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Sandia National Laboratories

Development of SNAP potential for ZrC strengthened W

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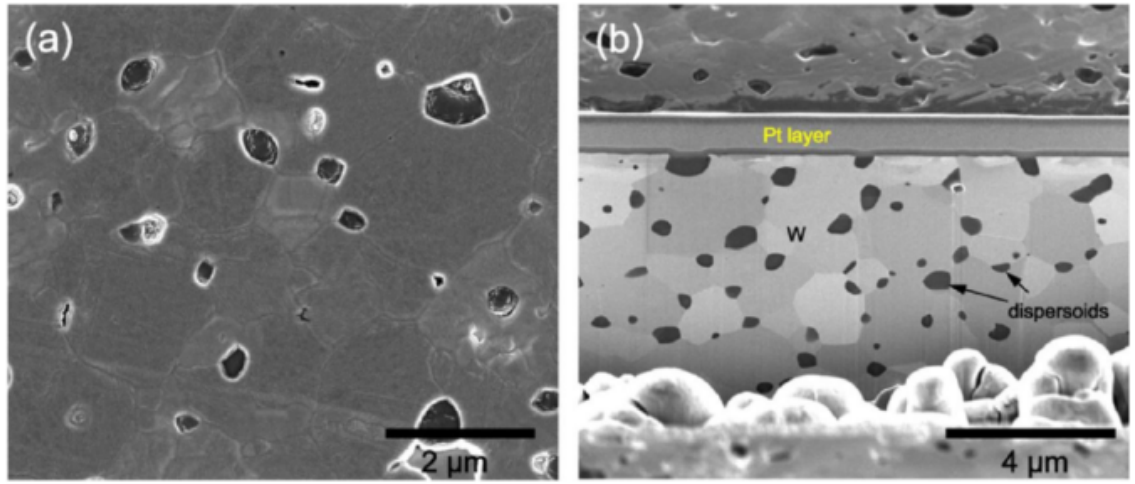
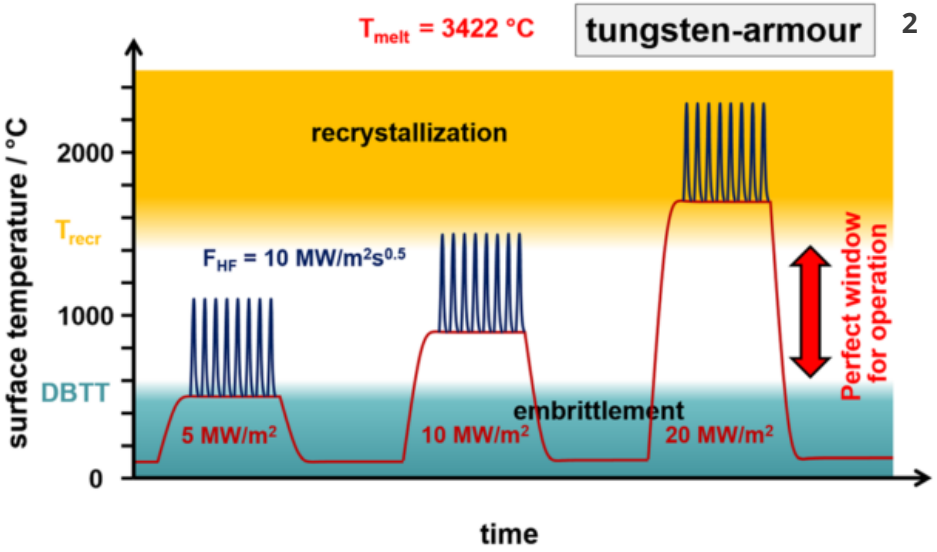
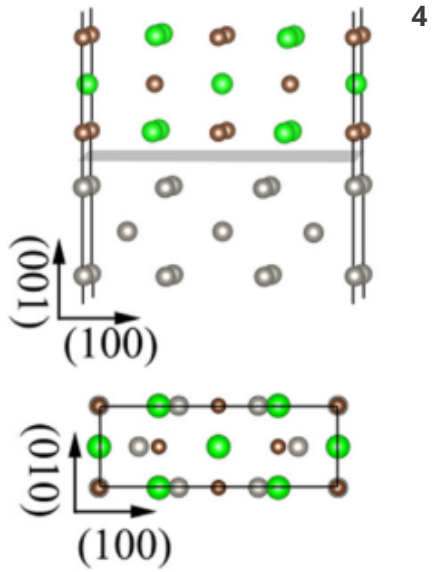
How can we investigate the mechanical properties of ZrC dispersoid-strengthened W?

