Predicting and Interpreting Energy Barriers of Metallic Glasses with Graph Neural Networks

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Abstract

Metallic Glasses (MGs) are widely used disordered materials. Understanding the relationship between the local structure and physical properties of MGs is one of the greatest challenges for both material science and condensed matter physics. In this work, we utilize Graph Neural Networks (GNNs) to model the atomic graph structure and study the connection between the structure and the corresponding local energy barrier, which is believed to govern many critical physical properties in MGs. One of our key contributions is to propose a novel *Symmetrized GNN* (SymGNN) model for predicting the energy barriers, which is invariant under orthogonal transformations of the structure, e.g., rotations and reflections. Such invariance is a desired property that standard GNNs like Graph Convolutional Networks cannot capture. SymGNNs handle the invariance by aggregating over orthogonal transformations of the graph structure for representation learning, and an optimal distribution over all 3D orthogonal transformations $\mathcal{O}_3$ is learned to maximize the benefit of invariance. We demonstrate in our experiments that SymGNN can significantly improve the energy barrier prediction over other GNNs and non-graph machine learning models. With such an accurate model, we also apply graph explanation algorithms to better reveal the structure-property relationship of MGs. Our GNN framework allows effective prediction of material physical properties and bolsters material science research through the use of AI models.

1 Introduction

Metallic glasses (MGs) is a unique class of disordered materials that exhibit pronounced local atomic structures. It has been demonstrated that the complex local structures of MGs have a tremendous impact on their physical properties. Those properties, including local plastic deformation, glass state transition, and etc, have broad scientific impact and wide real-world applications. Nonetheless, it

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remains a challenge for material scientists and chemists to unveil the intricate role of local atomic structure in determining these properties. A typical way is using a descriptor characterizing local structural features inspired by the underlying physics (e.g., soft spot, free volume, local stress, etc.) [23, 6, 9, 29]. In contrast, machine learning (ML) approaches were explored to model the relationship between the local structure and the corresponding physical properties [7]. Since this approach does not require specific domain knowledge, it can provide a more general framework to identify the structure-property relationship of different disordered materials.

One route of the ML approach is model the structure-property relationship directly [1]. However, due to the complexity of the physical properties, it is often challenging to capture the correlation accurately and only limited explanation can be given. Another more promising route is to study the structure-property relationship through the *energy barrier* of the energy landscape. The energy barrier is a chemical quantity that describes the local roughness of the energy landscape by comparing the average energy difference around an atom's local neighbors. It has been shown that the energy barrier can act as an important intermediate step when predicting the important properties with the atomic structures as inputs [30, 8, 36]. However, the precise measurement of the energy barrier can be challenging and involves time-consuming computation. For example, computing the energy barriers for an MG with 3,000 atoms can take over a month even with a high-performance computing (HPC) cluster. To overcome the difficulty, we phrase the energy barrier prediction problem as a graph node regression problem and solve it with Graph Neural Networks (GNN). Under this formalization, atoms become nodes in a graph, and edges are constructed between nearby nodes. The node features are the atom types. The edge features are the 3D coordinate vectors of the relative position between two end nodes. Then the energy barrier prediction problem becomes a regression task on each node.

Using GNNs to predict the energy barrier of MGs is also a non-trivial task. The graph structure is the critical information for the prediction and is represented with 3D coordinates. The energy barrier labels should be invariant to orthogonal transformations of the graph coordinates, e.g., rotations or reflections. However, existing GNNs are not designed to automatically capture such invariance. As we show in our experiments, commonly used GNNs like GCN perform poorly for energy barrier prediction. We thus propose the Symmetrized GNN (SymGNN), which captures the invariance by introducing a symmetrization module to aggregate information from all orthogonal transformations of the graphs structure. We demonstrate in experiments that SymGNN on the MG dataset outperforms a variety of widely-used GNNs including GCN [15], EGNN [27], and non-GNN ML models such as a multi-layer perceptrons (MLPs). We also conduct an ablation study to show that the symmetrization module is the critical design for improving the performance. Furthermore, we generate explanations to better understand the relationship between the atomic structure and energy barriers, where we extend GNNExplainer [35] to fit the regression task and demonstrate our result through a case study. We summarize our contributions as the following:

1. We formulate the material science problem of MG energy barrier prediction into an ML problem of node regression on graphs.

