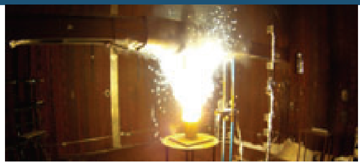
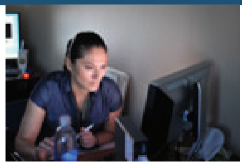
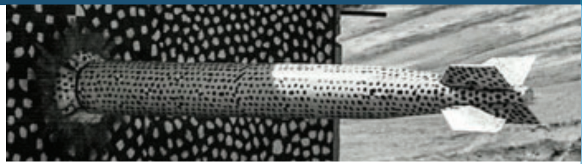
Multiscale Modeling of Materials for Fusion Energy

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Sandia National Laboratories

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ANS Lightning Talk

February 23, 2021

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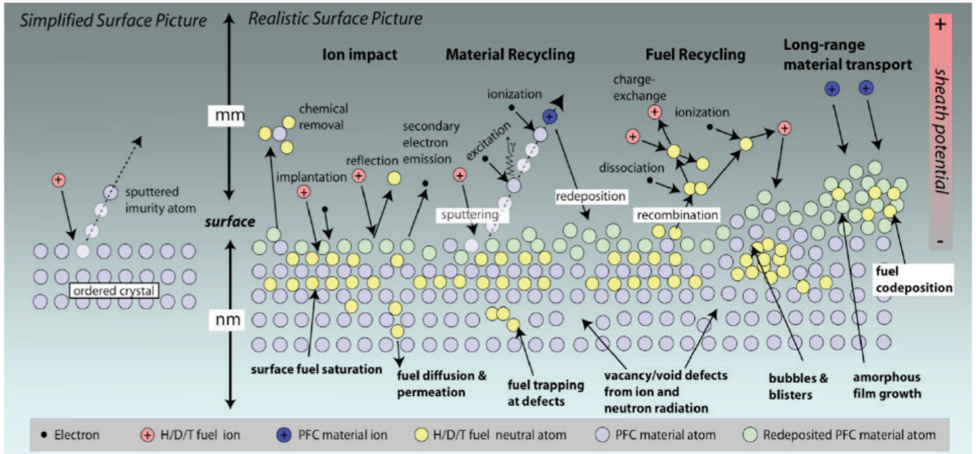
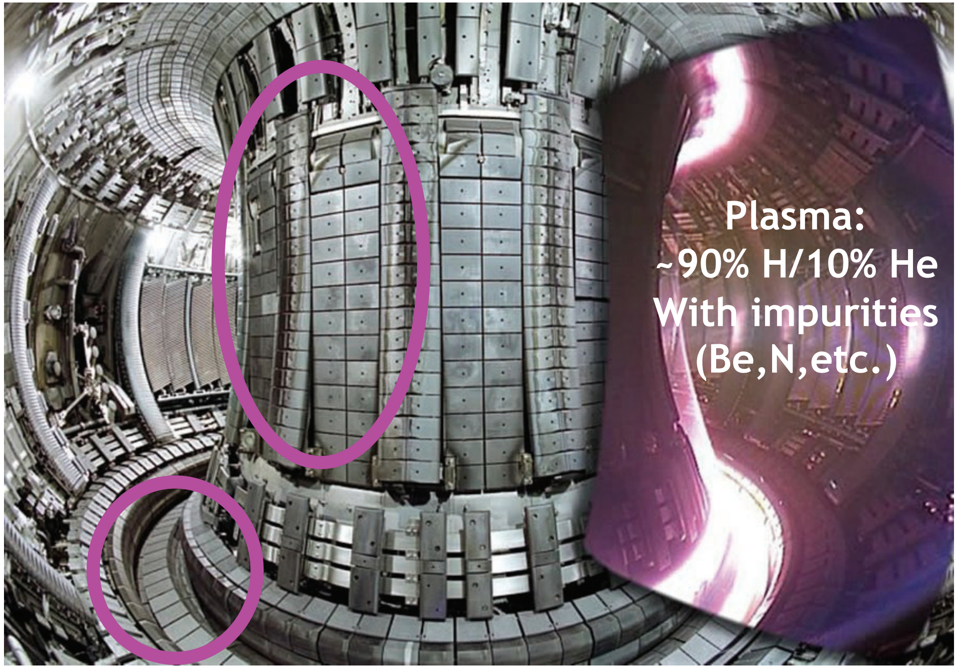
Materials for Fusion Energy

- 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

Beryllium First Wall



Tungsten Divertor

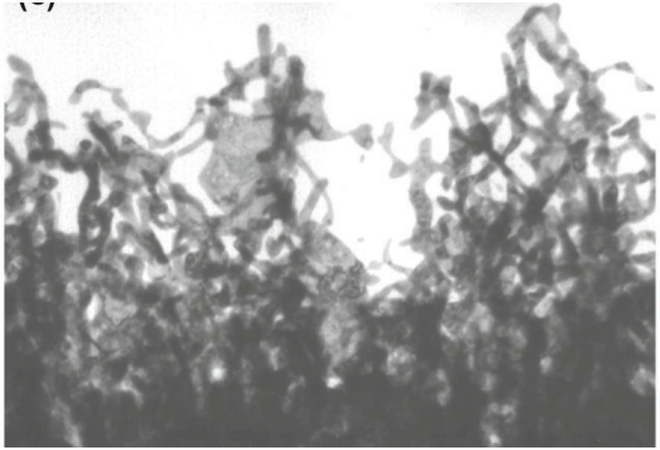
iter.org

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

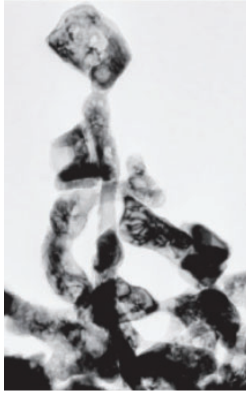
Plasma Material Interactions in Tungsten