- Plasma facing materials in ITER will experience high temperatures which may lead to W recrystallization and grain growth.[1,2]
- ZrC dispersoids have been shown to improve ductility and limit grain growth.[1,3]
- Effects on microstructure and mechanical properties are not fully understood and atomistic modeling can play a role in understanding these materials.



SEM of dispersoid strengthened W





Density Functional Theory (DFT) ~100 atoms

[1]E. Lang et al. / JNM 545 (2021) 152613
[2]J. Linke et al. / Matter Radiat. Extremes 4 (2021) 056201
[3]Z. Xie et al. / . Sci. Rep. 5 (2015) 16014
[4]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:

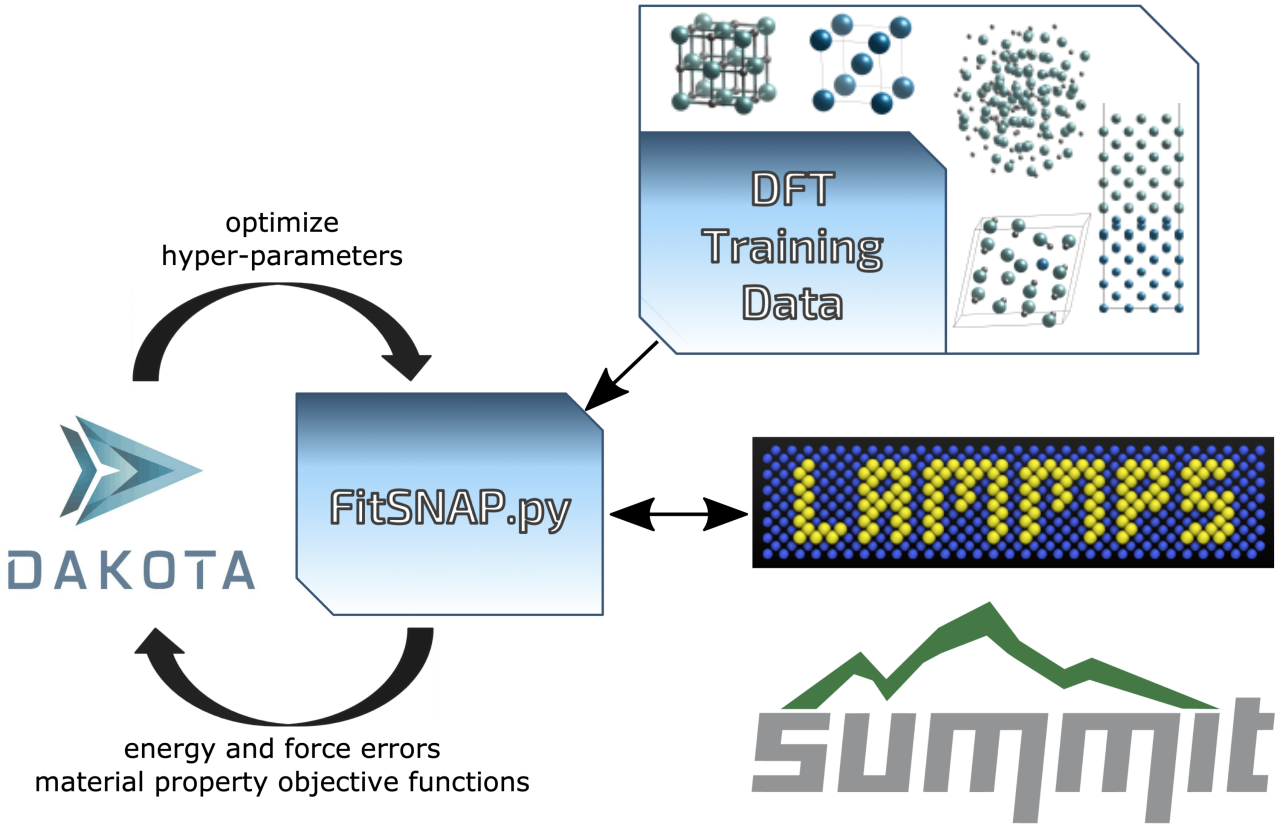
$$E_{SNAP}^i = \beta_0 + \sum_{k=1}^{K} \beta_k (B_k^i - B_k^i 0)$$