2. We propose a novel SymGNN model that is invariant to orthogonal transformations of the graph and achieves highly accurate energy barrier predictions for MGs.

3. We combine SymGNN with model explanation methods to generate insightful explanations and benefit scientific discovery.

2 Related work

Various ML methods have been applied to investigate the relationship between the atomic structures and physical properties in MGs. Previous work includes GNNs that attempt to directly capture their relationship [1], and XGBoost for modeling the connection between the atomic structure and the energy barriers [33]. Wang's work focused on classification of nodes with the highest 5 percent and lowest 5 percent activation energy. Our work furthers the investigation of [33] by leveraging the natural graph structure using GNNs to perform an regression with respect to energy barriers and generating insightful explanations.

2.1 Graph Neural Networks

Graph Neural Networks (GNNs) are special types of neural networks that are designed specifically to work on graph data. It leverages the structural information of the graph to make predictions utilizing a node's neighbors' information by the message passing mechanism [15, 12, 32]. In material science, molecule graphs are naturally constructed by considering the distance between molecules. Specific GNN architectures have been proposed to perform various tasks by utilizing the natural physical interaction between each individual molecule [1]. Different GNN structure differs in how the message from each node is computed and how the messages from different neighbors are aggregated. Among many GNN variants, Graph Attention Network (GAT) [32] introduces the attention mechanism into the aggregation to assign different importance to nodes in the same neighborhood and increase model capacity. Edge Graph Attention Network (EGAT) [14] further adds edge features to the attention calculation [14]. Other variants of GNNs were introduced to specifically handle the special characteristics of certain graphs. For example, $E(n)$ Equivariant GNN, Nequip, MACE, Equiformer were introduced to be equivariant under translation, rotation, reflection, and permutation, meaning that the network output will undergo the same transformation if one of these transformation is applied to the network input [27, 16, 4, 3].

2.2 GNN Explanation

Model explainability is crucial for complex modern ML models. It helps users to gain insights into the model's prediction. Popular explanation methods include local-approximation-based methods like LIME [26], and Shapley-Value-based methods SHAP [18]. Specifically for explaining GNNs, a wide range of explanation methods are proposed to select the most influential edges, nodes, features, and even subgraphs [35, 19, 37, 39, 17], for the prediction of one node in the sense that the most message passing happens. GNNExplainer is the pioneering work that achieves this goal by learning edge masks to maximize the mutual information between perturbed output and the original model output [35]. These works including GNNExplainer focus on explaining classification problems, whereas we focus on explaining node regression. To the best of our knowledge, the only work that targets GNN explanation for regression tasks is [38], but it is very different from ours because it focuses on graph-level regression, and it does not consider any invariance explanation nor any application to material science.

3 Preliminaries

3.1 GAT and EGAT

EGAT is a backbone architecture we build up on in this work. As discussed in the related work, GAT and EGAT extend the basic GNN by realizing a nonuniform contribution from different neighbors with the attention mechanism. Each EGAT layer employs a multi-head attention calculation for a node on each of its neighbors and incorporate the edge features in the calculation. After the message from each node is computed, EGAT first calculates an attention score a_{ij} over the edge between nodes i and j. Then the representation of node i in the $l+1$-th layer (h_i^{l+1}) is constructed as the attention-weighted average of the neighbor representations from the l-th layer. The formula is shown as the following with σ represents the non-linear activation function and $\mathcal{N}(i)$ represents the set of neighbors of node i.

$$h_i^{l+1} = \sigma(\sum_{j \in \mathcal{N}(i)} a_{ij} h_j^l) \tag{1}$$

3.2 GNNExplainer

GNNExplainer seeks to explain the graph neural network's prediction by selecting a edge-induced subgraph and a subset of node features that plays the most important role in the prediction of one node. GNNExplainer targets at classification task and achieves this by learning a fractional edge mask that minimizes the entropy. Mathematically, denote H to be the entropy and G_S to be a subgraph, then the objective can be written as

$$\min_{\mathcal{G}} \mathbb{E}_{G_S \sim \mathcal{G}} H(Y|G = G_S, X = X_S) \tag{2}$$

After learning the edge mask, a threshold filtering is done to select the most important edges.

4 Method

In this section, we present SymGNN for accurately predicting and elucidating the structure-property relationship of MGs. We first formulate the energy barrier prediction problem as a node regression problem on graphs in Section 4.1. Then we introduce the theory behind the symmetrization module in SymGNN for capturing the invariance in Section 4.2. The full SymGNN model is presented in Section 4.3. Finally, we discuss how we generate explanations to better reveal the connection between the atomic structure and the energy barrier in Section 4.4.

