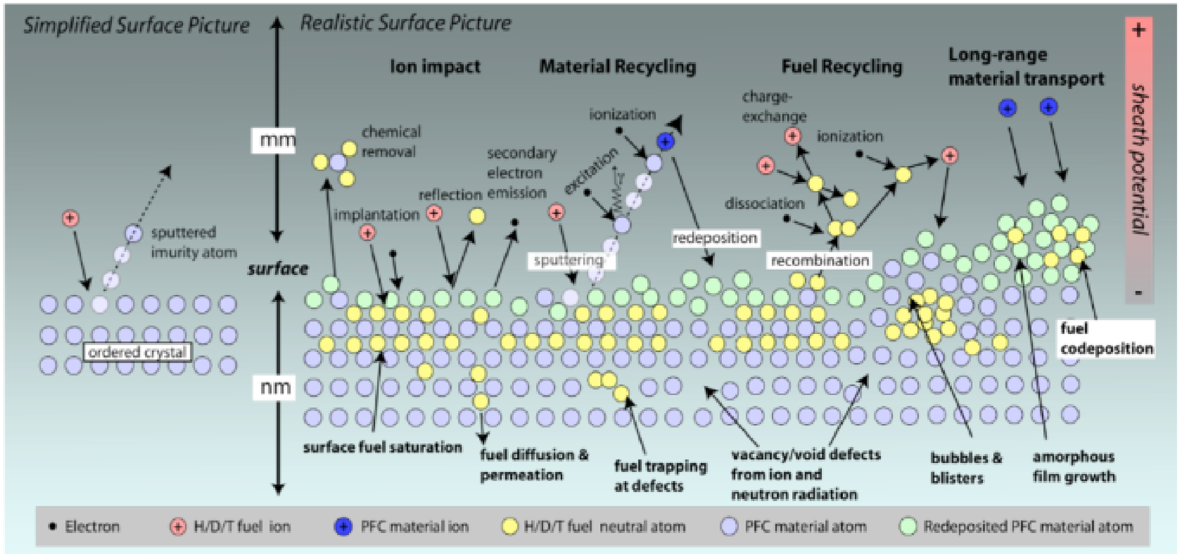
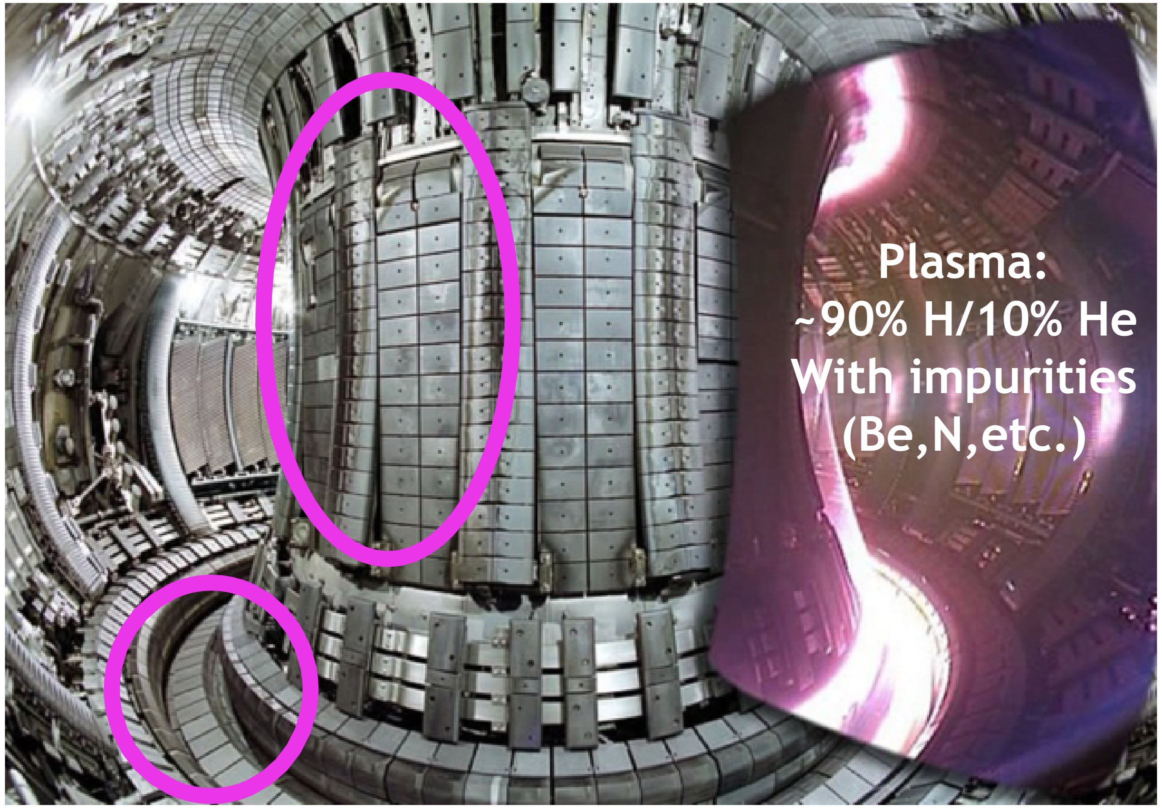
Materials for Fusion Energy

- Difficult to develop materials to handle extreme conditions within tokamak
- Large heat loads of 10-20 MW/m^3
- High particles fluxes of $\sim 10^{24}\ m^{-2}s^{-1}$ of mixed ion species (H/He/Be/N etc.)



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



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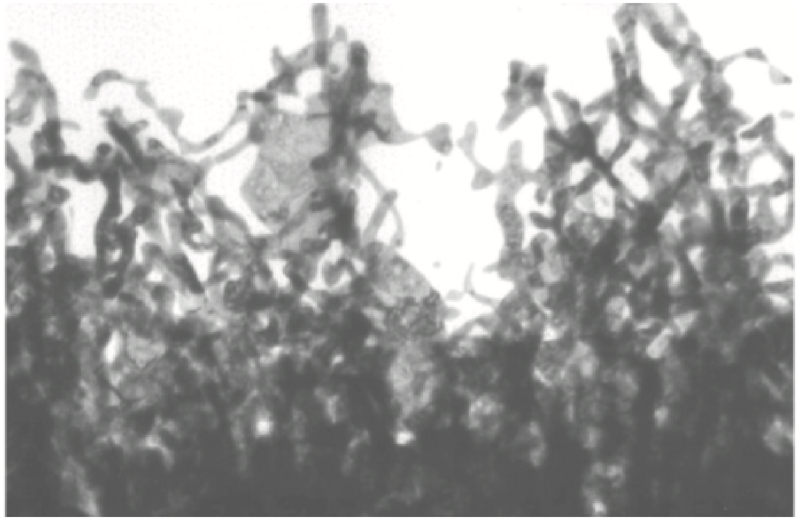
- Many complex processes that occur at the plasma/material interface that can lead to material degradation

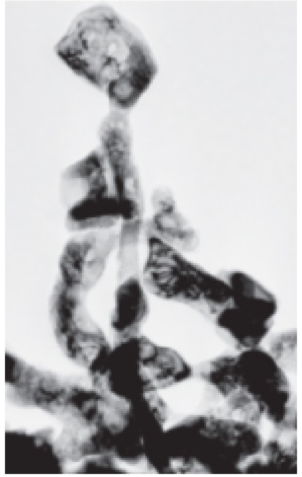
Plasma Material Interactions in Tungsten

Helium Fuzz Growth



Kajita, et al. J. Nucl. Mater, 418, (2011) 152-158

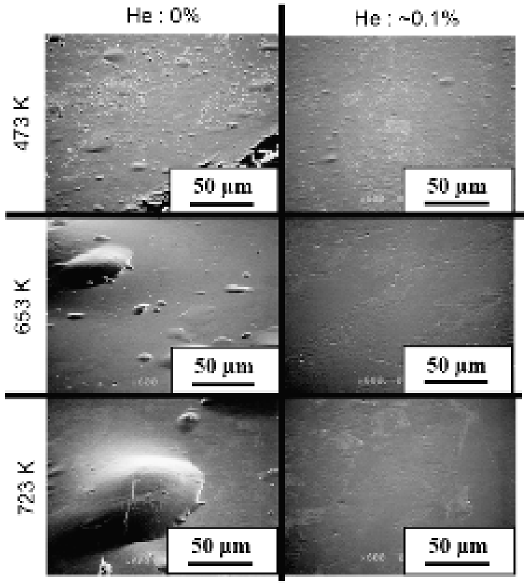
Material Degradation



Kajita, et al. Nucl. Fus. 471, 886-890 (2007)

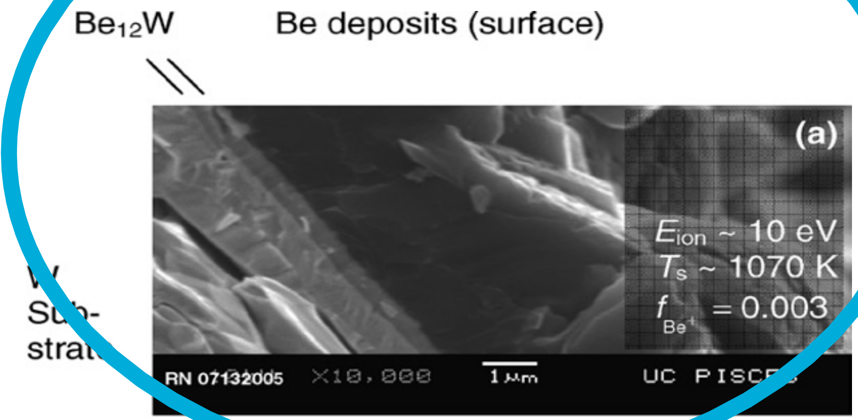
Tritium Retention

Effect of He on H Blistering



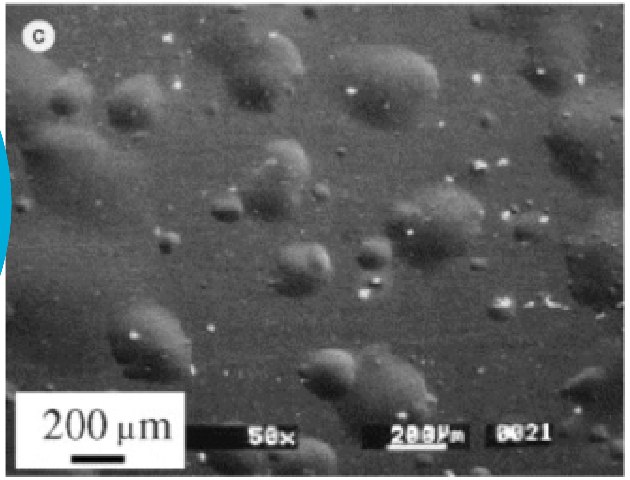
Ueda, et. al. J. Nucl. Mater. 386-388 (2009) 725-728