Linear Regression

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

group weight — descriptor prediction — DFT training

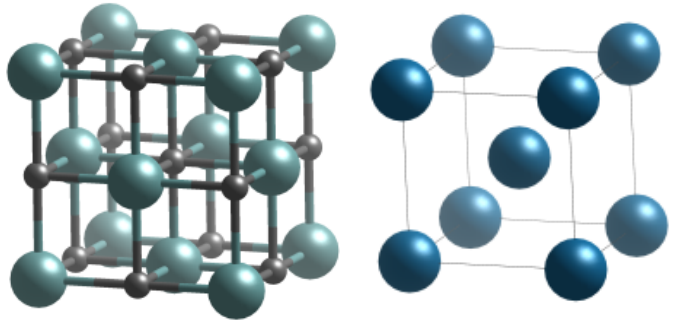
Work flow



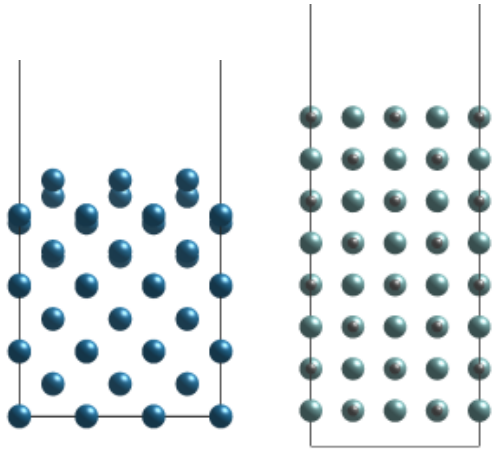
Code available: https://github.com/FitSNAP/FitSNAP

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

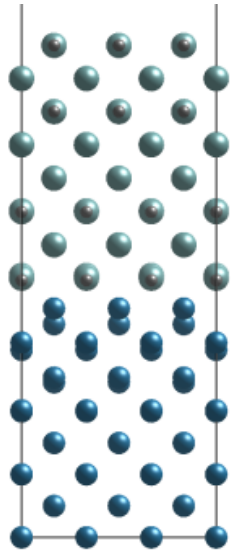
The SNAP W-ZrC potential is trained on a variety of first-principles data (~8,000 structures).