4.1 Metallic Glasses Energy Barrier Prediction with GNNs

The problem of predicting energy barriers of MGs can be formalized as a node regression problem on graphs and be solved with GNNs. Under this formulation, atoms become nodes in a graph, and edges are constructed between nearby nodes. The MG data thus becomes a graph G with n nodes and m edges. The node features are the atom types, which we represent with $\boldsymbol{Z} = \{\boldsymbol{z}^1, \boldsymbol{z}^2, \ldots, \boldsymbol{z}^n\}$. The edge features are the 3D coordinate vectors of the relative position between two end nodes, which we represent with $\boldsymbol{X} = \{\boldsymbol{x}^1, \boldsymbol{x}^2, \ldots, \boldsymbol{x}^m\}$. The regression task is to predict the energy barrier y of each node with the graph structure and features as inputs.

4.2 Symmetrization for Invariance

The energy barrier is the average energy needed for a node to hop between the current and nearby energy subbasins, and it describes the local roughness of the energy landscape. Therefore, it should be invariant to orthogonal transformations of the 3D coordinates of the graph, for example, rotations or reflections. However, regular GNNs are not designed to automatically capture such invariance. We thus propose a symmetrization module to better capture it. We now present the theory behind the symmetrization module for capturing the invariance of orthogonal transformations. First, recall some mathematical definitions.

Definition 4.1 (Orthogonal Transformation)**.** A linear function $T : \mathbb{R}^d \to \mathbb{R}^d$ is called an orthogonal transformation if for all $a, b \in \mathbb{R}^D$, it satisfies $\langle T(a), T(b)\rangle = \langle a, b\rangle$. The set of orthogonal transformation on $\mathbb{R}^D$ is denoted as $\mathcal{O}(D)$. An orthogonal transformation T that has $\det(T) = 1$ is called a rotation, and a non-rotation otherwise. The set of all rotations is denoted as $SO(n)$.

Definition 4.2 (Invariant/Equivariant Function)**.** Given a group G, a G-action, and two G-sets X, Y. A function $f : X \to Y$ is said to be equivariant if $g \cdot f(x) = f(g \cdot x)$ and invariant if $f(x) = f(g \cdot x)$.

In our case, as the map we are investigating are a function from $\mathbb{R}^3 \to \mathbb{R}$ under the action of $\mathcal{O}_3$, equivariant is not applicable as there is no corresponding group action in the codomain. More specifically, there are no corresponding notion of rotation or reflection for element in $\mathbb{R}$. Therefore, the primary goal of our method will be to achieve invariance.

To predict a node label y with graph structure G, edge features $\boldsymbol{X}$, and node features$\boldsymbol{Z}$, we fit ML models, e.g., GNNs, for $P(Y = y|\, G, \boldsymbol{Z}, \boldsymbol{X})$. However, in this setting, $\boldsymbol{X}$ only represents the 3D vectors under one particular coordinate. To have the model learn the invariance under orthogonal transformations of edge features, we reformulate the problem as marginalizing over all orthogonal transformations of graph positions in Equation 3,

$$P(Y = y \,|\, G, \boldsymbol{Z}, \boldsymbol{X}) = \int_{T \in \mathcal{O}(3)} P(Y = y \,|\, G, \boldsymbol{Z}, \boldsymbol{X}, T(\boldsymbol{X}))P(T)\, dT \tag{3}$$

In this way, the model will learn the desired invariance by foreseeing different possibilities that can be exhibited by the graph. To parameterize over all the orthogonal transformations, we adopt the following theorem by Euler,

Theorem 4.3. *(Euler [28]) Define the rotatins around the three cooridinate axes x_1, x_2, x_3 in $\mathbb{R}^3$ by*

$$O_{x_1}(\alpha) = \begin{bmatrix} 1 & 0 & 0 \\ 0 & \cos(\alpha) & -\sin(\alpha) \\ 0 & \sin(\alpha) & \cos(\alpha) \end{bmatrix}$$