W-Be Intermetallics



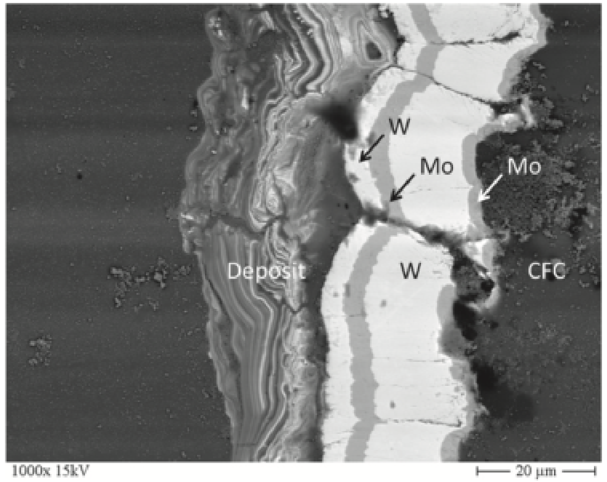
Baldwin, et. al. J. Nucl. Mater. 363-365 (2007) 1179-1183

Hydrogen Blisters



Ye, et al. J. Nucl. Mater. 313-316, 72-76 (2003)

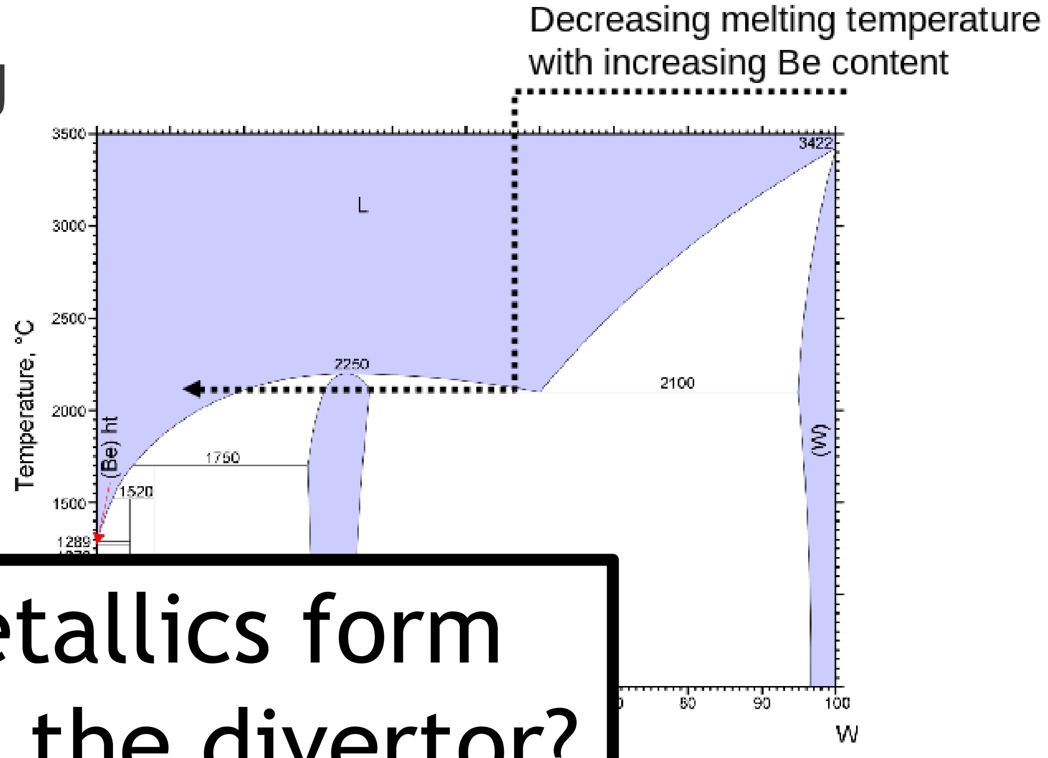
Co-Deposit Layer at Divertor Surface



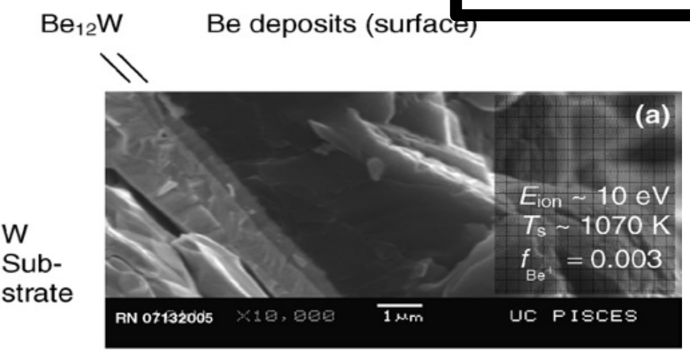
M Mayer *et al* 2016 *Phys. Scr.* **2016** 014051

Beryllium Effect on Tungsten Melting

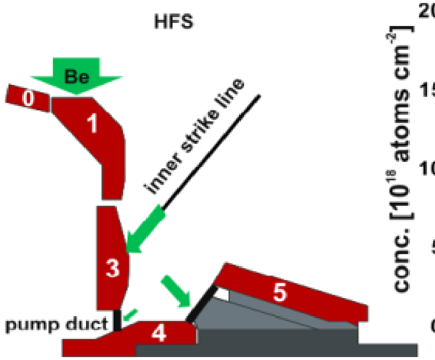
- W-Be intermetallics observed in linear plasma experiments
- Tokamak experiments indicated beryllium deposition on the divertor
- Phase diagram indicates decreasing melting temperature w

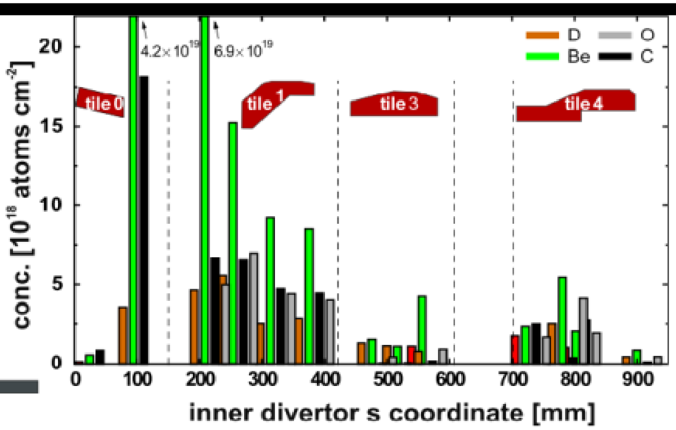


How do W-Be Intermetallics form and how do they affect the divertor?



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

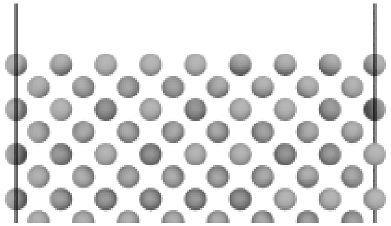




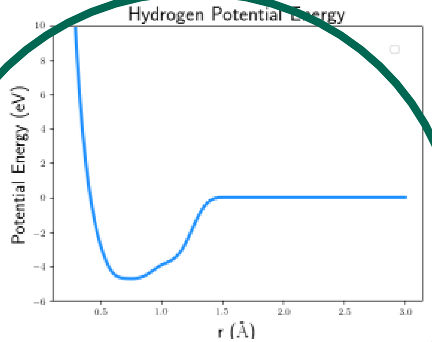
Brezinsek, et. al. J. Nucl. Mater. 463 (2015) 11-21