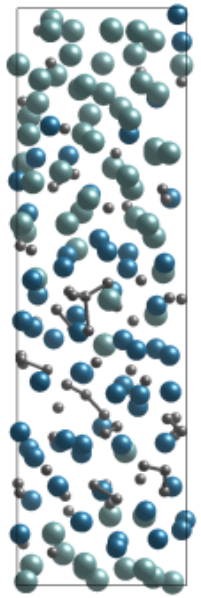
Bulk



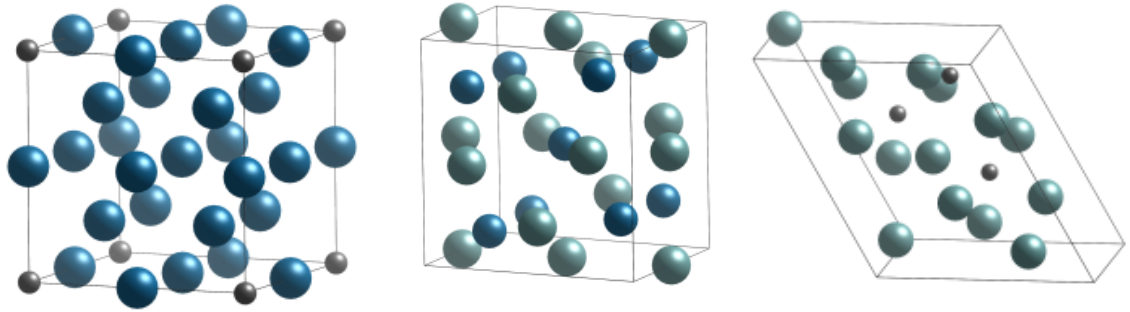
Surfaces



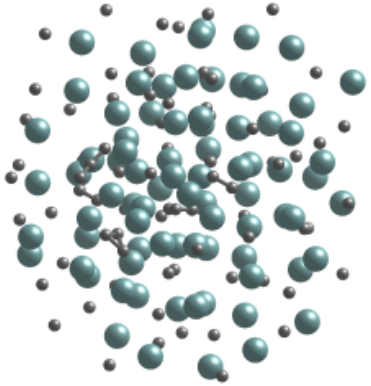
Interfaces



Liquids



USPEX[1]



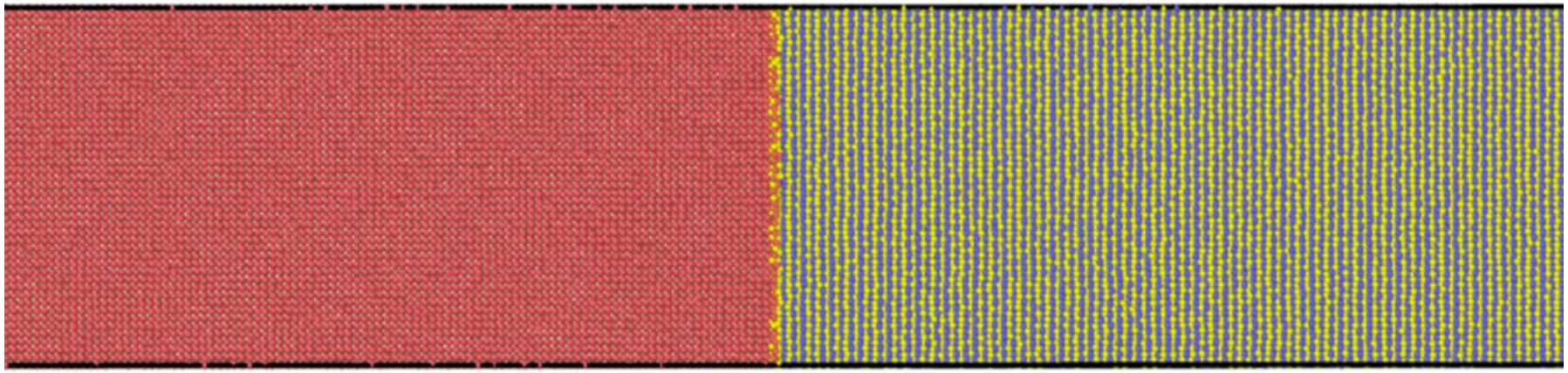
“active learning”

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

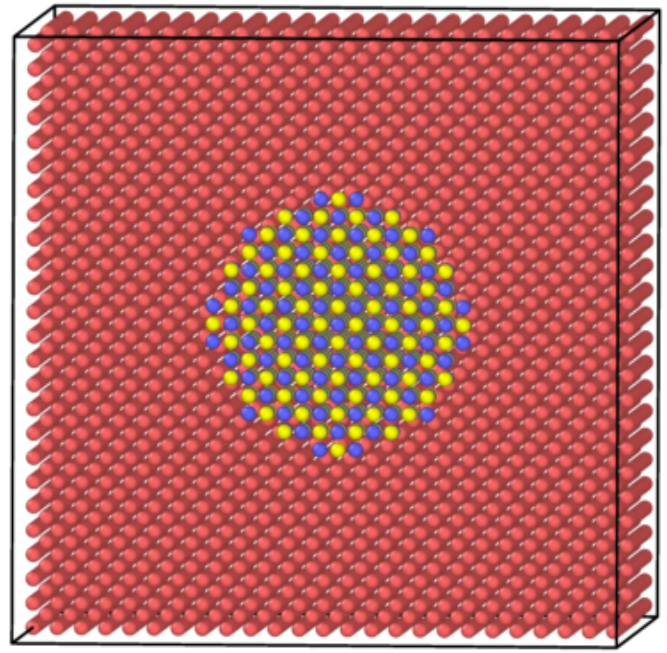
The W-ZrC SNAP potential agrees with DFT and runs Molecular Dynamics (MD) simulations at 2000K.

