High Pressure Material Phase Classification with Spatially Weighted Dynamic Graph Convolutional Neural Networks

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Background

- Phase identification is a process of classifying a certain spatial configuration of atoms as a certain type of 'phase'
- Common methods for phase identification compare an observed structure to an ideal structure, such as Polyhedral Template Matching (PTM)
- These approaches are specialized to a few simple structures, and do not work for nonperiodic structures like amorphous
- Erhard et al. presented a method for crystal identification by using Dynamic Graph Convolutional Neural Networks (DGCNN)
- While Erhard's method for classifying simple crystals is effective, it has various shortcomings that we confront

Motivations

- Develop a neural network approach based off Erhard's original work
- Improve accuracy and inference speed
- Solve coarseness problem

Local Environment Based Approach

- For each atom a Molecular Dynamics (MD) trajectory sample, a local environment is created, containing the k nearest neighbors, with the focal atom at the center of the coordinate system
- A DGCNN model classifies the structure of the focal atom, using the absolute and relative positions of the surrounding atom

Erhard's Process Overview

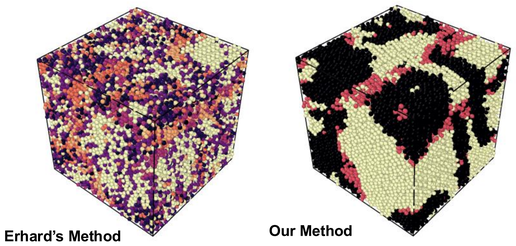
- Local environments $l_i \in R^{N\times 3\times k}$ are extracted from simulations of pure phase samples being heated, and the model $F: R^{N\times 3\times k} \rightarrow R^{N\times C}$ is trained to classify which structure the local environment belongs to
- Local environments are extracted from multiphase, or unknown phase samples, and their phase is predicted
- Extracting a local environment for every single atom is slow, and there is an accuracy-coarseness trade off for large samples

Our Process Overview

- Local environments $l_i \in R^{N\times 3\times k}$ from pure phase samples are used for model training, however the model $F: R^{N\times 3\times k} \rightarrow R^{N\times k\times C}$ generates a prediction for every atom in the environment
- For multiphase sample inference, the entire sample is treated as a single environment $l \in R^{N\times 3\times P}$, and predictions are generated for every atom, so $F(l) \in R^{N\times P\times C}$
- The goal of this method is to provide 'good' predictions as $P \rightarrow \infty$

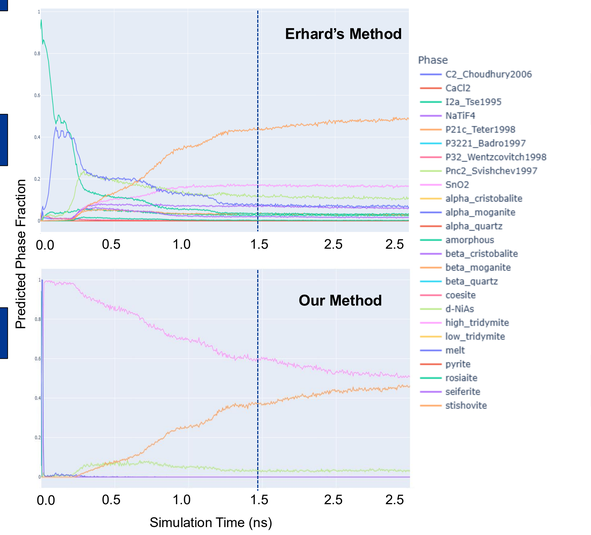
Model	Test Accuracy After 10 Epochs
Erhard's method, 32 point environments	0.81
Our method, 32 point environments	0.85
Erhard's method, 64 point environments	0.89
Our method, 64 point environments	0.93
Our method, 128 point environments	0.95

SiO2 shock experiment



Erhard's Method

Our Method



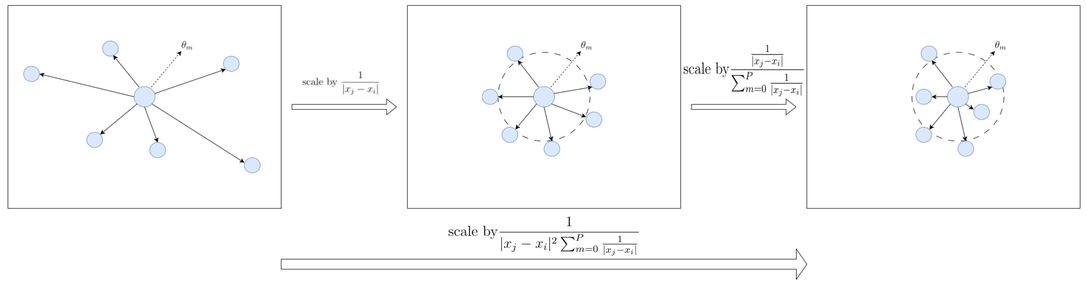
Confusion Matrix

Erhard's Method

Our Method

Spatial Weighting Mechanism

- For our approach, only relative positions in the input space could be used, however we observed that training with only relative positions was extremely detrimental to model performance
- The spatial weighting method was implemented to overcome this issue



Architectural Overview

Rotation Invariance Optimization

- The DGCNN architecture is not inherently rotation invariant, however phase classification does not depend on absolute orientation of atoms
- Environments are randomly rotated, and the standard deviation of predictions across all rotations is added to the loss function

$$\mathcal{L}_{\text{combined}}(\theta) = -\phi \sum_{i=0}^{N} \log \mathcal{F}_\theta(x_i) + (1-\phi)\alpha \sum_{i=0}^{N} \sqrt{\frac{1}{C}\sum_{j=0}^{C} (\mathcal{F}_\theta(x_{ij}) - \mu_i)^2}$$

$N =$ Number of batches

$C =$ Possible phases

$\mathcal{F}_\theta(x_i) =$ Model predictions

$\phi \in [0, 1]$

$\mu_i =$ Mean predictions

Rotation Optimization	Nearest Neighbors Graph	Spatial Weighting Mechanism	Included Relative Positions (Input space)	Included Absolute Positions (Input Space)	Included Relative Positions (Embedding Space)	Included Absolute Positions (Embedding Space)	Cross entropy after 100 batches
No	Embedding Space	No	Yes	Yes	Yes	Yes	1.93
No	Embedding Space	No	Yes	No	Yes	No	2.33
No	Embedding Space	No	No	Yes	No	Yes	2.13
No	Embedding Space	Yes	Yes	No	Yes	Yes	1.86
Yes	Embedding Space	Yes	Yes	No	Yes	Yes	1.69
Yes	Input Space	Yes	Yes	No	Yes	Yes	1.63

References

- Erhard, L. C., Utt, D., Klomp, A. J., & Albe, K. (2024). Crystal structure identification with 3D convolutional neural networks with application to high-pressure phase transitions in sio2. *Modelling and Simulation in Materials Science and Engineering*, *32*(6), 065029. https://doi.org/10.1088/1361-651x/ad64f3
- Wang, Y., Sun, Y., Liu, Z., Sarma, S.E., Bronstein, M.M., Solomon, J.M. (2018). Dynamic Graph CNN for Learning on Point Clouds. arXiv preprint arXiv:1801.07829.
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