	MD Melt T. (C)	Expt. Melt T (C)
W	3130	3422
Be	1630	1289
WBe_2	1830	2250

Multiscale Modeling of Materials



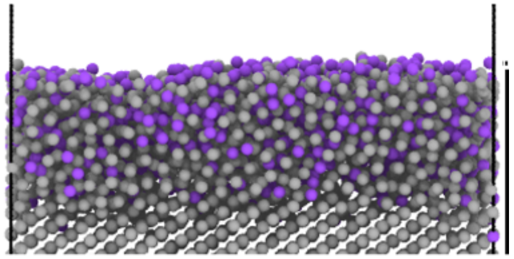
Initial Atom Positions and Velocities

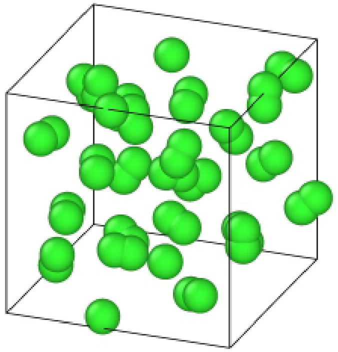


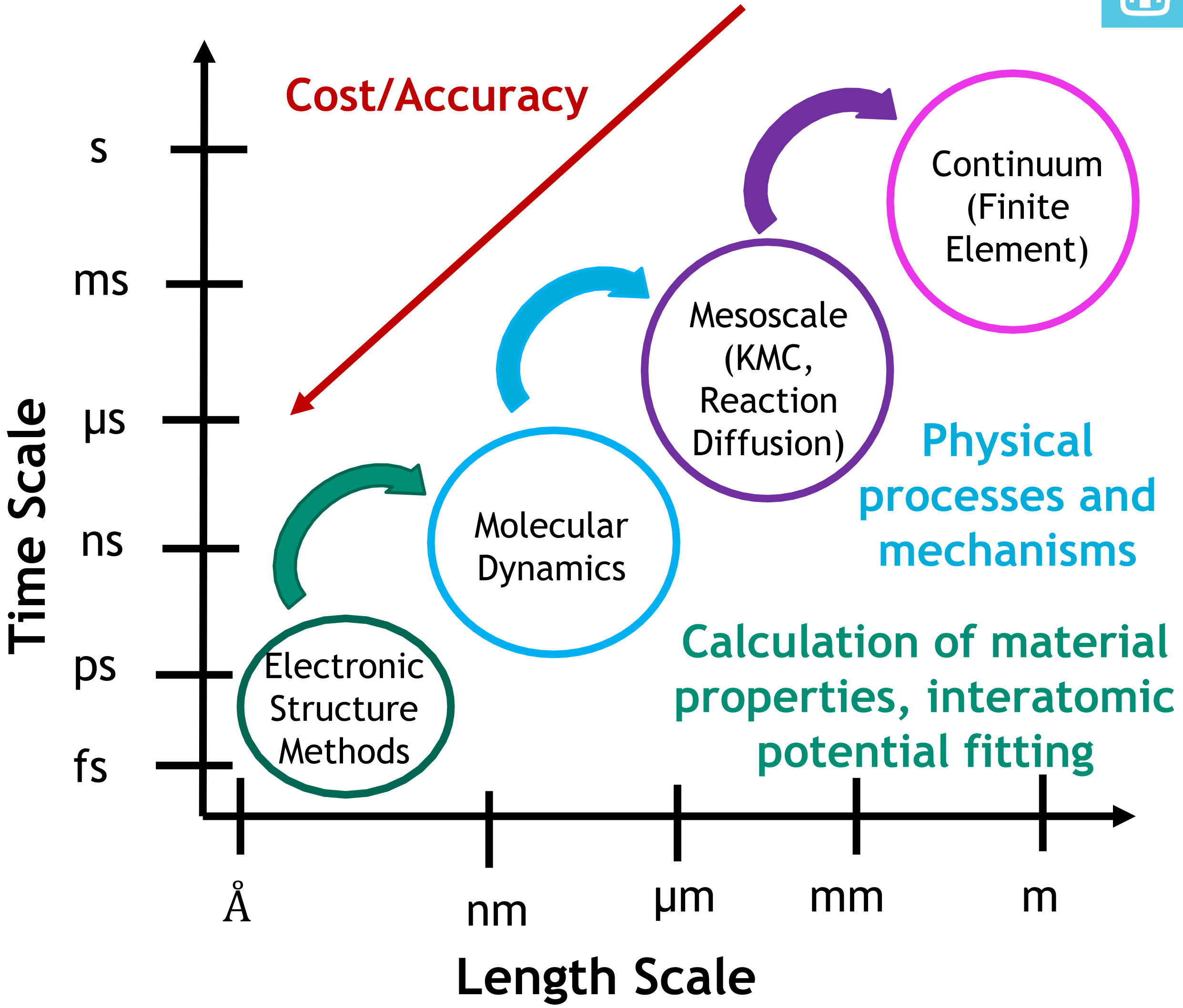
Interatomic Potential

Molecular Dynamics (LAMMPS)

Evolution of Material System Over Time





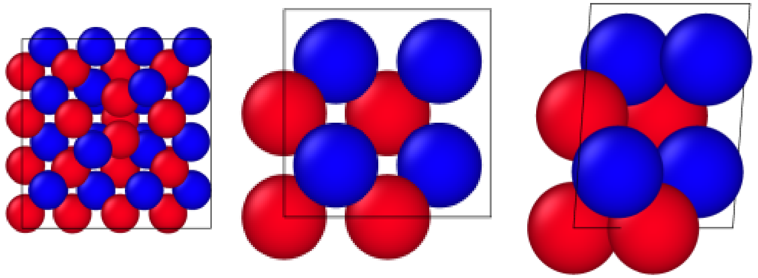


Each simulation technique can provide information to the next scale up

What Makes a Machine Learned Interatomic Potential?

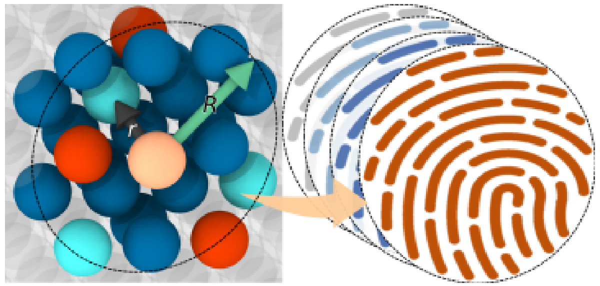
Training Data

- Generated using quantum methods
- Can include:
  - Energies
  - Forces
  - Stresses
- Variety of atomic configurations
  - Bulk structures, liquids, surfaces, defects, etc.



Descriptor

- Describes the local atomic environment
- Requirements
  - Rotation/Translation/. Permutation invariant
  - Equivariant forces
  - Smooth differentiable
  - Extensible
- Some Examples
  - Bispectrum, SOAP, ACE, Moment Tensors, etc.



Regression Method

- Linear regression
- Kernel ridge regression
- Gaussian process
- Non-linear optimization
- Neural Networks

SNAP

- Energies, forces, and stresses from DFT
- Bispectrum component descriptors
- Linear regression

SNAP Definition and Work Flow

Model Form

No Image

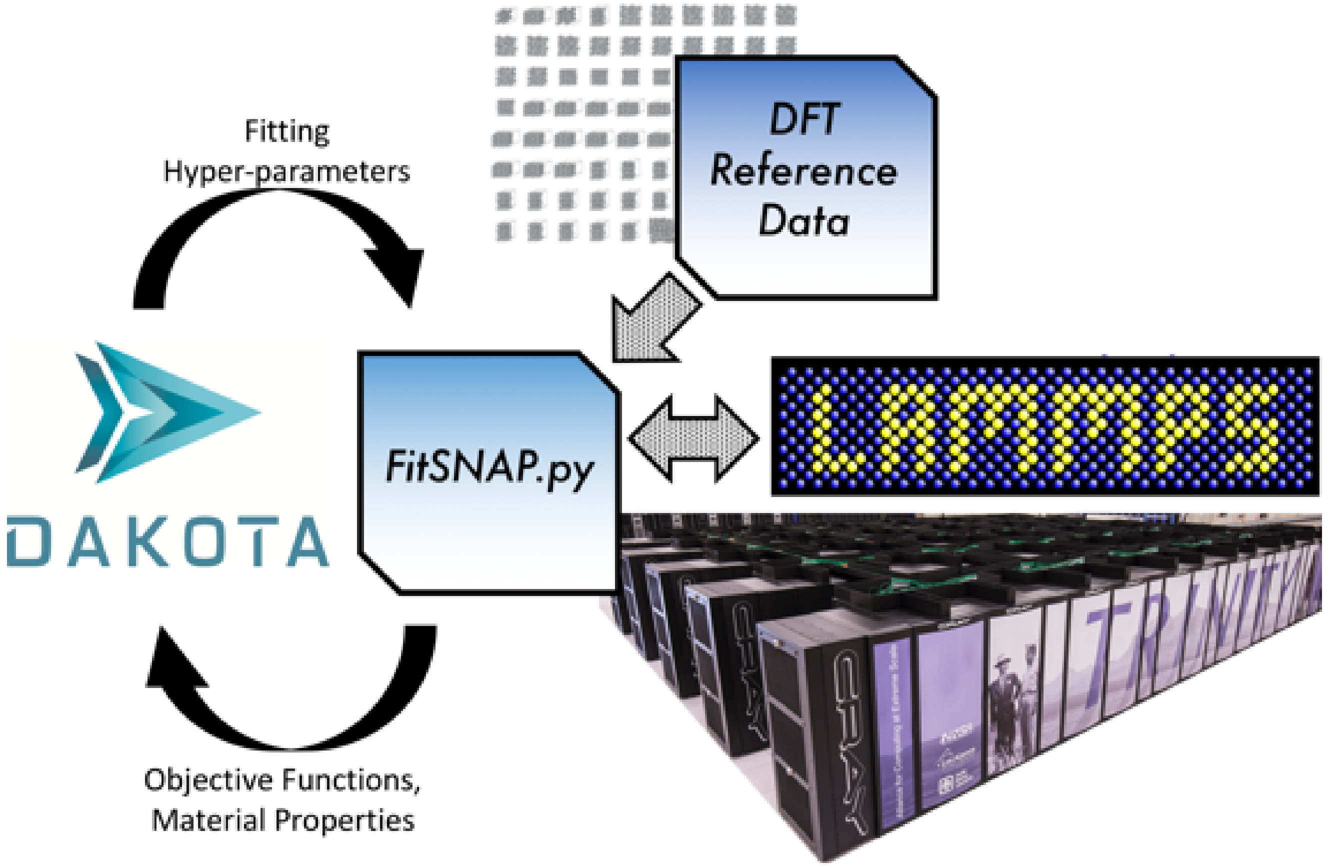
$$E^{i}_{SNAP} = \beta_0 + \sum_{k=1}^{K} \beta_k (B^{i}_{k} - B^{i}_{k0})$$

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



Code available: https://github.com/FitSNAP/FitSNAP

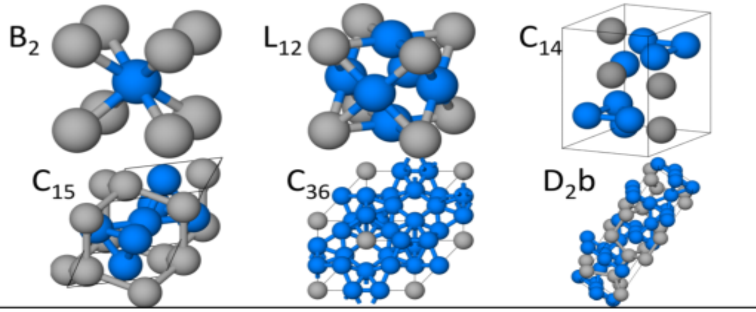
M. A. Wood, M.A. Cusentino, B.D. Wirth and A.P. Thompson, Phys. Rev. B 99, 184305