- Performance of the latest potential on 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 (100)	E_{surf} ZrC (110)
DFT	301.4	216.0	4.13	3.18	1.63	3.31
SNAP	300.9	221.9	3.68	3.38	1.77	3.15



Bicrystal simulation at 2000K (~400,000 atoms)

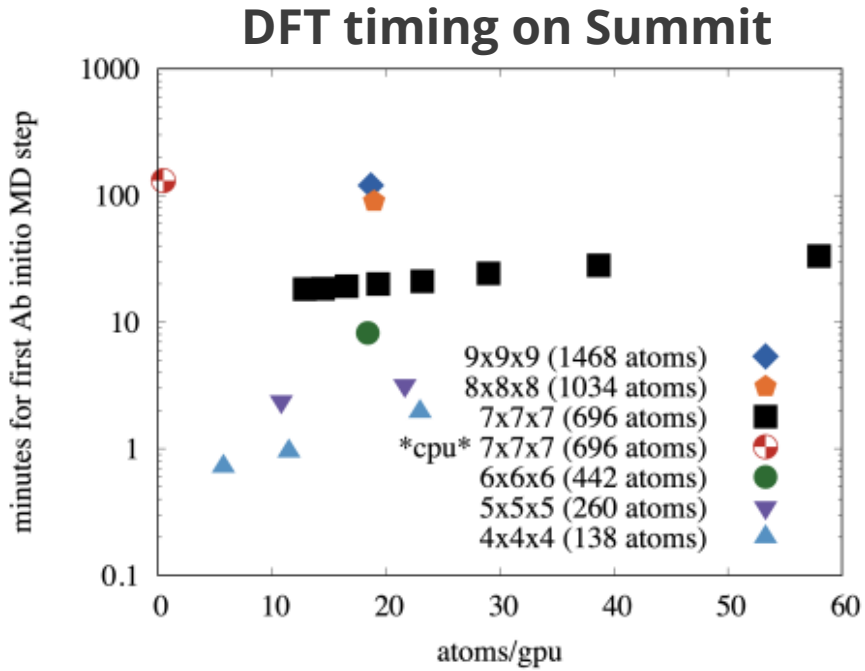


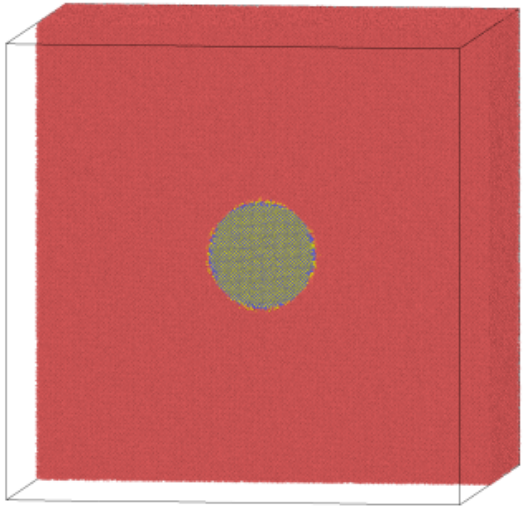
Embedded ZrC sphere - minimize followed by 2000K (~31,000 atoms)

W Zr C

Next steps: simulations on Summit (Oak Ridge National Lab)

- GPU acceleration
  - Generate DFT training data
  - Run large scale MD simulations out to nanoseconds, e.g. 10 million atoms on 256 nodes can run 5 ns in ~18 hours
- Geometries
  - Pure W with embedded ZrC
  - Polycrystalline W with embedded ZrC
  - Bicrystals of expected W-ZrC interfaces from experiment and DFT
- Investigate
  - Accommodation of strain at ITER temperatures
  - Effect of ZrC on thermal expansion





Spherical ZrC in crystalline W (~10 million atoms)

Thank you for your time.

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