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Sandia National Laboratories

Machine Learned Interatomic Potential Development for W -ZrC

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1444 Computational Multiscale

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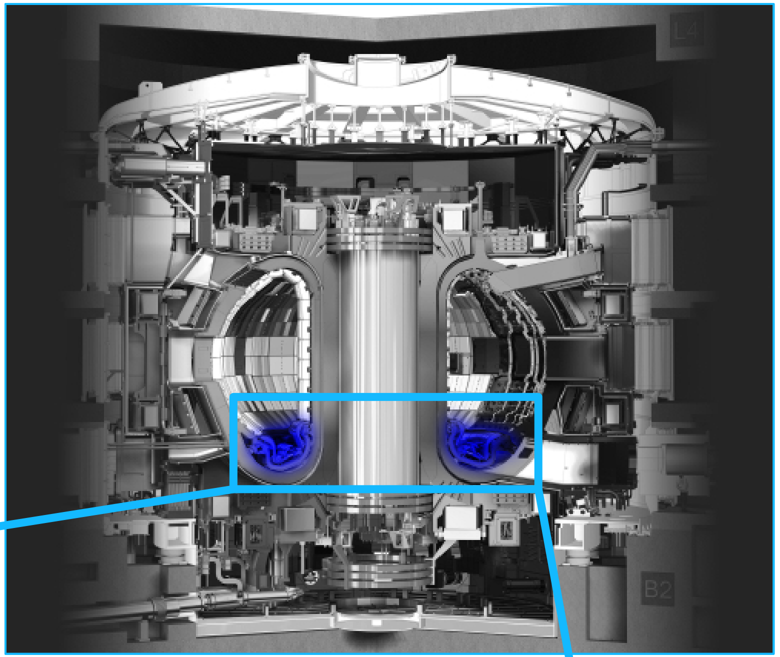
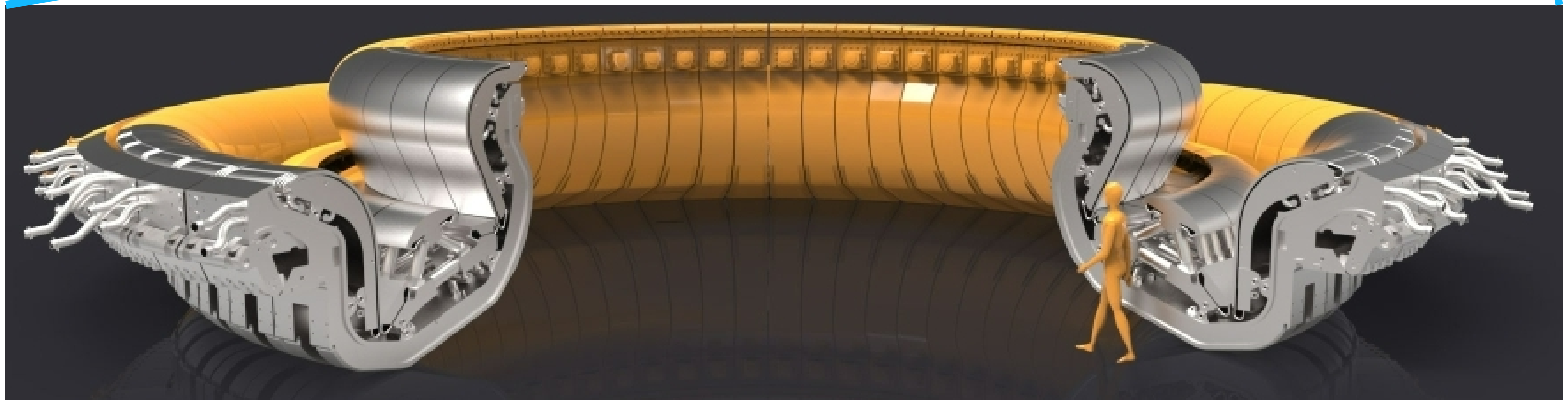
Divertor Materials for ITER and Future Fusion Reactors