Material Degradation

Helium Fuzz Growth

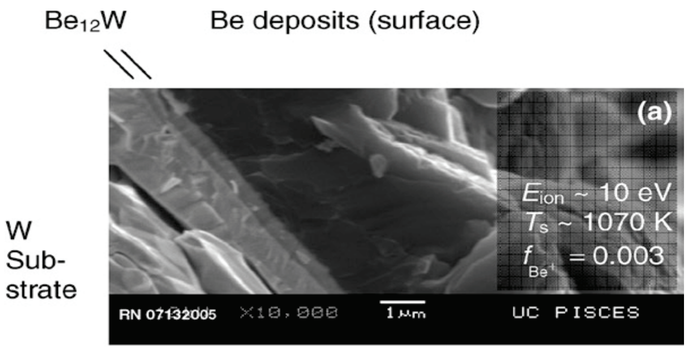


Kajita, et al. J. Nucl. Mater, 418, (2011) 152-158



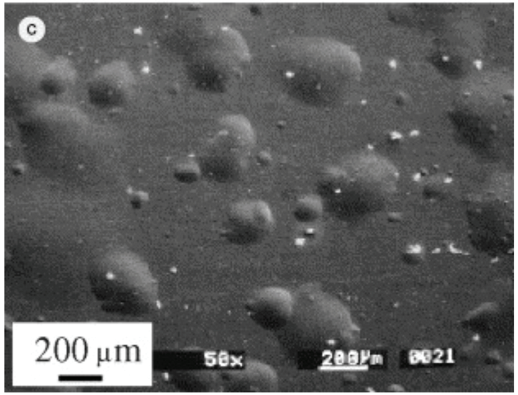
Kajita, et al. Nucl. Fus. 471, 886-890 (2007)

W-Be Intermetallics



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

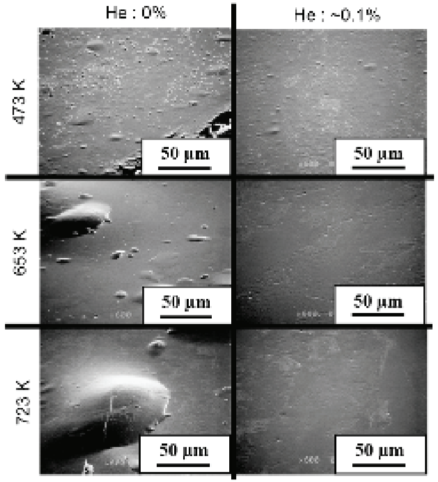
Hydrogen Blisters



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

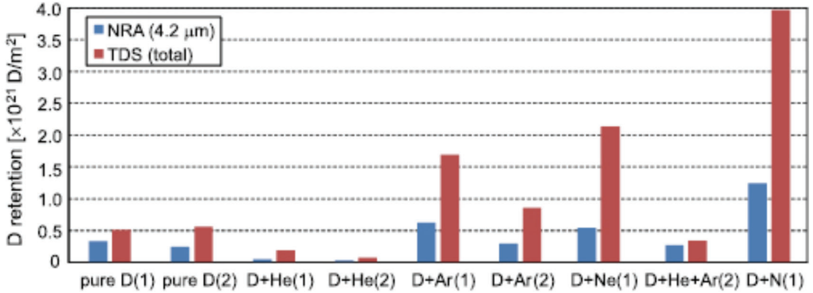
Tritium Retention

Effect of He on H Blistering



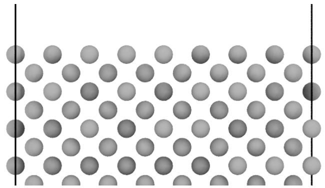
Ueda, et. al. J. Nucl. Mater. 386-388 (2009) 725-728

Effect of Plasma Impurities on Hydrogen Retention

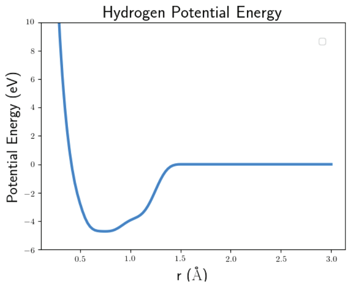


Kreter, et al. Nucl. Fus.. 59, 086029 (2019)