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:



W-Be Intermetallic Formation Energies (eV)

Phase	Composition	DFT[1]	SNAP[1]	BOP[2]
B_2	WBe	0.67	0.30	-2.20
C_{14}	WBe_2	-0.87	-1.27	-4.20
C_{15}	WBe_2	-0.92	-1.15	-4.19
C_{16}	WBe_2	-0.90	-1.22	-4.20
L_{12}	WBe_3	-0.51	-0.15	-4.58
D_2B	WBe_{12}	-0.96	-0.34	-6.69

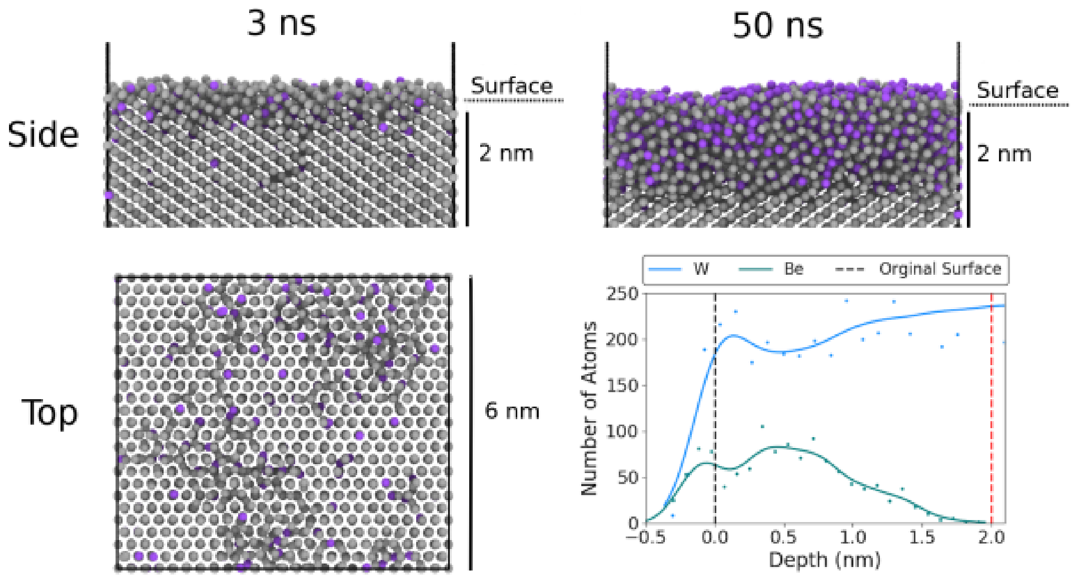
Be Defect Formation Energies in W (eV)

	DFT[1]	SNAP[1]	BOP[2]
[111] Dumbbell	4.30	3.66	0.67
Substitution	3.11	3.29	-2.00
Surface Hollow Site	-1.05	-1.39	-3.52
Tetrahedral	4.13	4.20	-0.28
[110] Dumbbell	4.86	4.29	-0.03
Octahedral	3.0	5.11	0.34
Surface Bridge Site	1.01	0.44	-1.30

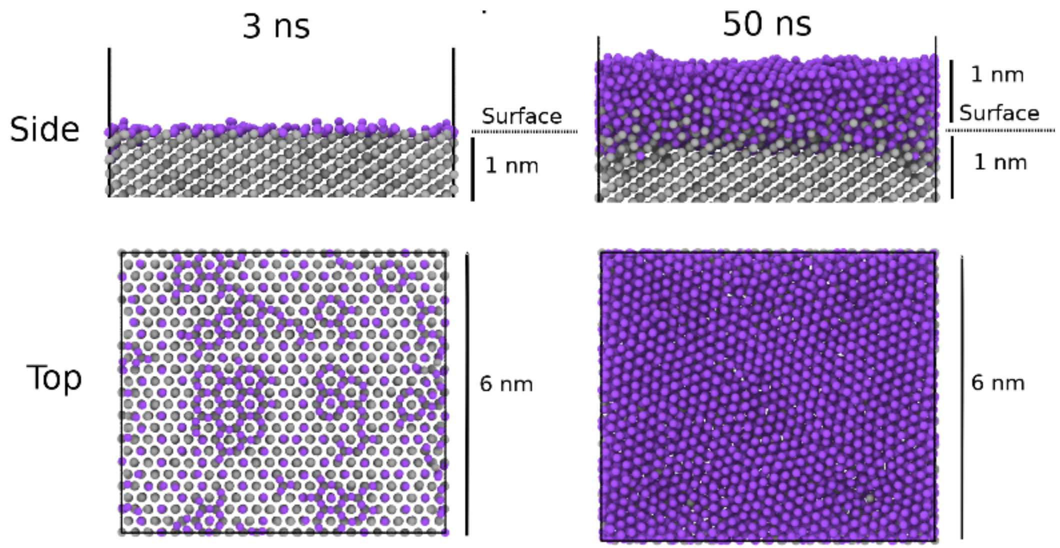
[1] M. A. Wood, M.A. Cusentino, B.D. Wirth and A.P. Thompson, Phys. Rev. B 99, 184305
[2] C. Björkas et al 2010 J. Phys.: Condens. Matter 22 352206

Beryllium Deposition Results in Near Surface Mixed Layer

75 eV Implantation

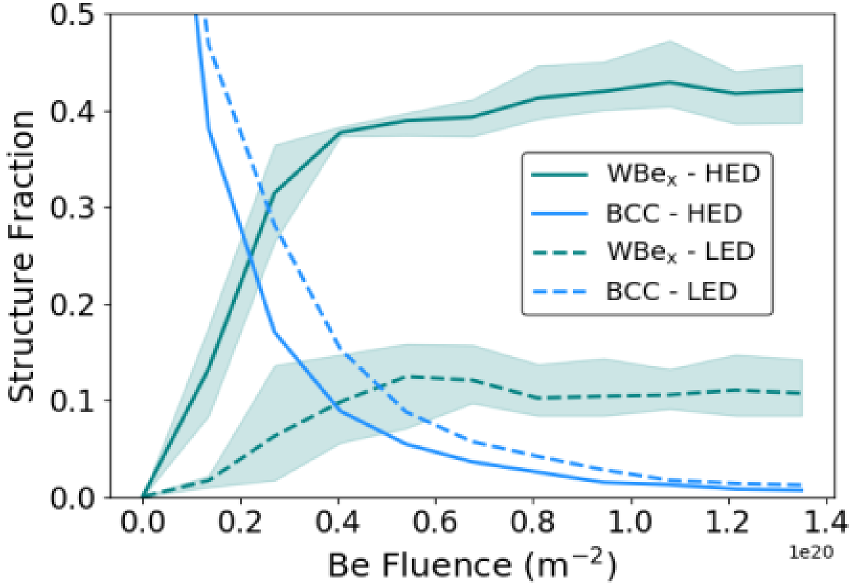


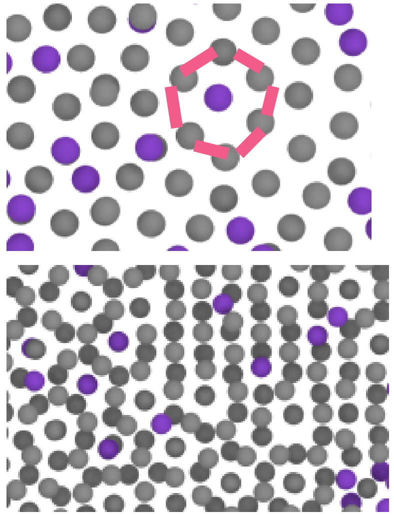
Athermal Deposition



- High energy (75 eV) and low energy (0 eV) beryllium deposition on tungsten surfaces
- Formation of disordered mixed materials layer in first 2 nm of surface
- Some intermetallic growth observed within mixed materials layer
- However, mixed materials layer appears to be kinetically trapped at MD time scales

Intermetallic Growth





Fluence: 1.4 x 10^{20} m^{-2}

Cusentino, et al. Nucl. Fusion, 61, 046049 (2021)