- The divertor controls the exhaust of waste gas and impurities
- Withstands the highest surface heat loads, up to 20 MW/m^2
- Tungsten (W) has optimal thermomechanical properties for a plasma-facing material, but has a high ductile-to-brittle transition temperature
- Strengthening W with **zirconium carbide (ZrC) dispersoids** can improve mechanical properties





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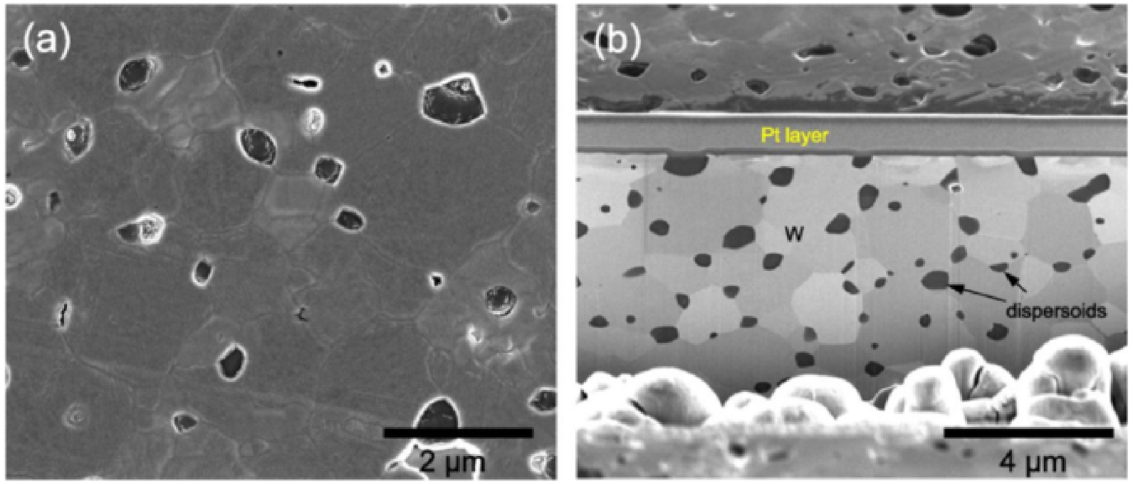
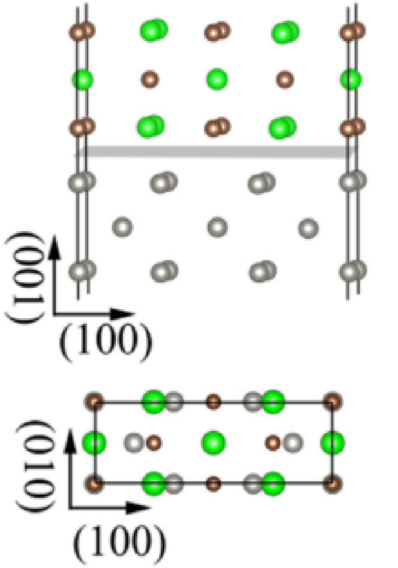
How can we investigate the mechanical properties of ZrC dispersoid-strengthened W?

- Plasma facing materials in ITER may experience temperatures > 2000 °C[1] which leads to W recrystallization and grain growth.
- W microstructural changes degrade strength, decrease fracture toughness, and enhance embrittlement.
- ZrC dispersoids have shown to improve ductility and limit grain growth.
- Mechanisms for these are still unknown and atomistic modeling can play a role in understanding these materials.



SEM of dispersoid strengthened W



[2]

DFT ~100 atoms

[1]E. Lang et al. / JNM 545 (2021) 152613
[2]X. Zhang et al. / Appl. Surf. Science 499 (2020) 143995

The Spectral Neighbor Analysis Potential (SNAP) can map quantum data to a classical interatomic potential.