Multiscale Modeling of Materials



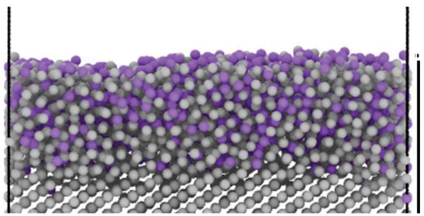
Initial Atom Positions and Velocities

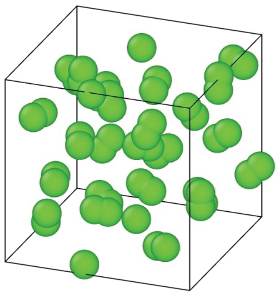


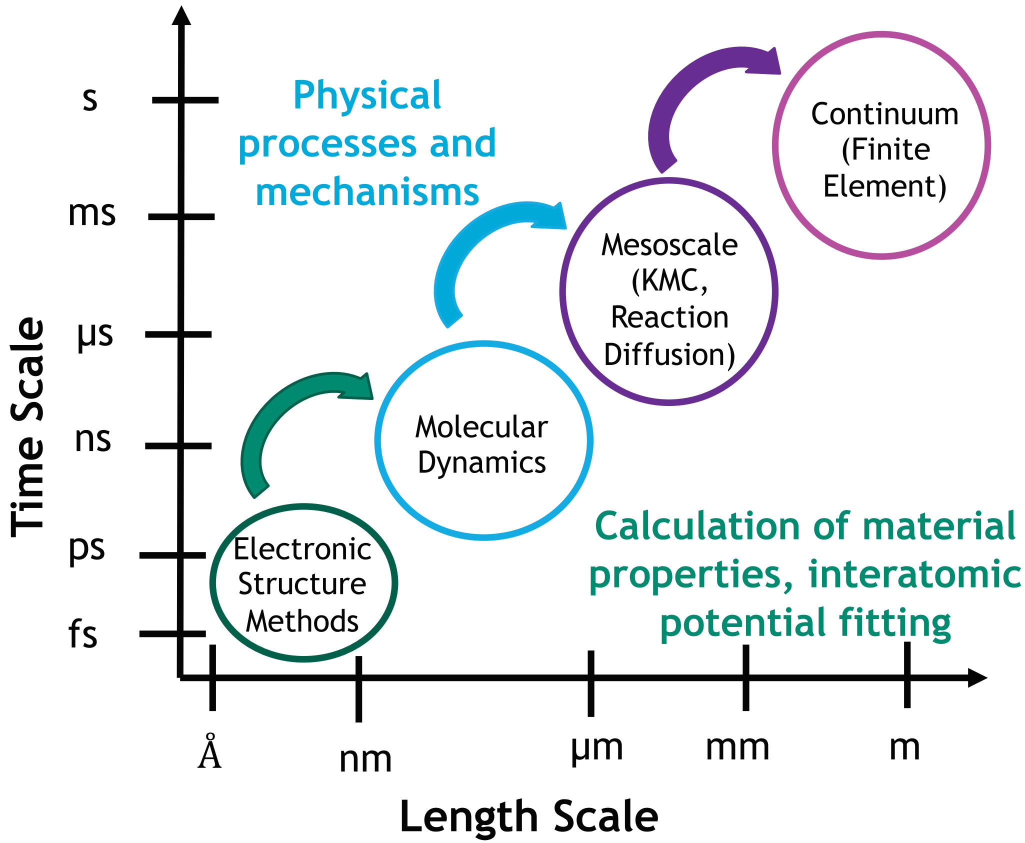
Interatomic Potential

Molecular Dynamics (LAMMPS)

Evolution of Material System Over Time



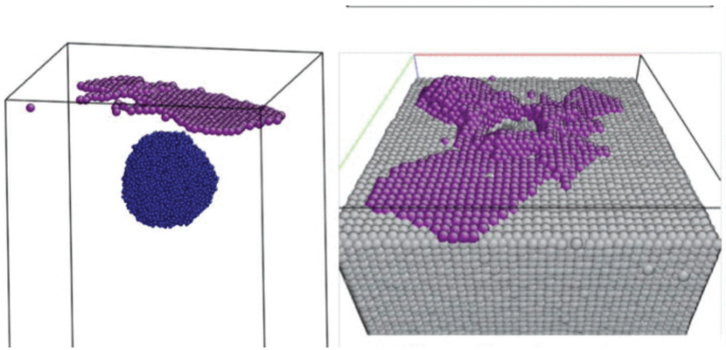




Each simulation technique can provide information to the next scale up

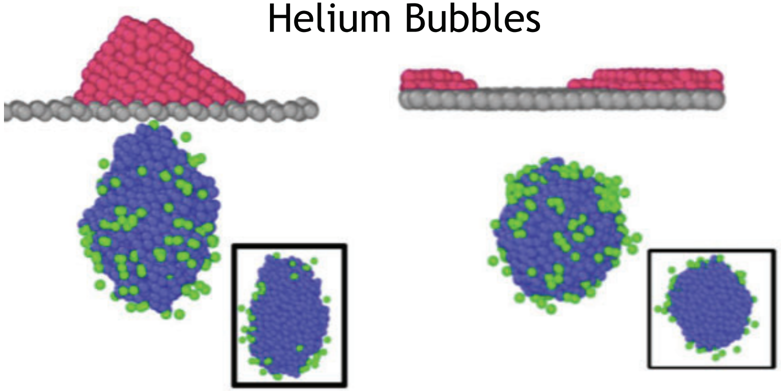
What Can MD Tell Us About Plasma Material Interactions?

Helium Bubbles Deform Tungsten Surface



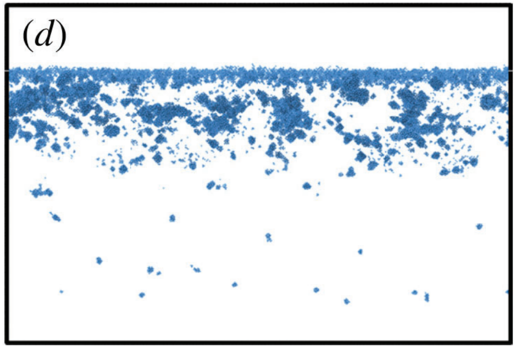
Sefta et al 2013 J. Appl. Phys 114 243518

Hydrogen Trapping at Helium Bubbles



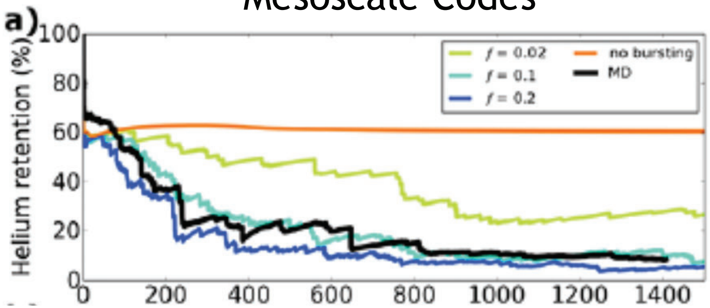
Bergstrom,et al. Fus. Sci. Tech., 71, 122-135, (2017)