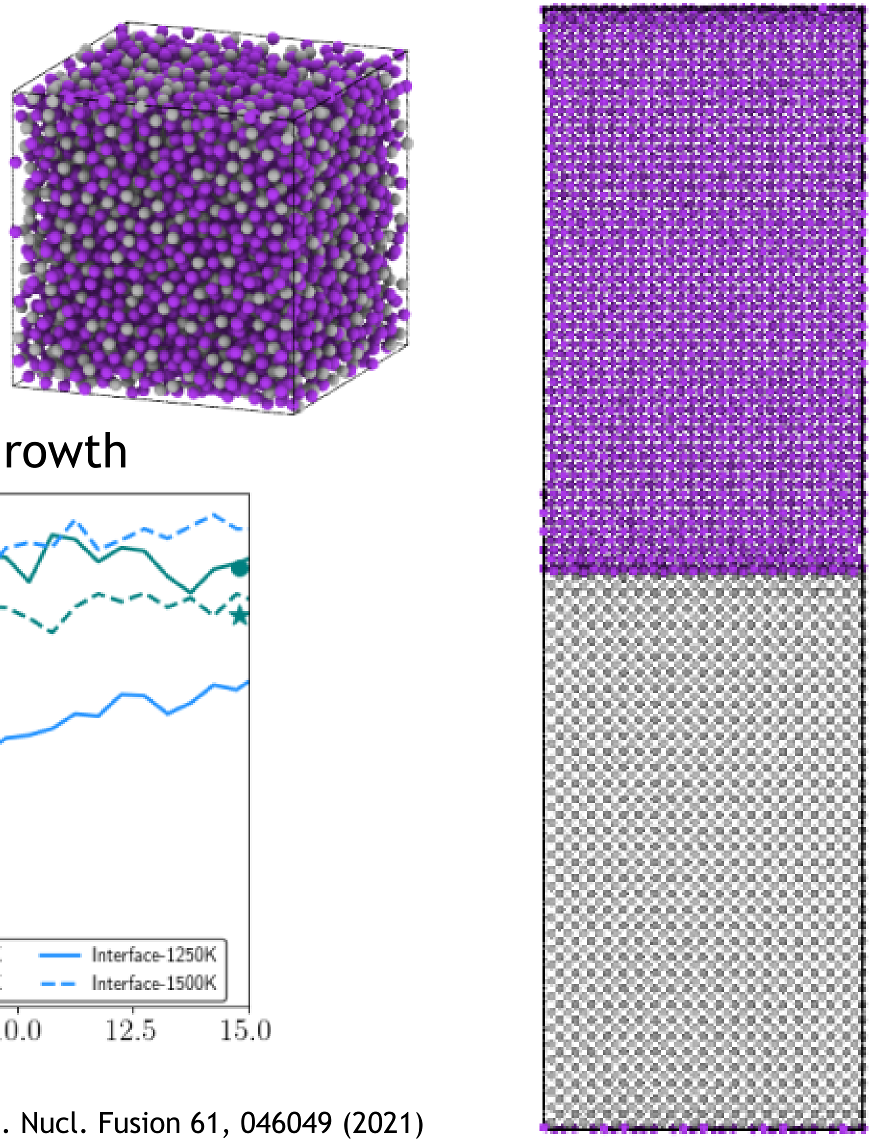
How Does Be Diffuse Within the Mixed Materials Layer?

- How quickly does beryllium diffuse within the MML and how does this impact intermetallic formation over longer periods of time?
- Diffusion was found to be limited in the pre-mixed case and higher in the interface
- However, intermetallic growth saturates and further growth is likely beyond MD timescales

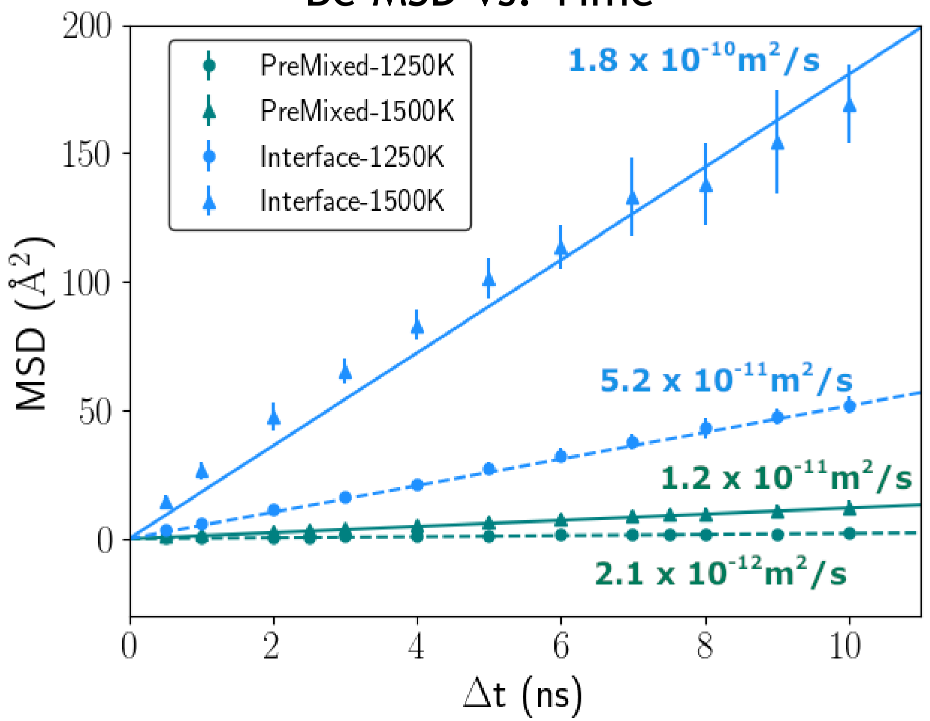
Purple: Be
Gray: W

Pre-Mixed W-Be

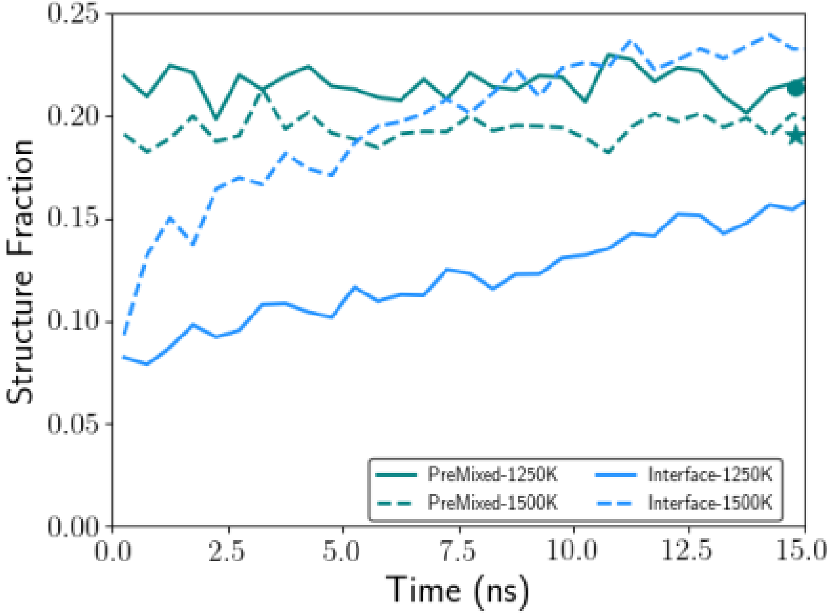
W-Be Interface



Be MSD vs. Time

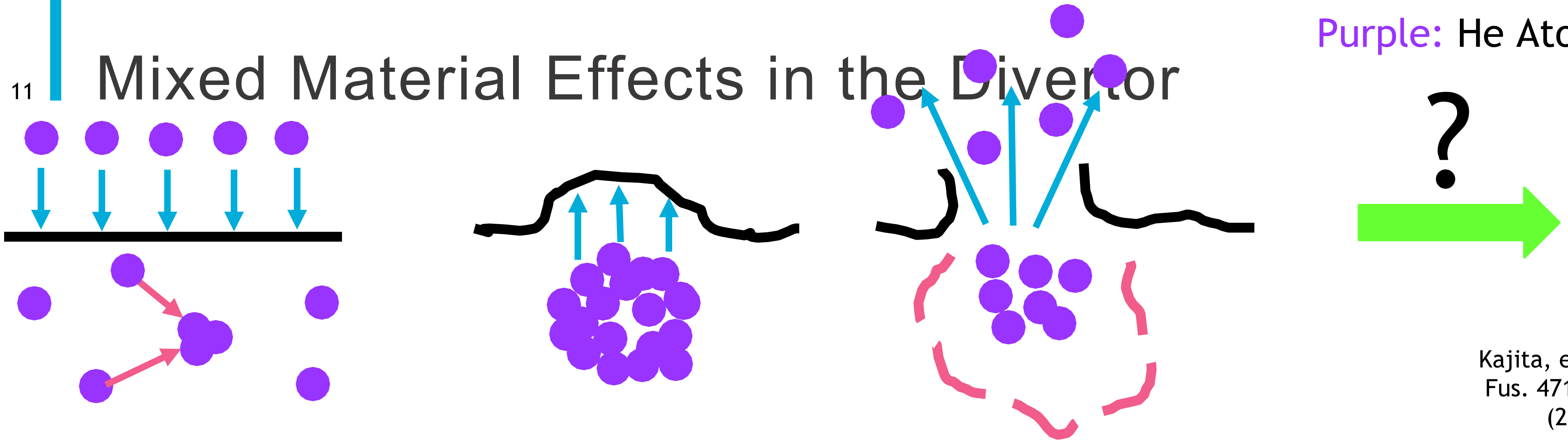


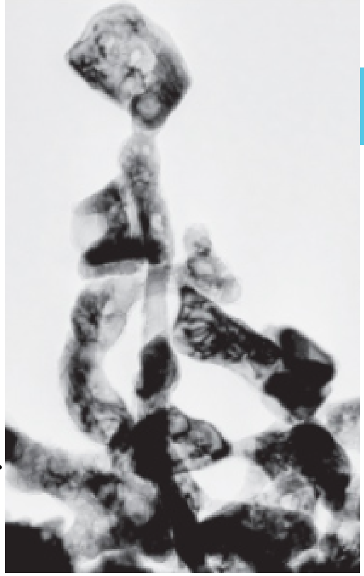
Intermetallic Growth



Cusentino, et al. Nucl. Fusion 61, 046049 (2021)