Model Form

- Each neighbor position, (r, θ, ϕ), is mapped to a point, (θ_0, ϕ, θ), on the unit 3-sphere.
- The basis can be described with bispectrum components, B_k^i.
- Fitting the linear coefficients, β_k, produces the SNAP potential:

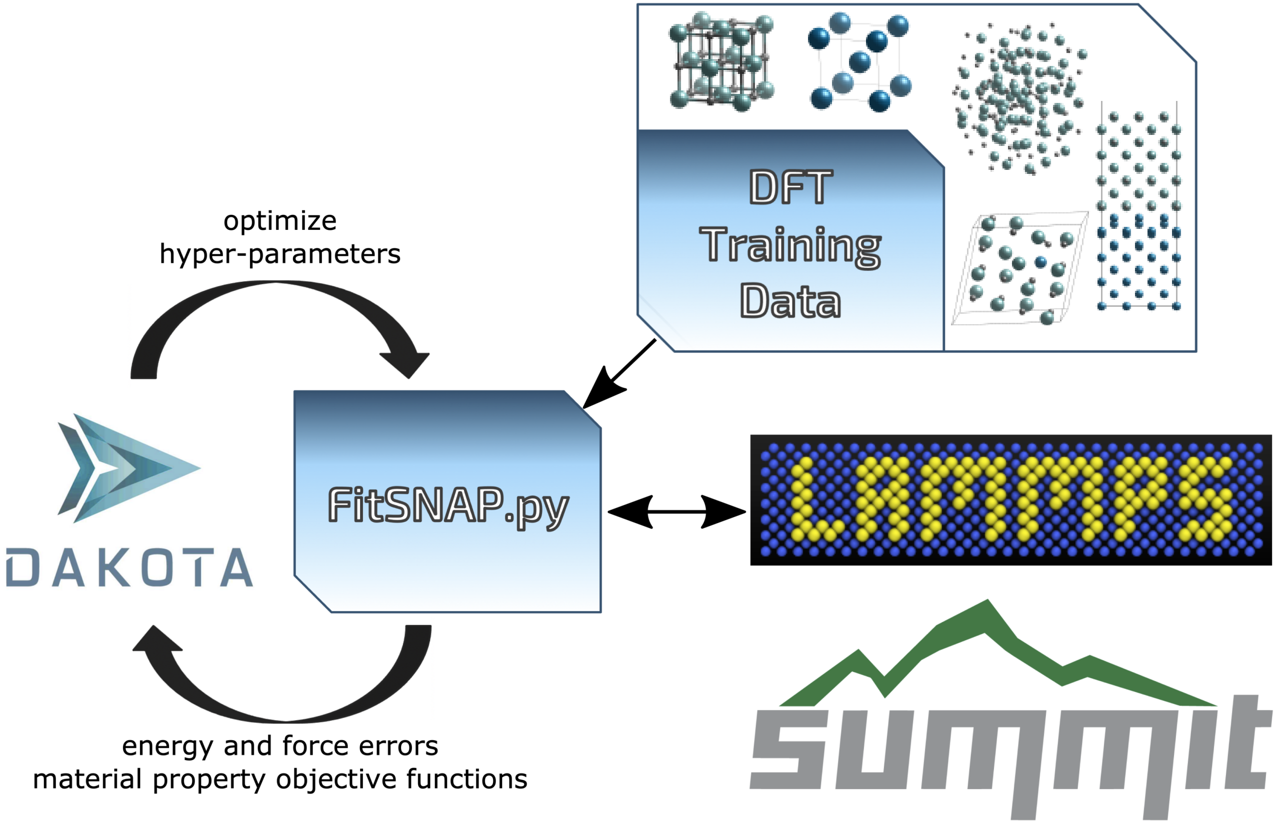
$$E_{SNAP}^{i} = \beta_0 + \sum_{k=1}^{K} \beta_k (B_k^i - B_k^i 0)$$