Large-scale simulations of He implantation in W



Hammond et al 2019 Nucl. Fusion 59 066035

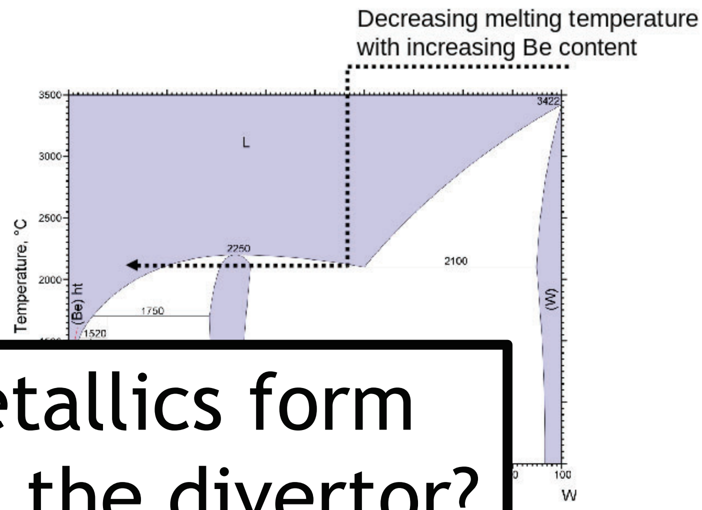
Using MD to Benchmark Mesoscale Codes



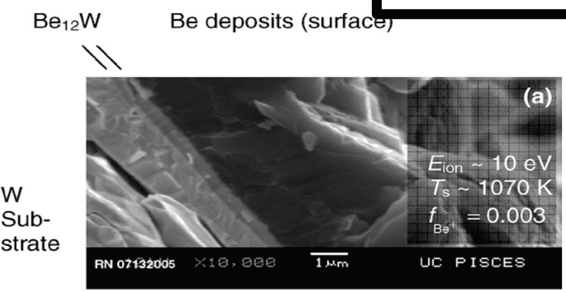
Blondel et al 2018 Nucl. Fus. 58 126034

Beryllium Effect on Tungsten Melting Temperature

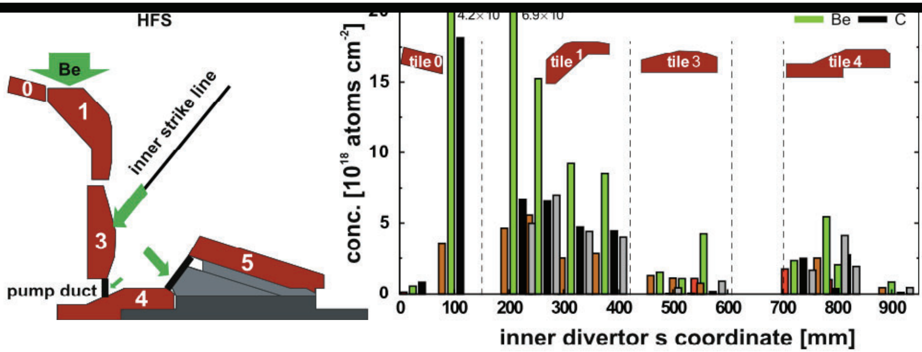
- W-Be intermetallics observed in linear plasma experiments
- Tokamak experiments indicated beryllium deposition on the divertor
- Phase diagram indicates decreasing melting temperature wit



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



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

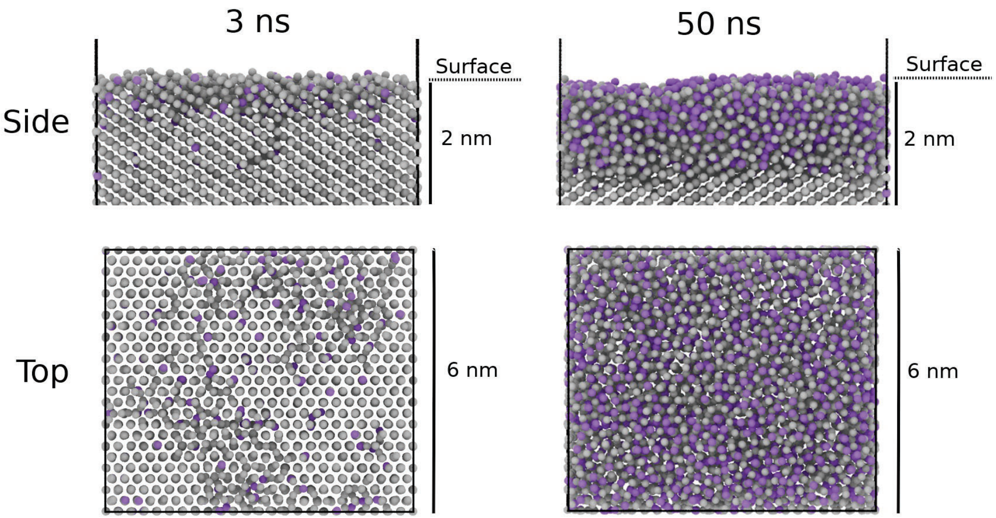


Brezinsek, et. al. J. Nucl. Mater. 463 (2015) 11-21

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

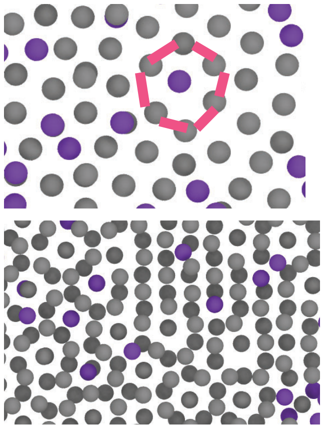
Beryllium Deposition on Tungsten Surfaces

Purple: Be
Gray: W

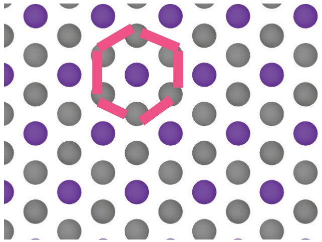


- **75 eV Beryllium Deposition**
  - Be implantation (75 eV) creates near-surface disordered layer
  - No Be diffusion beyond 2 nm
  - Ordered structures emerge within disordered layer
  - Clear restructuring of near-surface region occurs within nanoseconds