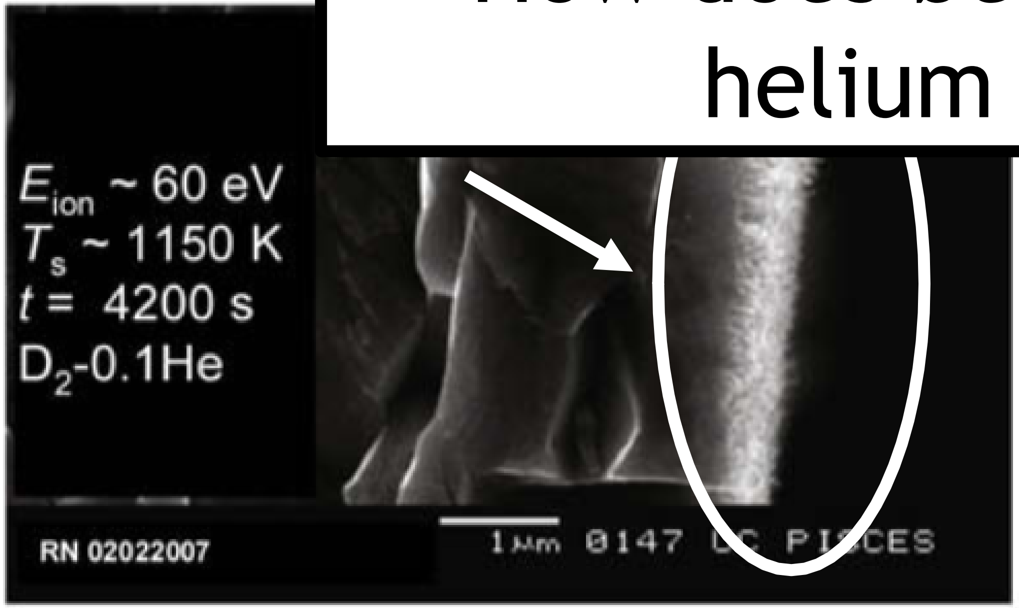
Mixed Material Effects in the Divertor





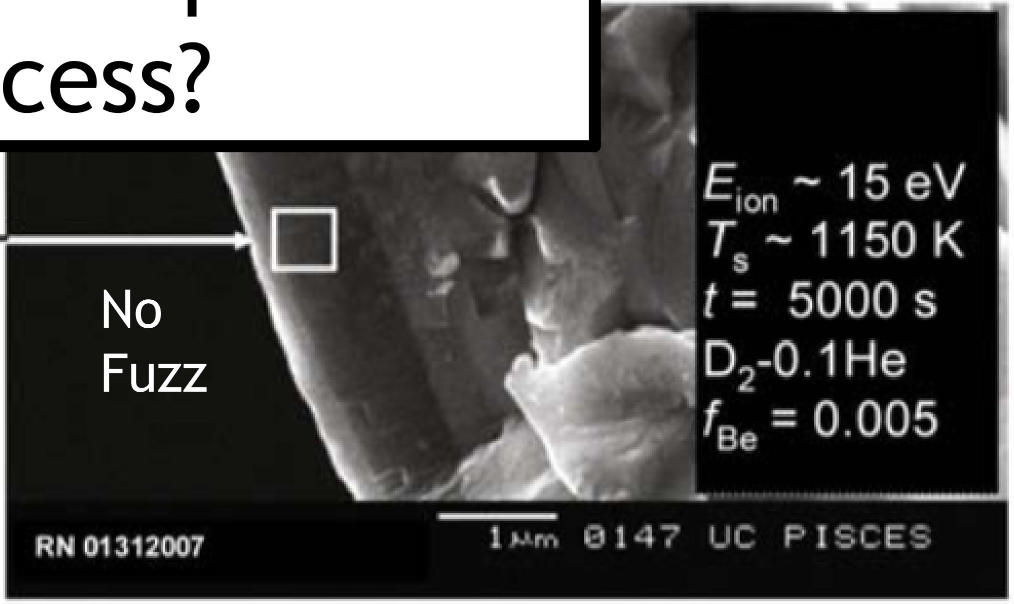
Kajita, et al. Nucl. Fus. 471, 886-890 (2007)

D_2 - 0.1 He Plasma



How does beryllium disrupt the helium fuzz process?

D_2 - 0.1 He with Be Plasma

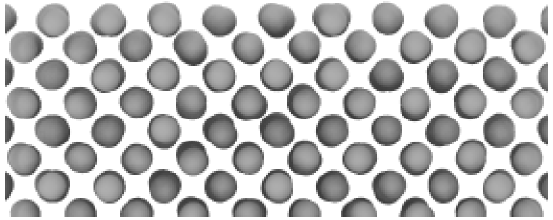


Baldwin, et al. J. Nucl. Mater 390-391, 886-890 (2009)

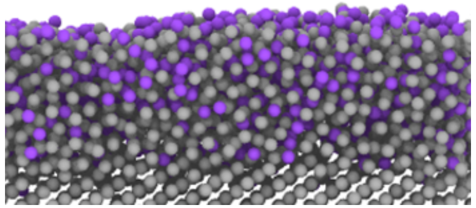
Cumulative He Implantation in W and W-Be at 2.5 x 10^{19} m^{-2}

Increasing TIme

Crystalline W

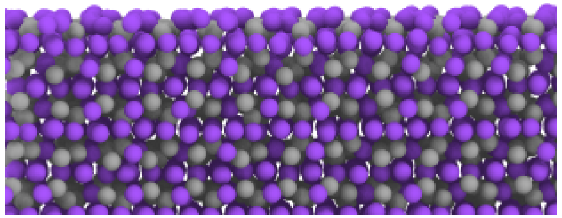


Amorphous W-Be

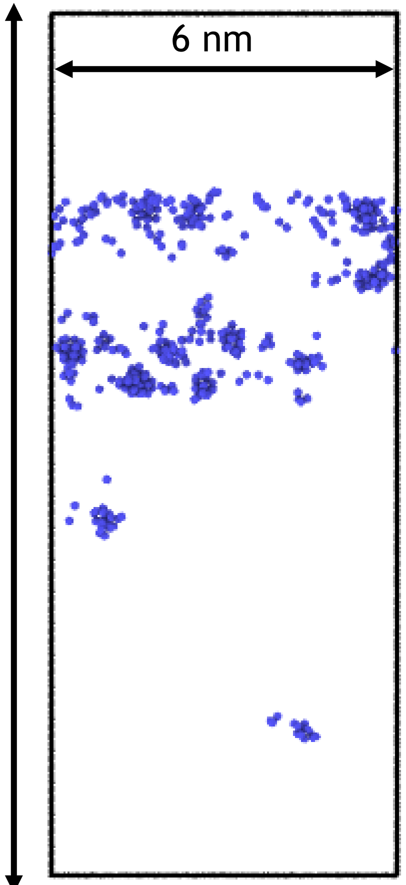


Blue: He
Purple: Be
Gray: W

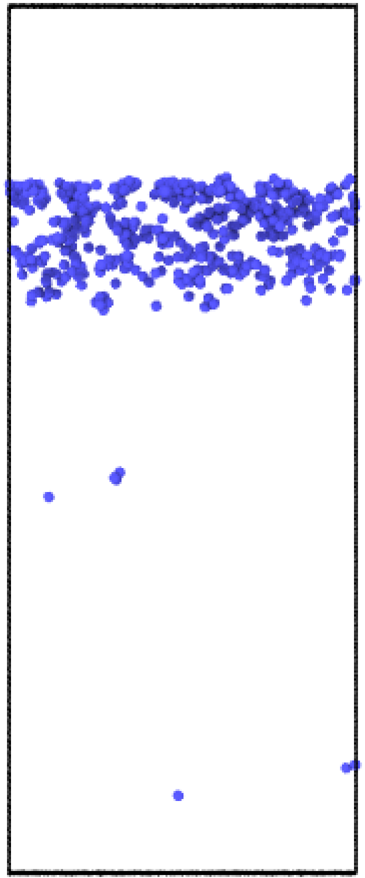
WBe_2 C14 Structure



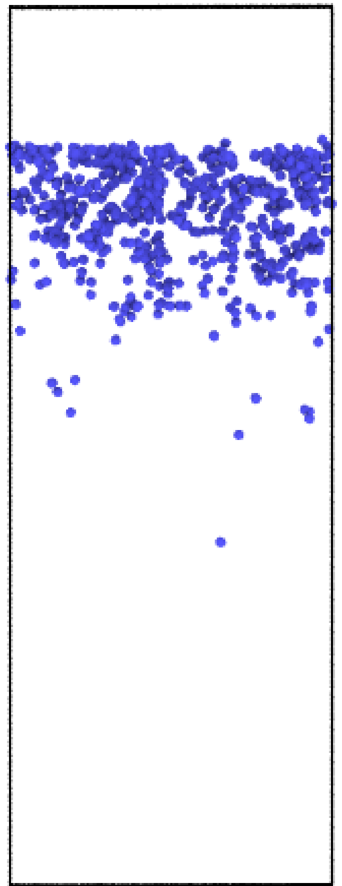
12 nm



<u>Tungsten:</u>
Larger He clusters distributed throughout simulation cell

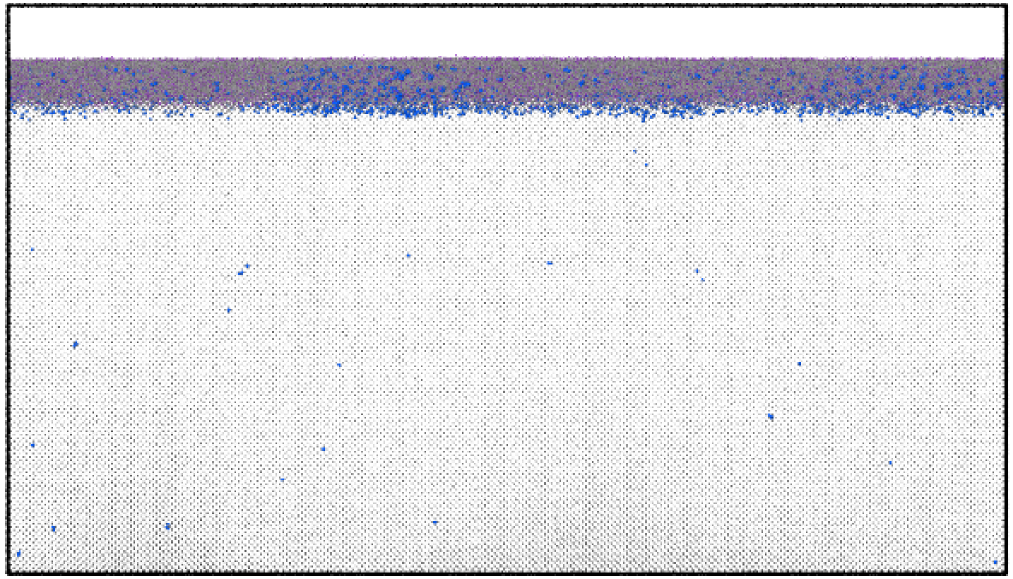


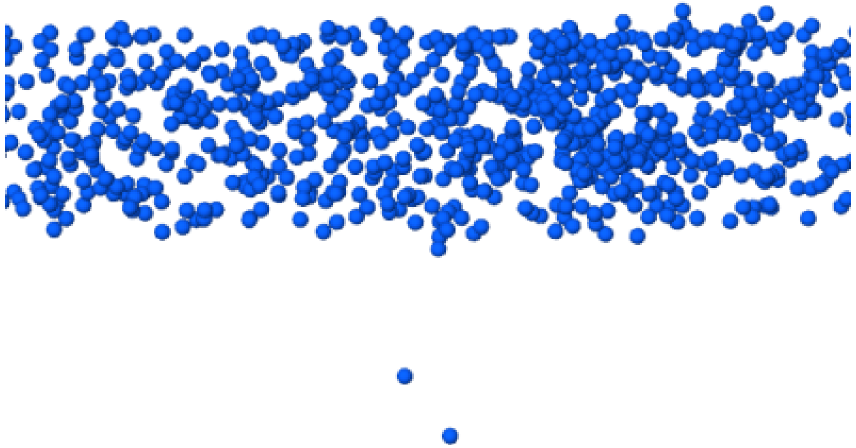
<u>Laves/Deposited Layer:</u>
Smaller He clusters mostly located near the surface



