Modeling Solidification Shrinkage of Metals with Machine Learned Force Fields

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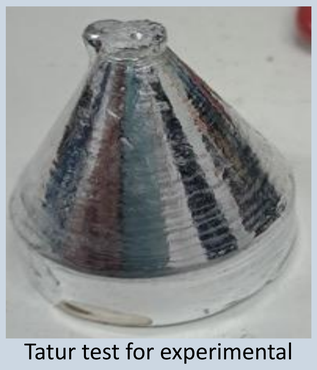
Background

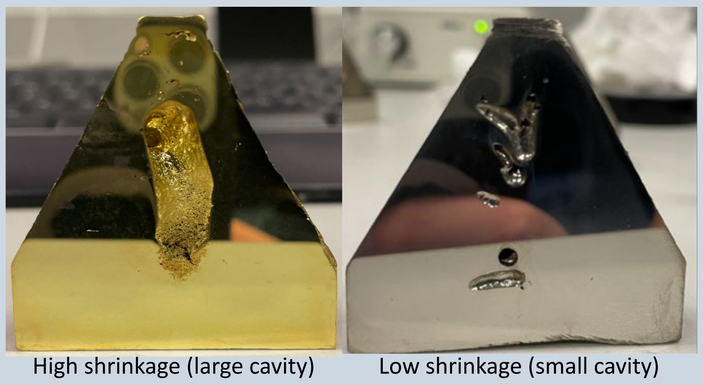
Our research seeks to understand alloy casting shrinkage by simulating atomic scale structures undergoing temperature changes.

- Volumetric shrinkage during the liquid-to-solid phase transition causes imperfections in cast metal products.
- High temperatures of liquid phase metal make experimental study difficult.
- Our group developed single-phase, high-entropy brasses (based on [1]) with a reduction in casting shrinkage.
- This work focuses on the liquid-to-FCC phase transition where the greatest shrinkage occurs.



Tatur test for experimental shrinkage

Cut in half



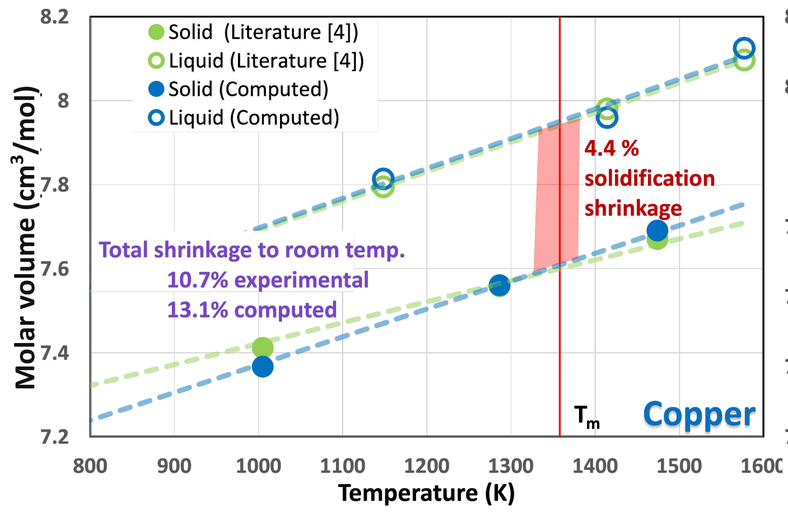
High shrinkage (large cavity) | Low shrinkage (small cavity)

Ab-Initio Molecular Dynamics

Copper and Binary Cu-Zn Alloys

- Using ab-initio (first principles) molecular dynamics (AIMD) in VASP [2], structures are equilibrated near the experimental melting point (T_m).
- **Plotting computed volume vs temperature creates two thermal expansion curves** – one solid-phase, and one liquid-phase.
- Separation between the solid and the liquid curves at T_m predicts the volume changes for the liquid-solid phase change.
- Comparison to experimentally-based curve fitting data [4,5] verifies **AIMD predicts shrinkage for pure copper and a binary Cu-Zn** brass.

- AIMD alone is too computationally expensive to predict shrinkage of compositionally complex multicomponent alloys.
- A combination of **AIMD**, Density Functional Theory (**DFT**) and Machine Learned Force Fields (**MLFF**) can create the thermal expansion curves.