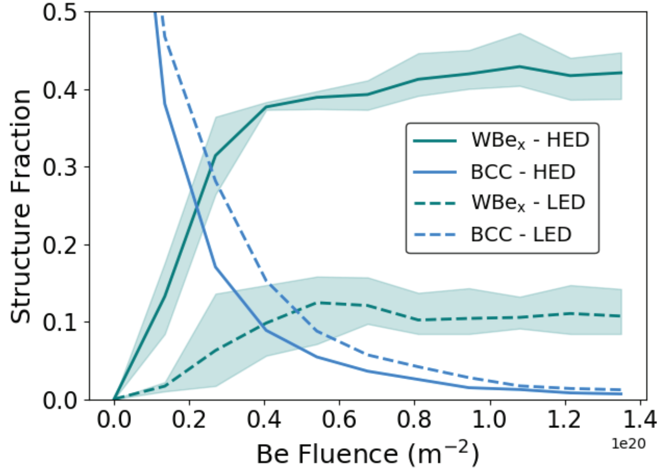
Implantation Simulations



Expected Ordered Intermetallic Structure

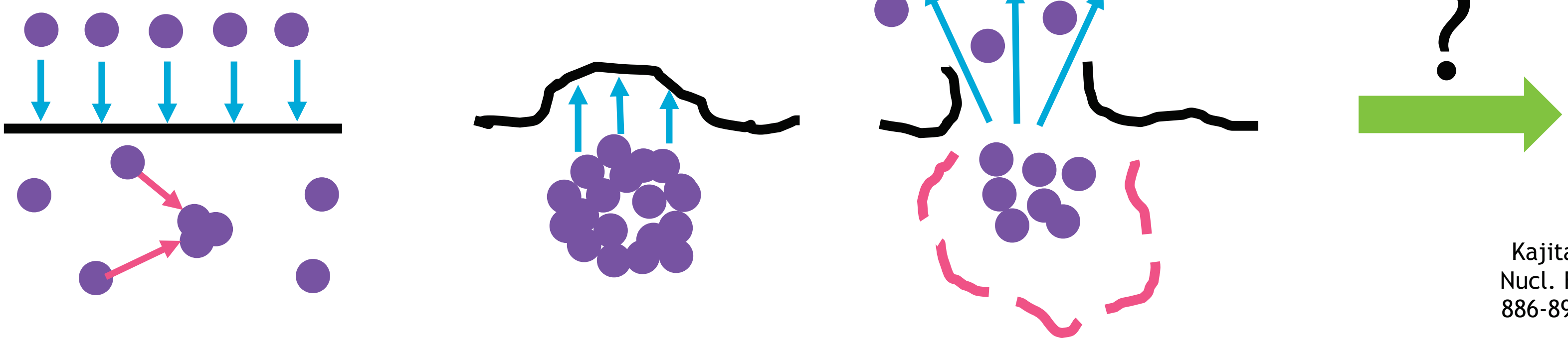


Intermetallic Growth Over Time

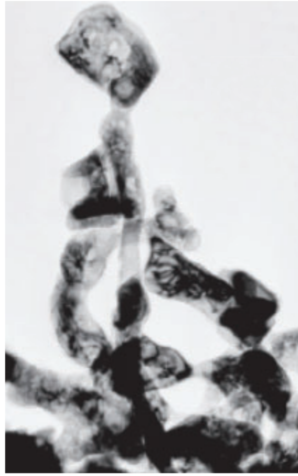


Mixed Material Effects in the Divertor

Purple: He Atom



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

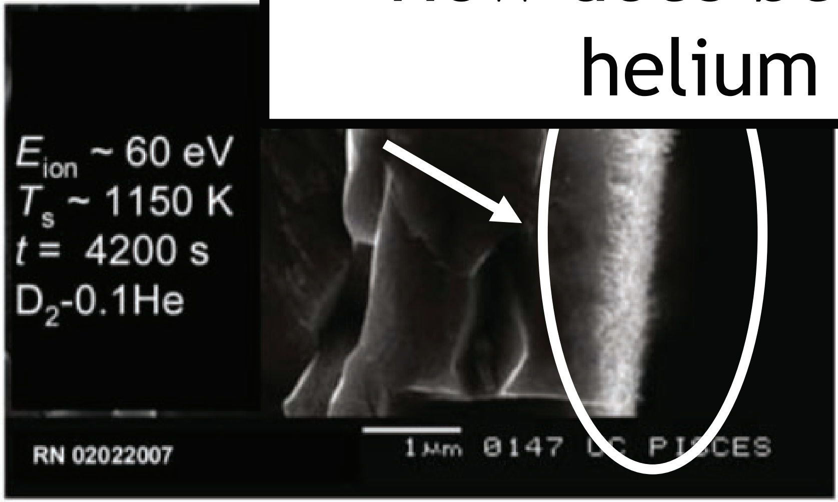


D$_2$ - 0.1 He Plasma

D$_2$ - 0.1 He with Be Plasma

How does beryllium disrupt the helium fuzz process?