Large Scale Be/He Implantation Simulations in W

He Implantation in Be Pre-Implanted W Surface



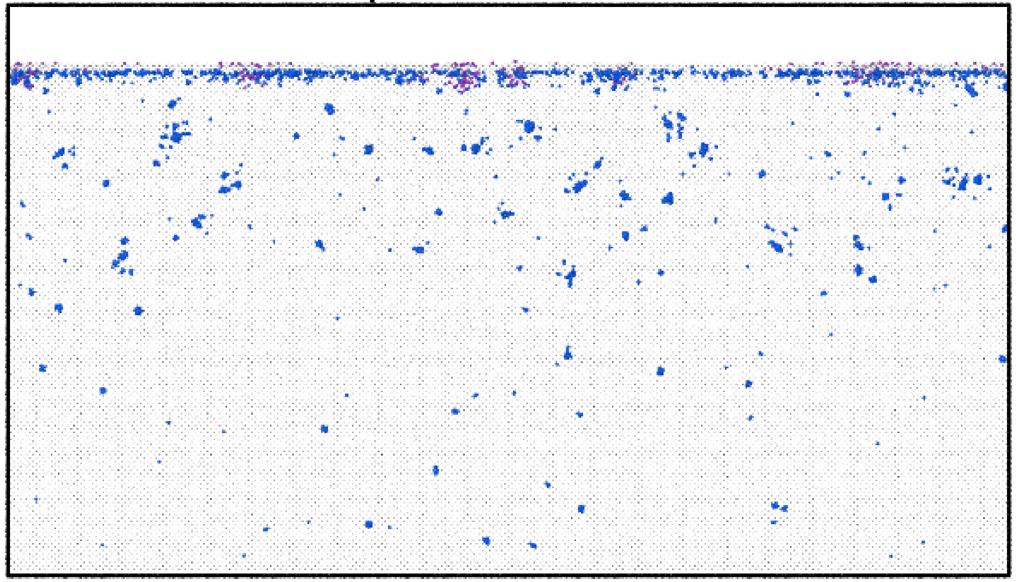


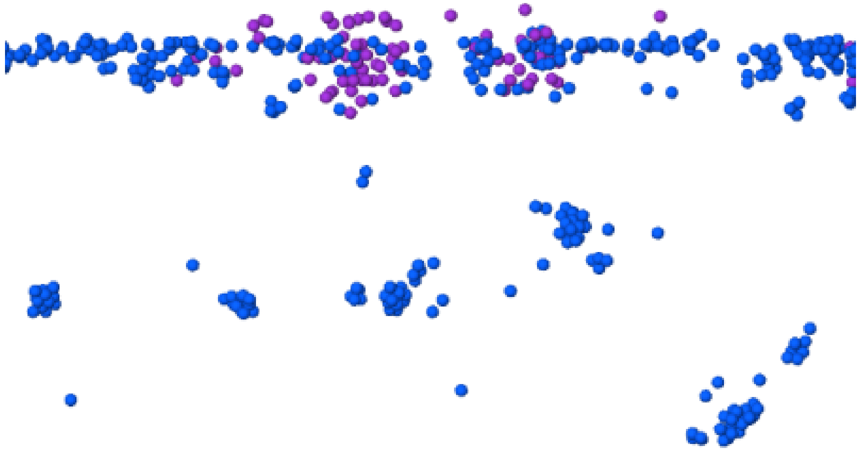
- Helium resides in W-Be layer
- No clustering of He atoms

Blue: He
Purple: Be
Gray: W

Time: 90 ns
Fluence:
3.56 x 10^{18} m^{-2}

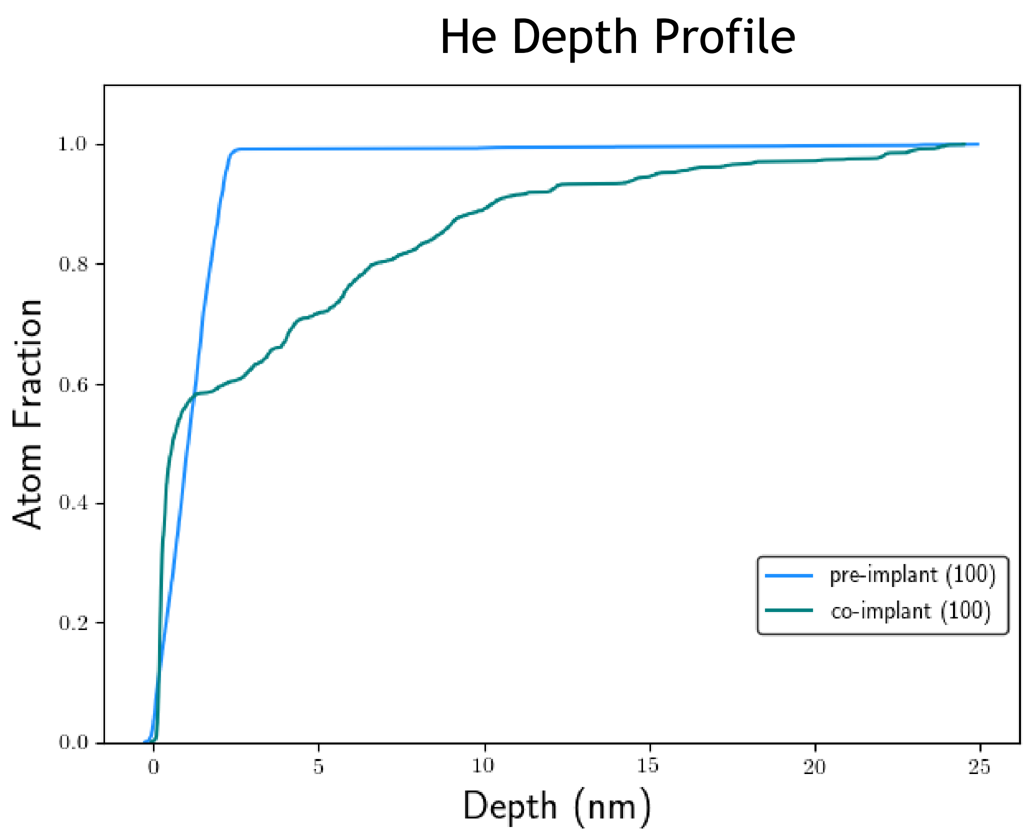
90% He/10% Be Implantation onto Clean W Surface





- Helium distributed throughout material
- He bubbles forming
- Be has created some local disorder

W-Be Mixed Materials Layer Alter He Bubble Nucleation



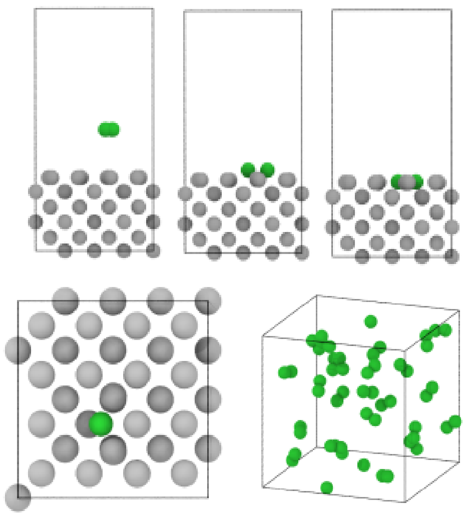
	Pre-(100)	Co-(100)
% Retention	46.4	23.1

m^2/s	W	WBe_2
Diffusion Coefficient	1.2×10^{-8}	1.8×10^{-11}

- W-Be mixed materials layer results in:
  - Smaller helium clusters
  - Helium remaining near the surface
  - Higher helium retention
  - Slower helium diffusion
- This will results in changes to helium bubble nucleation and will likely affect fuzz growth

