Development of SNAP Potentials for Fusion Reactor Materials

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²Center for Computing Research

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August 12 2021
Materials for Fusion Energy

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

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- High particles fluxes of $\sim 10^{24} \text{m}^{-2}\text{s}^{-1}$ of mixed ion species (H/He/Be/N etc.)

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

Plasma Material Interactions in Tungsten

**Helium Fuzz Growth**

![Image](image1.png)


**Material Degredation**

![Image](image2.png)


**W-Be Intermetallics**

Be$_{12}$W
Be deposits (surface)


**Hydrogen Blisters**

![Image](image3.png)

Plasma Material Interactions in Tungsten

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**Hydrogen Blisters**


**Tritium Retention**

Effect of He on H Blistering


**Effect of Plasma Impurities on Hydrogen Retention**


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Be₁₂W

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

**Tritium Retention**

**Effect of He on H Blistering**

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**

- $\beta$ vector fully describes a SNAP potential
- Decouples MD speed from training set size

\[
\min(||w \cdot D\beta - T||^2 - \gamma_n ||\beta||^n)
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Weights  Set of Descriptors  DFT Training
SNAP Definition and Work Flow

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Weights  Set of Descriptors  DFT Training

DFT Training

Set of Descriptors

Weights

Fitting

Hyper-parameters

DFT Reference Data

FitSNAP.py

DAKOTA

LAMMPS

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

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

<table>
<thead>
<tr>
<th>Description</th>
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<td>W-Be:</td>
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Be Defect Formation Energies in W (eV)

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<td>Tetrahedral</td>
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<td>[110] Dumbbell</td>
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<td>Octahedral</td>
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<td>Surface Bridge Site</td>
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W-Be Intermetallic Formation Energies (eV)

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Beryllium Deposition Results in Near Surface Mixed Layer

- High energy (75 eV) and low energy (0 eV) beryllium deposition on tungsten surfaces

Experimentally Observed W-Be Intermetallics

Beryllium Deposition Results in Near Surface Mixed Layer

- 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

Fluence: $1.4 \times 10^{20} \text{ m}^{-2}$

Cusentino, et al. Nucl. Fusion, accepted

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- Some intermetallic growth observed within mixed materials layer
- However, mixed materials layer appears to be kinetically trapped at MD time scales

**Experimentally Observed W-Be Intermetallics**

**Fluence**: 1.4 x 10^{20} m^{-2}
Cumulative He Implantation in W and W-Be at $2.5 \times 10^{19} \text{ m}^{-2}$

- Crystalline W
- Amorphous W-Be (Blue: He, Purple: Be, Gray: W)
- WBe$_2$ C14 Structure (Increasing Time)
Cumulative He Implantation in W and W-Be at $2.5 \times 10^{19}$ m$^{-2}$

**Crystalline W**

**Amorphous W-Be**

- **Blue:** He
- **Purple:** Be
- **Gray:** W

**WBe$_2$ C14 Structure**

- **Tungsten:** Larger He clusters distributed throughout simulation cell
Cumulative He Implantation in W and W-Be at $2.5 \times 10^{19}$ m$^{-2}$

**Crystalline W**

- Larger He clusters distributed throughout simulation cell

**Amorphous W-Be**

- Blue: He
- Purple: Be
- Gray: W

**WBe$_2$ C14 Structure**

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

Increasing Time
Extending SNAP for W-H and W-N

- Additional training data needed

- Pure H/N data:
  - Dimers, trimers, DT-MD of gas dimers

W: Grey  H: Green  N: Pink
Extending SNAP for W-H and W-N

- Additional training data needed
- Pure H/N data:
  - Dimers, trimers, DT-MD of gas dimers
- W-H and W-N data:
  - Bulk defects, monomers/dimers on surface, liquids
  - $W_xN_y$ bulk configurations
Extending SNAP for W-H and W-N

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• W-H and W-N data:
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• Additional objective functions added:
  • W-H/N bulk defect formation energies
  • H/N surface adsorption energies
  • $W_xN_y$ cohesive energies
Challenges in Developing W-H and W-N SNAP Potentials

- Have never used SNAP for gaseous species before
- Hydrogen and nitrogen training data is also more sparse compared to crystalline structures i.e. tungsten
- Difficult resides in how to get correct gas behavior (like forming dimers but not trimers) without inherent physics built-in to potential form
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Poor Clustering Behavior

Hydrogen Binding Curves

Poor Energetics

Atoms colored by potential energy
- Green is nominal H2 energy
- Reproduces correct binding curves
Changes to Fitting Results in Better Hydrogen and Nitrogen Potentials

- Modifications to fitting workflow yielded better results in reproducing correct gas species behavior
- Adjustments included:
  - Only including training data near potential energy well
  - Making radial cutoff much shorter (1.5 Å for H and 2.0 Å for N) compared to W (4.6 Å)
  - Adding extra objective function for dynamics behavior
  - Adjusted ZBL cutoff
  - Adjusted objective function for binding curves
### Tradeoff Between Surface and Bulk Behavior

**Potential for H on Surfaces**

<table>
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<tr>
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<tbody>
<tr>
<td>(100) Ads. Site Bridge</td>
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<td></td>
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<tr>
<td>(110) Ads. Energy -0.96</td>
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**NEB Surface Hop**

**Top-down Surface View**
Tradeoff Between Surface and Bulk Behavior

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<tr>
<td>$E^f_{Tot}$ (eV)</td>
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### NEB Surface Hop

**Top-down Surface View**

![Top-down Surface View](image1)

**NEB Bulk Hop**

![NEB Bulk Hop](image2)

**Bulk Tungsten**

![Bulk Tungsten](image3)
### Tradeoff Between Surface and Bulk Behavior

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#### Run DFT

- **Add To Training Data**

#### NEB Surface View

- **Top-down Surface View**
- **Bulk Tungsten**
- **NEB Bulk Hop**
- **NEB Surface Hop**

- **Bad** Surface
- **Bad** Bulk
Summary

- SNAP is a versatile ML interatomic potential that has been applied to a variety of materials including materials for fusion energy.
- 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.
- The current SNAP potential is being extended for W-H and W-N and SNAP can reproduce gas species behavior both in vacuum and in metals.
- Future work entails the development of one W-Be-H-He-N potential for studying fusion energy materials.

Contact: mcusent@sandia.gov
Backup Slides
MD Approximations Change Over Time

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<tr>
<td>Lennard-Jones, Hard Sphere, Coulomb, Bonded</td>
<td>Stillinger-Weber, Tersoff, Embedded Atom Method</td>
<td>REBO, BOP, COMB, ReaxFF</td>
<td>GAP, SNAP, NN,…</td>
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**GPU Timings**

- **EAM Copper**
  - 4M atoms
  - Speed: 80 ns/day
  - Best Speed: 4 ns/day
  - 30k atoms/node

- **SNAP Tungsten**
  - 4M atoms
  - Speed: 400 ns/day (20x faster)

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

![Graph showing computational cost vs. test error]

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
Testing Potentials: Hydrogen Implantation in Tungsten

- Interested in studying hydrogen implantation in tungsten and how it interacts within the material, especially with other plasma species or defects
- Initial testing of W-H SNAP potentials for hydrogen implantations
- 100 eV H implanted every 10 ps at 1000 K for (100) W surface
- Hydrogen correctly initially resides at tetrahedral interstitial site
- Diffusion barrier is somewhat high so diffusion is lower than expected
- EAM does not predict correct surface behavior and desorbs as H atoms as opposed to H₂ molecules