W bulk



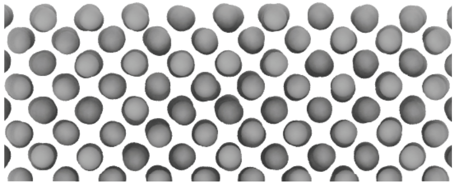
W bulk

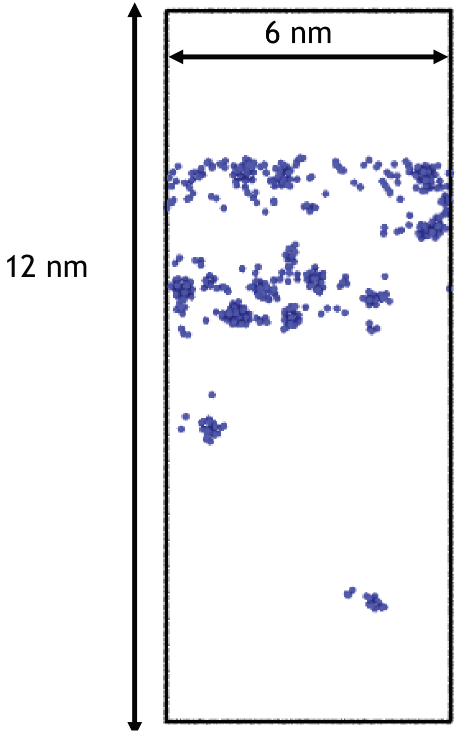
Baldwin, et al. J. Nucl. Mater 390-391, 886-890 (2009)

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

Increasing TIme

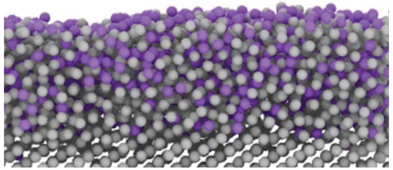
Crystalline W

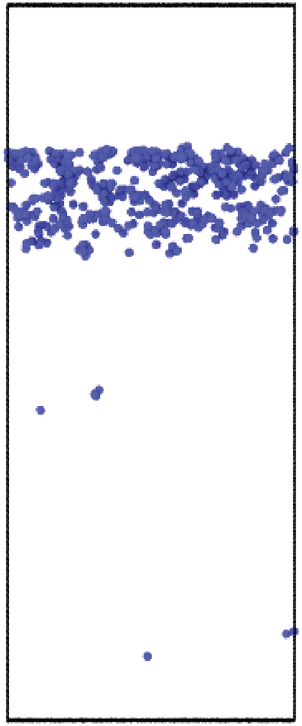




Tungsten:
Larger He clusters distributed throughout simulation cell

Amorphous W-Be

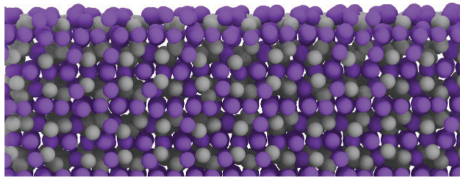


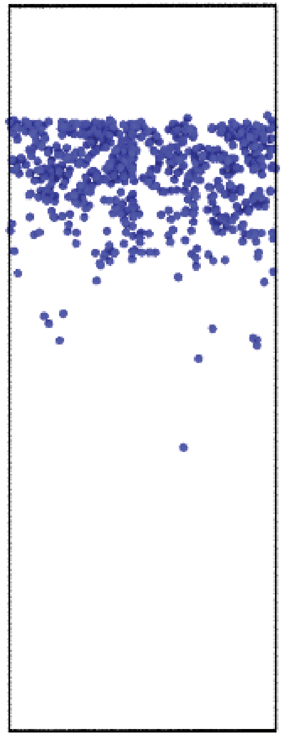


Blue: He
Purple: Be
Gray: W

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

WBe_2 C14 Structure

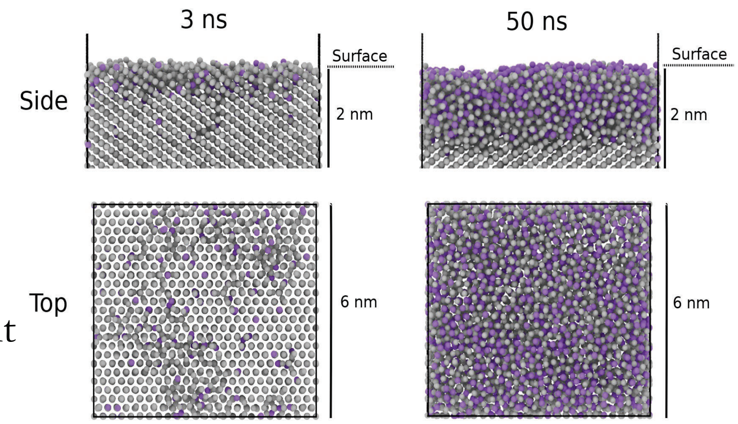


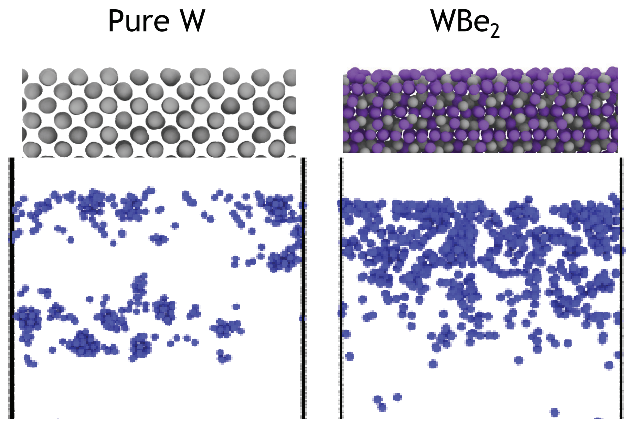


Cusentino, Wood, and Thompson, Nucl. Fusion, 60, 126018 (2020)

Summary

- Fusion reactor components are subject to high temperatures and high fluxes of multiple plasma species
- Understanding material degradation and tritium retention in these components is critical for designing fusion reactor components
- Atomistic modeling is a powerful tool that can provide insight into small/short scale processes that drive material degradation and are difficult to observe in experiments
- Simulations of beryllium deposition in tungsten indicated the formation of a disordered layer comparable to experimental observations
- The mixed W-Be layer affected the initial helium diffusion and bubble nucleation and growth which may affect helium fuzz growth





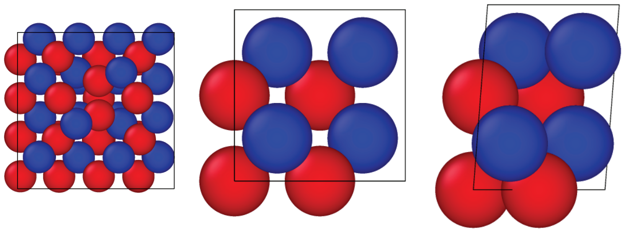
Contact:
mcusent@sandia.gov

SciDAC4-PSI2

What Makes a Machine Learned Interatomic Potential?