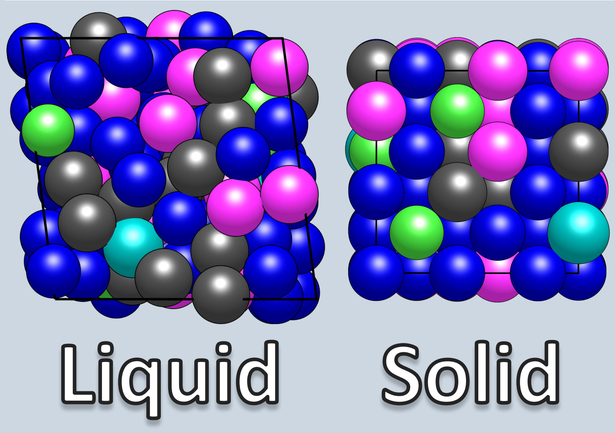
Machine-Learned Force Field Method

Training

VASP On-the-Fly Machine Learned Force Field (AIMD + MLFF) is computationally cheaper, with the accuracy of AIMD [2].

Liquid:
Liquid phase configurations are sampled by heating the system > 2500 K (above the target temperatures).

Solid:
Low energy configurations are sample for the training set with solid phase structures.

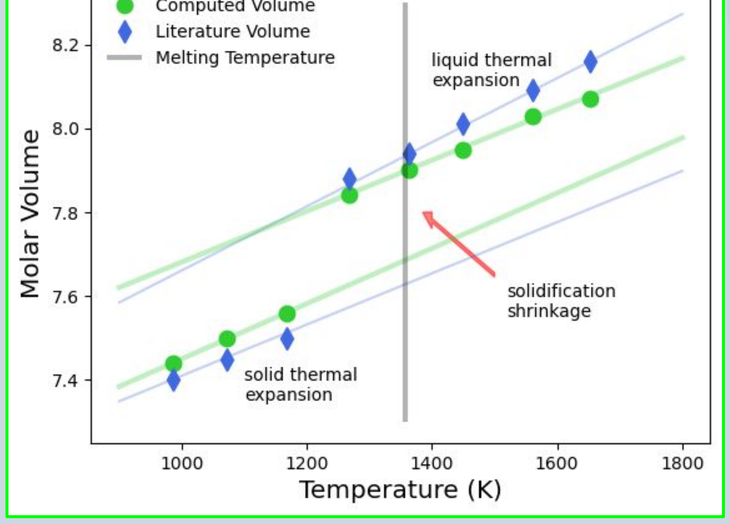


Refitting

The force field is created during hyperparameter optimization. The ML fitting parameters can be tuned for the system.

Production

Structures are equilibrated at temperatures near the melting point (All MLFF).



Extract Data

Volume and temperature data creates thermal expansion curves. The gap between curves at the melting temperature is the solidification shrinkage.

ML Validation (Errors)

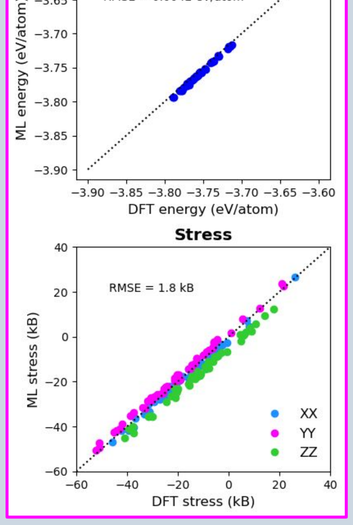
Training Set:

RMSE of ML vs DFT energy, forces and stress for training structures.

Test Set:

Structures are sampled from the production run. Static ML and DFT calculations are run. Energy, force and stress RMSE are calculated.

The training set error must be less than test set error to avoid overfitting.



References & Acknowledgments

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Fellowship in Applied Mechanics

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Ongoing Work

We will apply this method to novel high entropy brass alloys. The method may be a new tool to optimize alloy composition to minimize solidification shrinkage.

Cu-Ni-Mn-Zn-Al
Cu-Zn
Cu