Linear Regression

$$\min(||\epsilon \cdot (D\beta - T)||^2)$$

group weight — descriptor prediction — DFT training

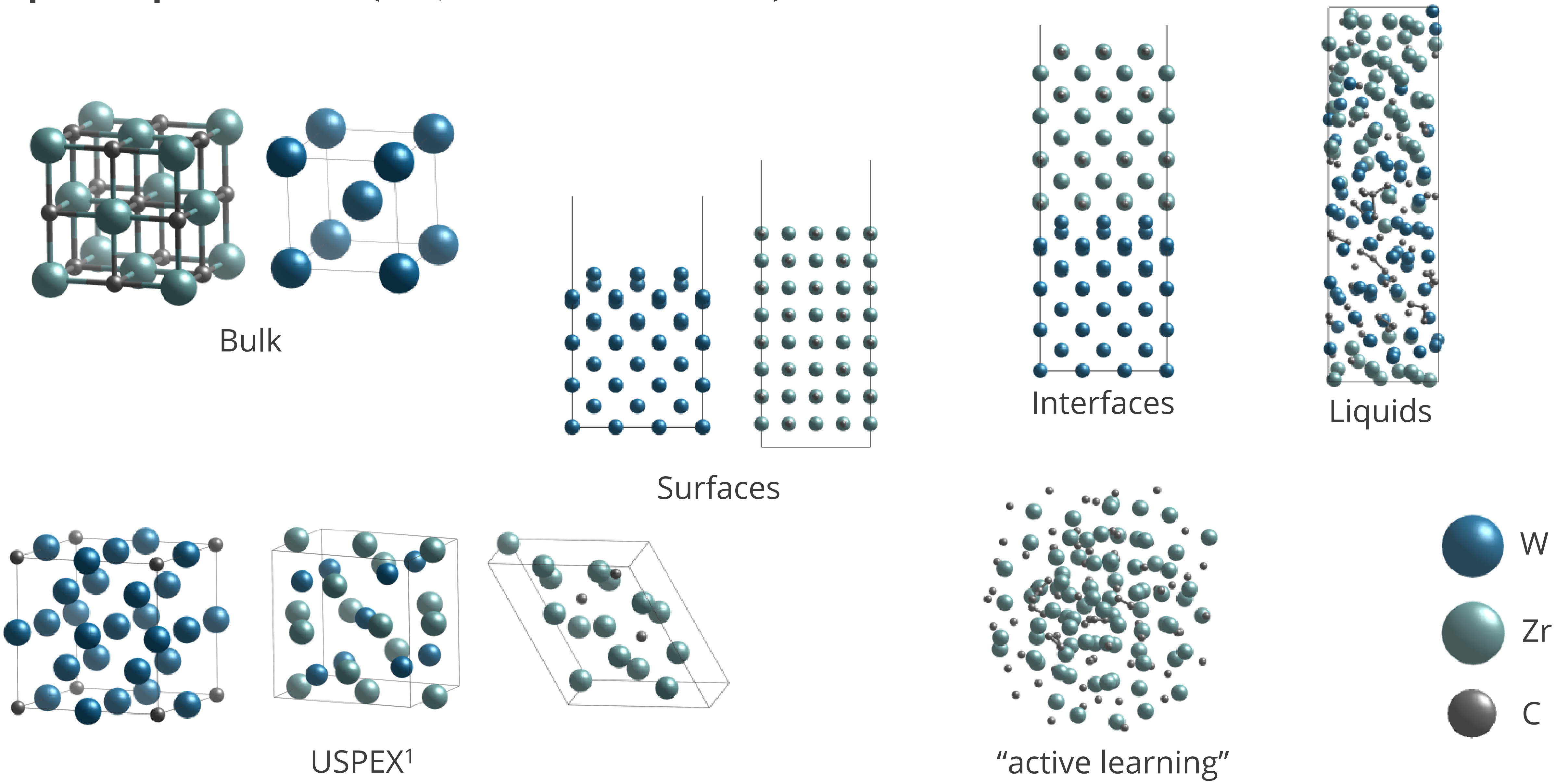
Work flow



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

M. Wood et al. / Phys. Rev. B **99** 184305 (2019)

The SNAP W-ZrC potential is trained on a variety of first-principles data (~8,000 structures).