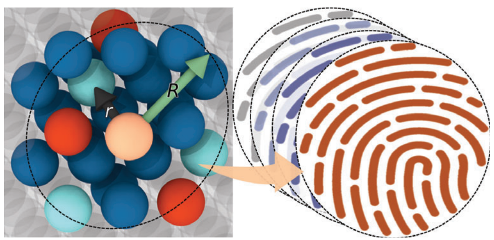
Training Data

- 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

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

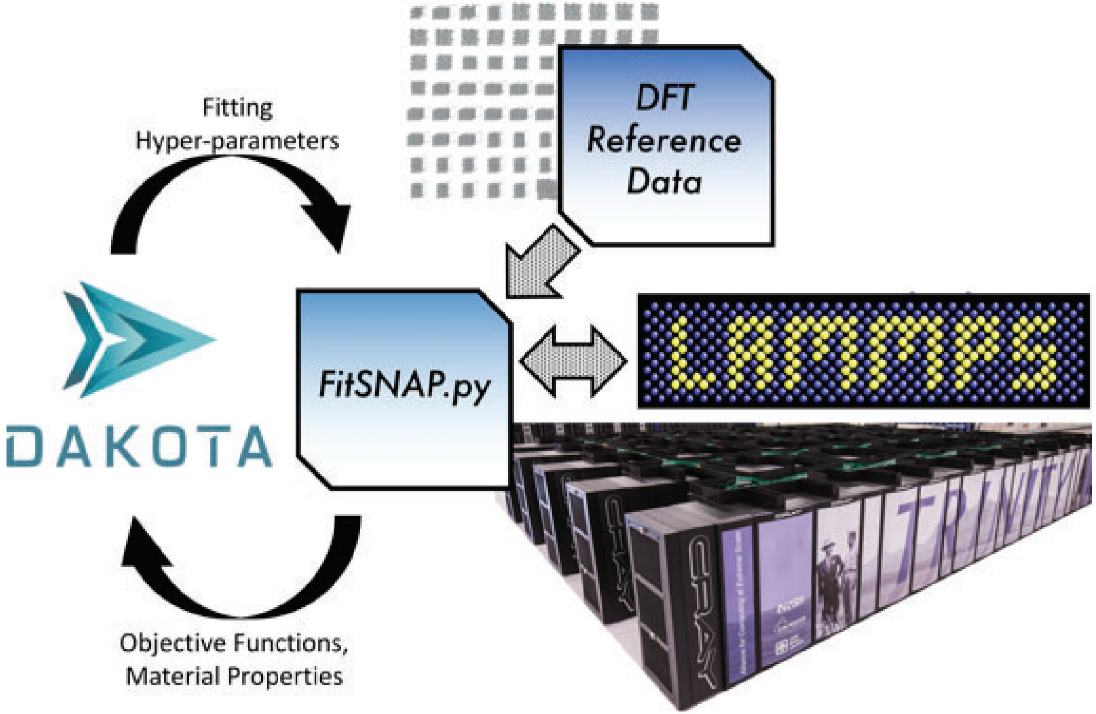
$$E_{SNAP}^i = \beta_0 + \sum_{k=1}^{K} \beta_k (B_k^i - B_{k0}^i)$$

Regression Method

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

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

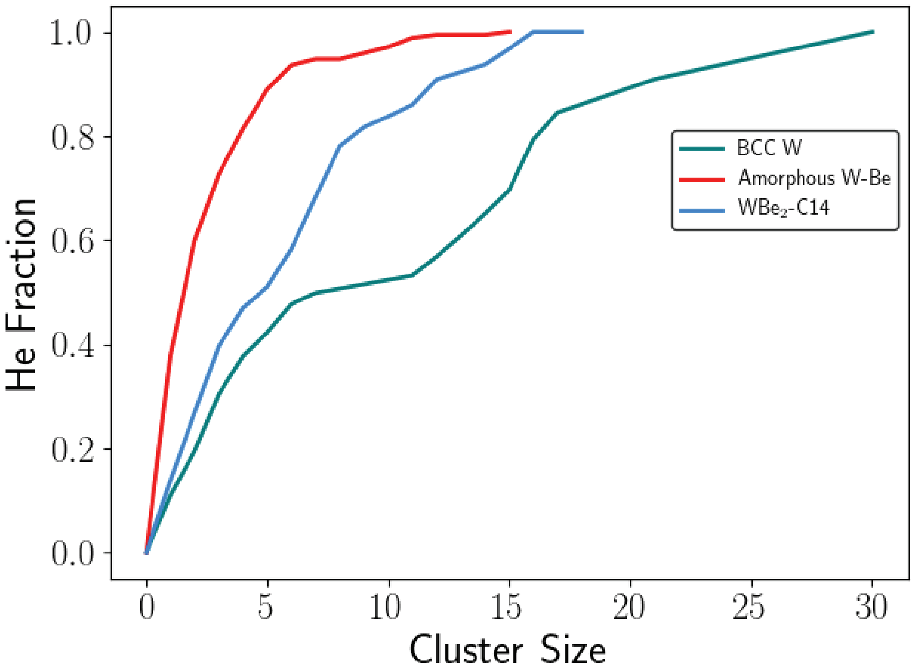
Weights   Set of Descriptors   DFT Training