Next Steps: Incorporating Other Plasma Species in SNAP

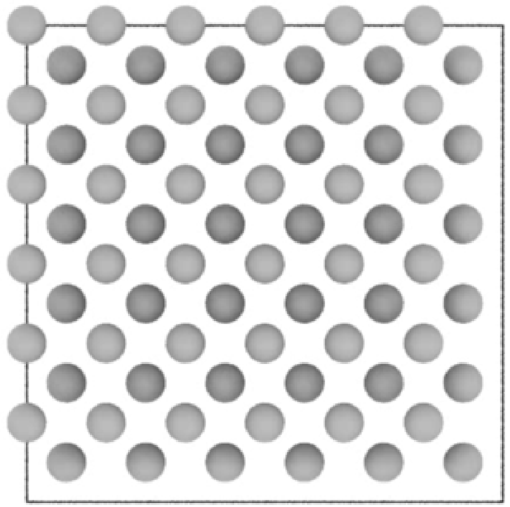
Hydrogen



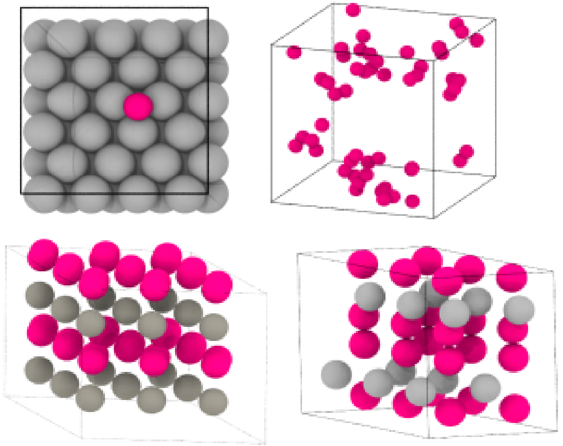
H Defect Formation Energies

H Defectx	DFT	SNAP
E_f^{Tet}(eV)	0.88	0.74
E_f^{Oct}(eV)	1.26	1.06
E_f^{Sub}(eV)	4.08	4.05
E_f^{H2}(eV)	-4.75	-4.77

H Diffusion in Bulk W



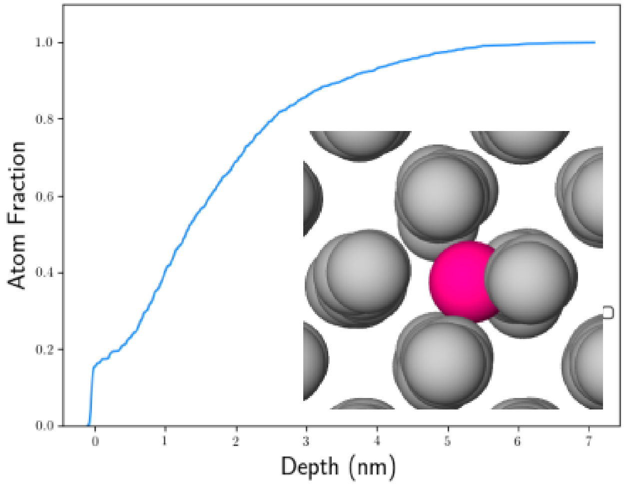
Nitrogen



W_xN_y Formation Energies

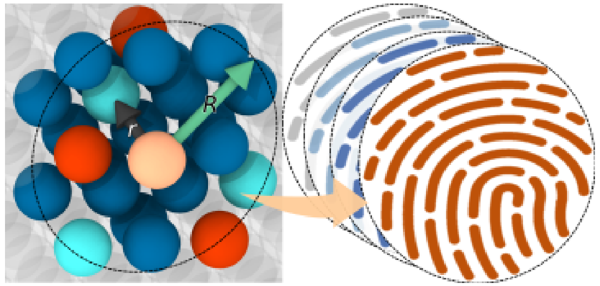
	DFT (eV)	SNAP (eV)
WN_2- P62mmc	-1.82	-2.17
WN_2- P6m2	-0.91	-1.91
WN - NiAs	-0.84	-1.36
WN - WC	-0.23	-0.77
W_2N	-0.03	0.7

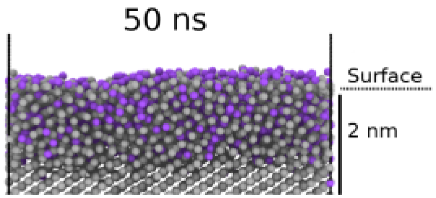
75 eV N Depth Profile

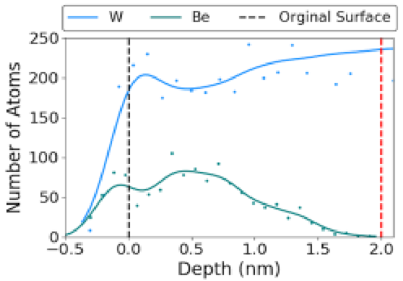


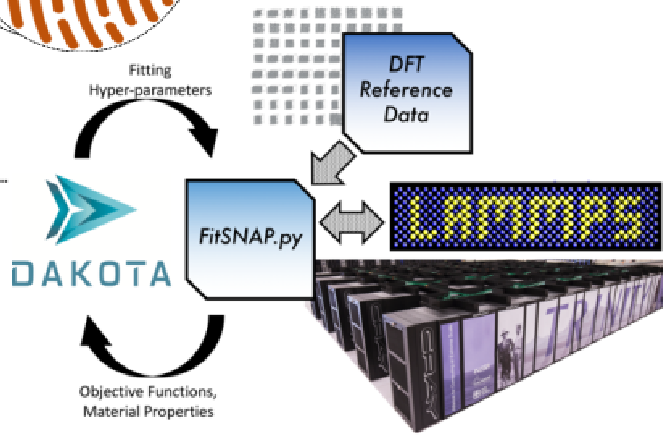
Summary

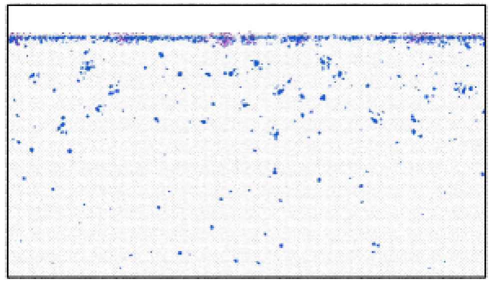
- Understanding material degradation in PFMs is critical for designing viable fusion reactors
- Atomistic modeling plays a key role in understanding relevant physical mechanisms for material degradation at the divertor
- A W-Be SNAP potential has been developed and used to study Be implantation in W and extended to simulation He implantation W-Be materials
- Beryllium will quickly form a mixed material layer in the near surface region which has some intermetallic structure
- The W-Be mixed layer alters helium diffusion, cluster formation, and depth profile
- Future work entails the development of one W-Be-H-He-N potential for st l interactions

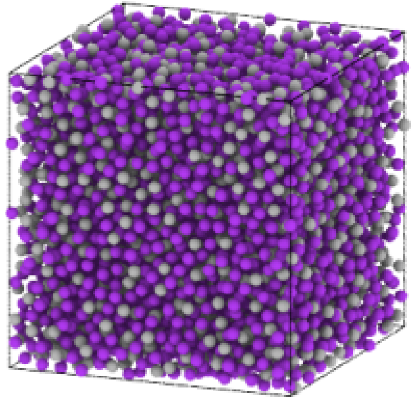












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EXASCALE COMPUTING PROJECT

Office of Science

Backup Slides

MD Approximations Change Over Time

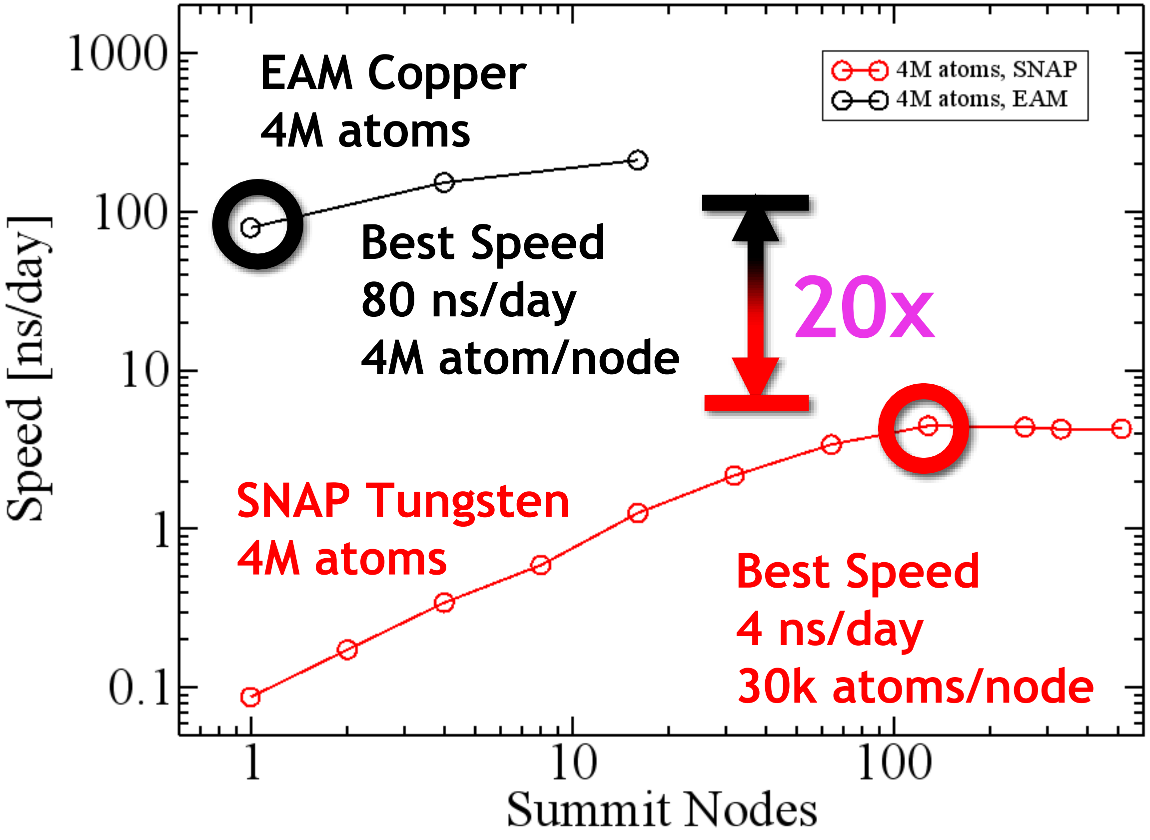
Twobody (B.C.)
Lennard-Jones, Hard Sphere, Coulomb, Bonded

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

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

Big Data / Deep / Machine Learning (2010s)
GAP, SNAP, NN,…

GPU Timings



Gayatri, Moore *et al.* (2020) https://arxiv.org/abs/2011.12875

Resources are limited, which is your best choice?