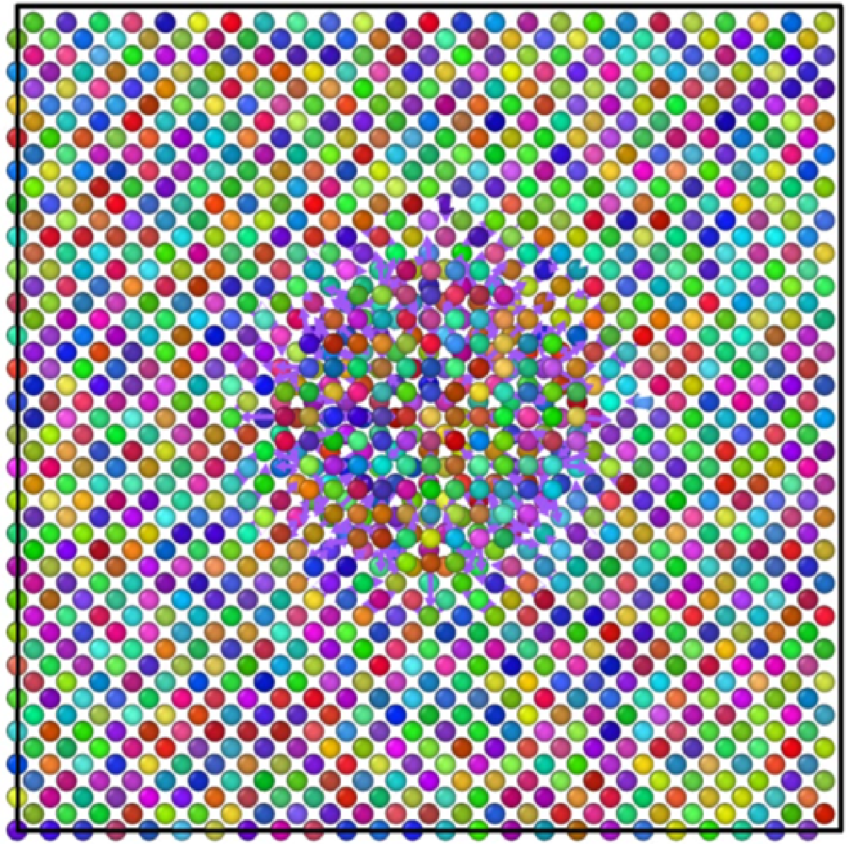


[1]A. Oganov et al. / J. Chem. Phys. **124,** 244704 (2006)

Candidate potentials need to be checked in NVT simulations for stability.

"Laminating"

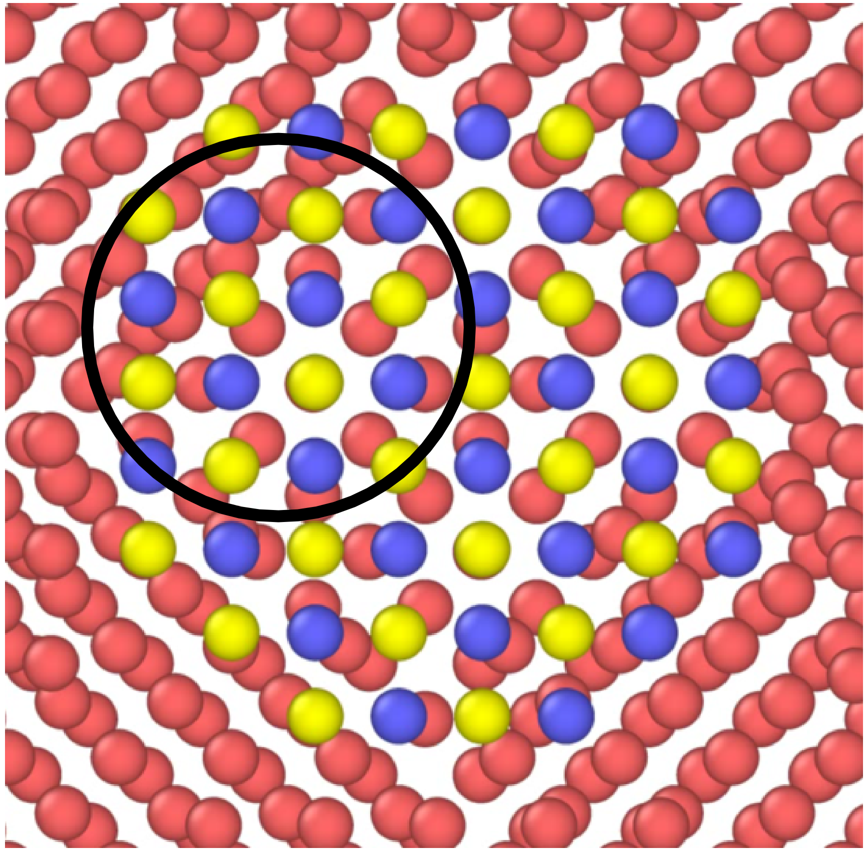
Cluster analysis <2.2 Å



$$\min\left(||\epsilon \cdot (D\beta - T)||^2\right)$$

- Increase group weight for forces on surface training data

"Black holing"