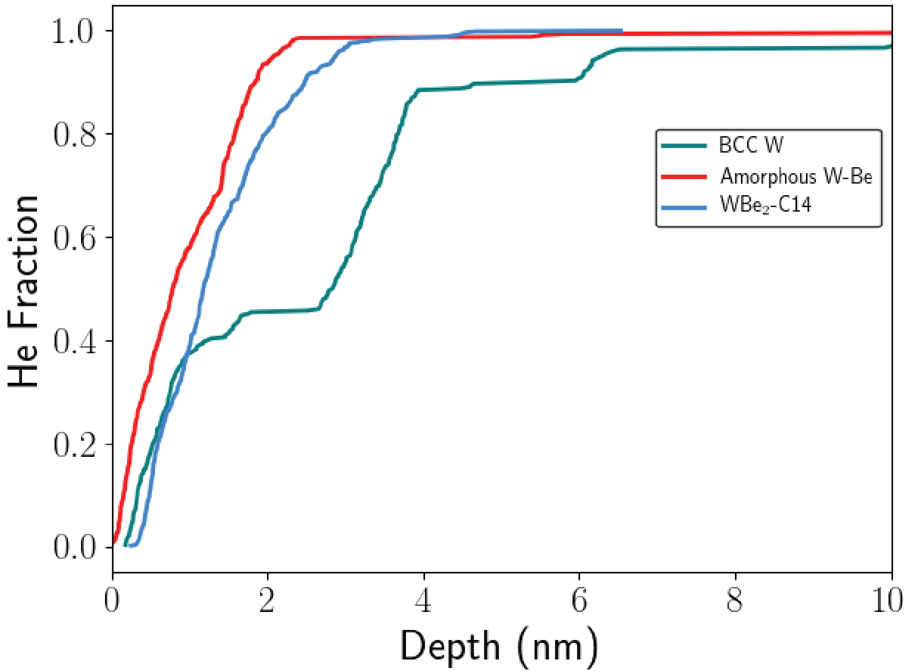
Code available: https://github.com/FitSNAP/FitSNAP

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

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



	He % Retention	Number of Clusters
W	36.7	85
Amorphous W-Be	49.3	172
WBe_2- C14	67.3	182



- Larger He clusters in pure tungsten and more, smaller clusters when Be is present
- Retention is much higher when Be is present
- He mostly remains within 2 nm of surface when Be is present

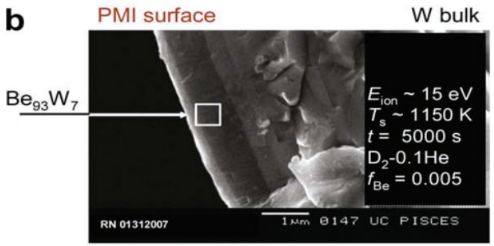
Cusentino, Wood, and Thompson, Nucl. Fusion, 60, 126018 (2020)

He Properties Change in W-Be Intermetallics

Lack of fuzz growth when Be is in plasma

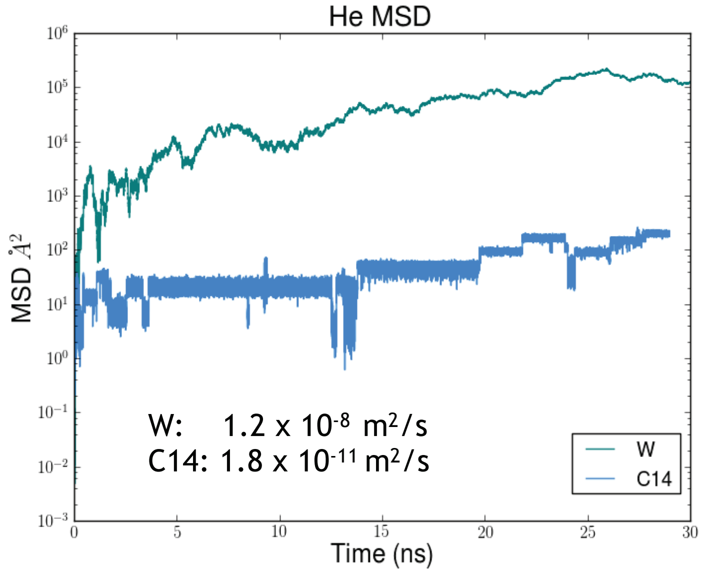
D_2 - 0.1 He Plasma

D_2 - 0.1 He with Be Plasma

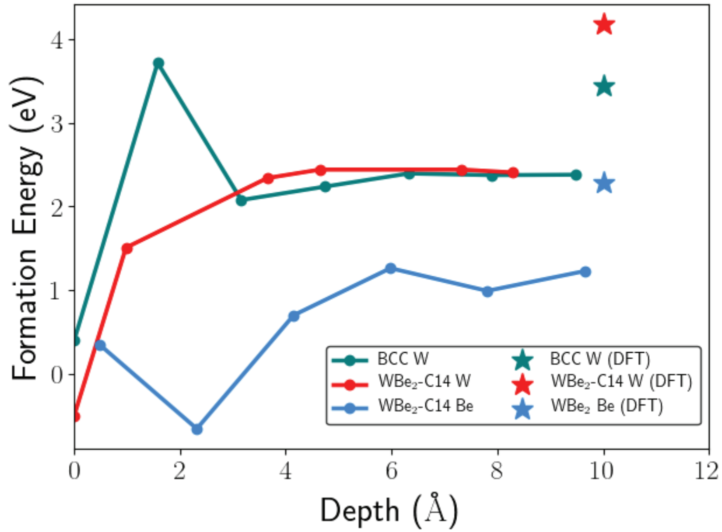


Baldwin, et al. J. Nucl. Mater 390-391, 886-890 (2009)

He diffusion is slower in WBe_2



Vacancy formation energy is lower in WBe_2



Combination of slower diffusion and lower vacancy formation energy in W-Be structures leads to smaller, more numerous He bubbles that remain near the surface