Modeling Superalloys using Machine Learned Potential

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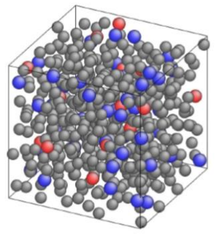
Introduction

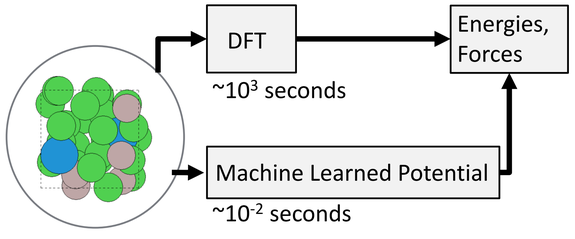
- Increasing demand for large aircraft engines and industrial gas turbines for power generation
- Turbine blades are made from superalloys, one of few materials that withstand the high temperatures and mechanical stresses in the engines

Above: Defects

- To understand conditions leading to defects, simulate local densities with quantitative models, the densities are difficult to measure experimentally

- Right Fig.: Previous work used molecular dynamics (MD) simulation with density functional theory (DFT), calculated densities to 2% agreement with available data[1]





- Machine learned (ML) potentials have been used in simulations successfully
- Previously, no ML potential for liquid alloys of several chemical elements
- This work will expand on knowledge of building ML potentials – learn physics otherwise not possible to simulate

Impacts

- Every turbine blade with a defect must be scrapped and reprocessed, equivalent to 49% loss in production costs[2]
- ML potentials save computing time on supercomputers
  Ex: ML potential decreased simulation cost from $185,000 to $500 [3]

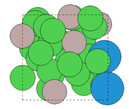
Objective

- Build neural network (NN) potential for Ni-Al-W
- Integrate ML potential with MD code to estimate thermodynamic properties of molten superalloys

Methods

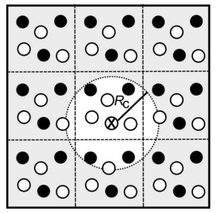
Select and generate relevant data required

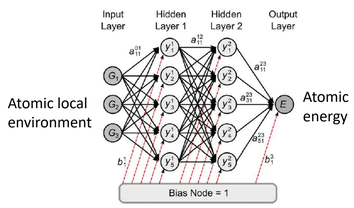
- MD trajectories using DFT (VASP)



Train model – Behler Parrinello NN

- Fingerprints characterize local atomic environments





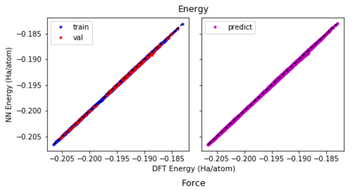
Validate potential and iteratively retrain

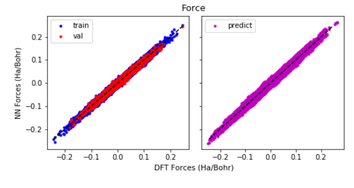
- Check error on atom configurations from MD trajectories not used during training

Results

Potential for Ni-Al-W

	Val	Predict
Energy RMSE (Ha/atom)	0.00009	0.00007
Force RMSE (Ha/bohr)	0.0047	0.0046

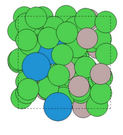




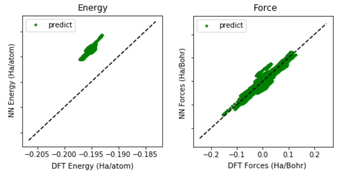
- Train/val: 90%/10% of 2080 points evenly sampled from 40 MD trajectories
- Predict: 10,920 points

Fingerprints contain radial and angular Behler symmetry functions (24 total) NN [24, 11, 11, 1]

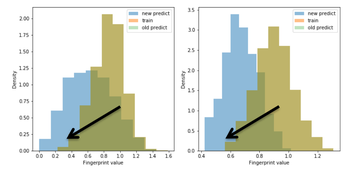
Model predictions on new data



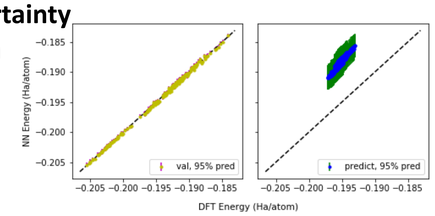
	New Predict
Energy RMSE (Ha/atom)	0.00656
Force RMSE (Ha/bohr)	0.0061



- New data has fingerprints outside the train distribution

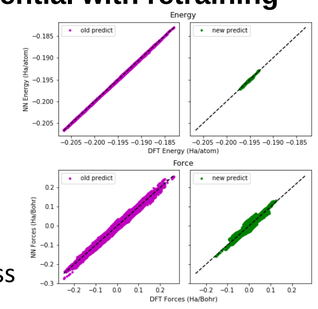


- ML potentials may extrapolate, which motivates a need for **quantitative model uncertainty**
- Uncertainty may be much larger if in extrapolation region

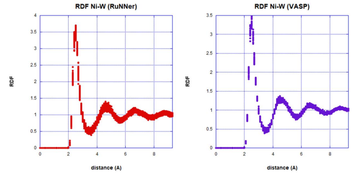


Systematically improve ML potential with retraining

- Model is more accurate after retraining with 5 – 10% of points added from each new trajectory.
- Current potential trained iteratively on atoms 32-500, temps 1720-2200K, different volumes
- Good parity on energy, force, stress



NVT simulation with ML potential agreed well with Ab Initio MD



- Calculated diffusion, viscosity, radial distribution function, coordination number, atomic volume
- 500 atoms simulation ran for 200,000 steps (10^5 fs) with energy conservation

Conclusions

- Determined parameters and procedures for building effective potentials
- ML potentials are accurate for Potential Energy Surface with enough training data
- ML potentials can be used with MD simulation to calculate material properties
- Uncertainty method can help determine prediction reliability and data regions of extrapolation

References

(1) Woodward et al. (2010) J. Appl. Phys. (2) Frueh et al. (2002) Mater. Sci. Eng. (3) Deringer et al. (2018) J. Phys. Chem. Lett. (4) Behler (2017) Angew. Chem., Int. Ed.