- Add compression data
- Tune zbl overlay
  - Increase repulsive diameter
  - Decrease radial cutoff

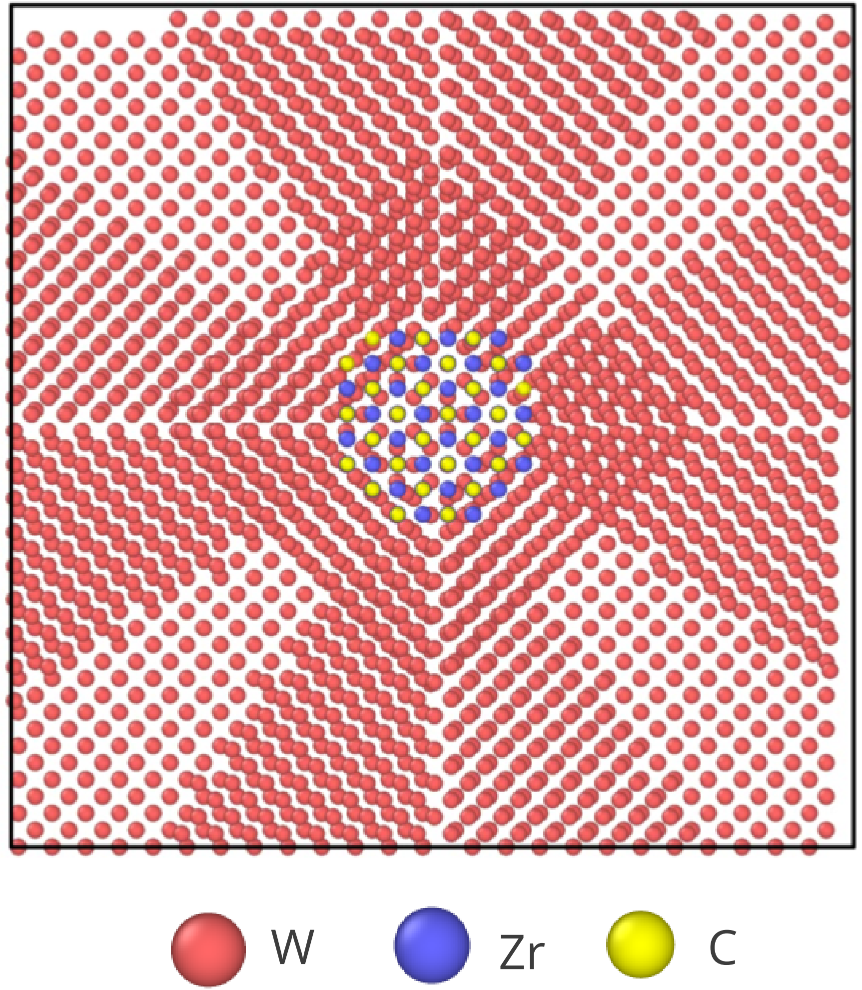
Genetic algorithm-generated SNAP potentials are narrowed down with MD tests.

- Potentials are tested on metrics including bulk modulus, *B* (GPa), and surface energies, E_{surf} (eV/Å^2).

	B_W	B_{ZrC}	E_{surf} W (100)	E_{surf} W (110)	E_{surf} ZrC (200)	E_{surf} ZrC (110)
DFT	301.4	216.0	4.13	3.18	1.63	3.31
SNAP	299.8	210.9	3.57	2.67	1.23	2.44

- MD minimization and NVT test simulations are performed to check potential stability.

- Best-performing potential is selected for large-scale tests and experiments.

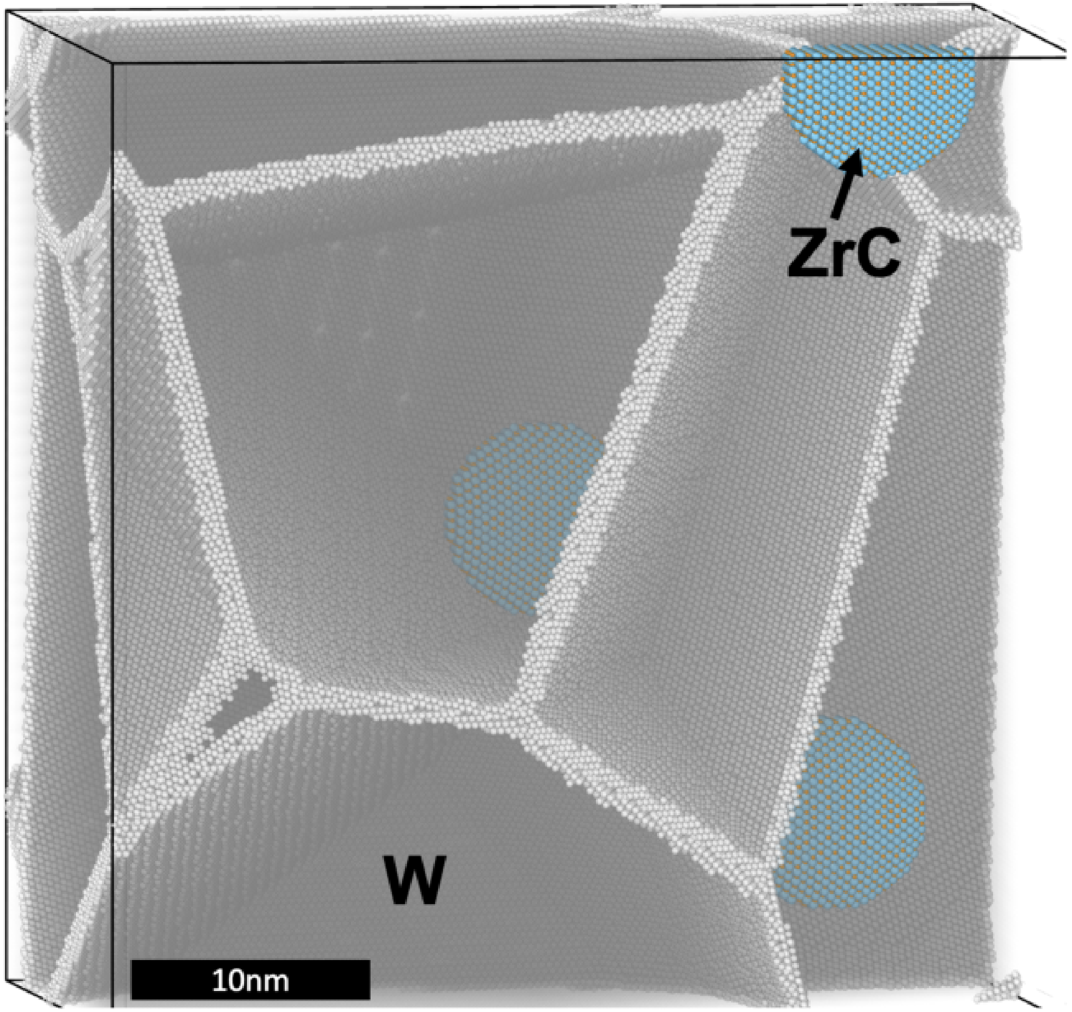


Example potential performance during minimize followed by NVT at 1000K.

Next steps: simulations on Summit (ORNL)

- Coherent interfaces
- Incoherent particles in W
- Material deformation at range of temperatures
  - 50 K (well below brittle--ductile transition)
  - 300 K (ambient conditions)
  - 1000 K (normal ITER operation)
  - 2500 K (approaching W melt)

- Other Summit simulations using SNAP:
  - Hydrogen (H) behavior in W in bulk and at interfaces
    - W-H SNAP: Mary Alice Cusentino
  - Radiation damage and recovery in refractory high-entropy alloys
    - Mo-Nb-Ta-Ti SNAP: Megan McCarthy



Example MD simulation geometry of ZrC dispersoid particles embedded in a polycrystalline W matrix

Thank you for your time.

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