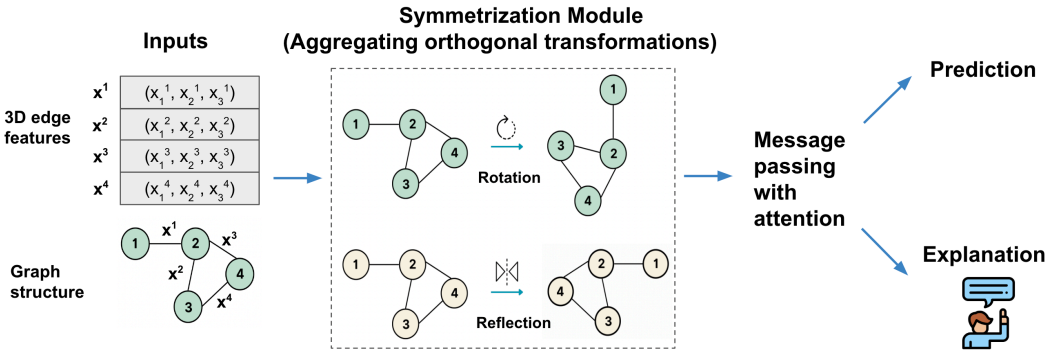

Figure 1: Illustration of the SymGNN framework.

$$O_{x_2}(\beta) = \begin{bmatrix} \cos(\beta) & 0 & -\sin(\beta) \\ 0 & 1 & 0 \\ \sin(\beta) & 0 & \cos(\beta) \end{bmatrix}$$

$$O_{x_3}(\gamma) = \begin{bmatrix} \cos(\gamma) & -\sin(\gamma) & 0 \\ \sin(\gamma) & \cos(\gamma) & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

Then any $3D$ rotation orthogonal matrix $T \in \mathbb{R}^{3\times 3}$ is of the form $T = O_{x_1}(\alpha)O_{x_2}(\beta)O_{x_3}(\gamma)$ for some α, β, γ. These angles are referred as the Euler angles.

Intuitively, this means that any rotation in 3D can be split into a combination of rotations that rotate only around the x_1-axis, x_2-axis, and x_3-axis. Using slight modification, we can also parameterize the non-rotations as shown in the following corollary.

Corollary 4.4. *Any $3D$ orthogonal matrix $T \in \mathbb{R}^{3\times 3}$ that is not a rotation has the form $T = -O_{x_1}(\alpha)O_{x_2}(\beta)O_{x_3}(\gamma)$ for some α, β, γ.*

Proof. Please refer to Appendix A.1. □

Therefore, we can decouple the integral in Equation 3 into two parts, where the first part controls the rotation, and the second part controls the reflections and any combination of rotations and reflections. The equation thus become

$$\begin{aligned} P(Y = y \,|\, G, \boldsymbol{Z}, \boldsymbol{X}) = &\int_{\alpha,\beta,\gamma} P(Y = y \,|\, G, \boldsymbol{Z}, \boldsymbol{X}, T_{\alpha,\beta,\gamma}(\boldsymbol{X}))P(T_{\alpha,\beta,\gamma})\, dT \\ &+ \int_{\alpha,\beta,\gamma} P(Y = y \,|\, G, \boldsymbol{Z}, \boldsymbol{X}, -T_{\alpha,\beta,\gamma}(\boldsymbol{X}))P(T_{\alpha,\beta,\gamma})\, dT \end{aligned} \tag{4}$$

where $T_{\alpha,\beta,\gamma} = O_{x_1}(\alpha)O_{x_2}(\beta)O_{x_3}(\gamma)$.

4.3 Symmetrized GNN

In this section, we present the full SymGNN model with an illustration shown in Figure 1. SymGNN consists of two sub-modules, the first is the symmetrization module mentioned above, and the second is a prediction module that takes the symmetrized representations to perform message passing with attention and then for node regression.

The symmetrization module learns two distinct distributions over the Euler angles α, β, and γ, where the first distribution controls the optimal set of rotations that can be applied to the graph and the second distribution controls the optimal set of non-rotations. As there are infinitely many orthogonal transformations, we approximate the integration in Equation 4 by sampling α, β, and γ from the

learned distributions.

$$P(Y = y \mid \boldsymbol{Z}, \boldsymbol{X}, G) = \sum_{i=1}^{K} P(Y = y \mid \boldsymbol{Z}, \boldsymbol{X}, G, O_{x_1}(\alpha_i) O_{x_2}(\beta_i) O_{x_3}(\gamma_i)) + \sum_{j=1}^{K} P(Y = y \mid \boldsymbol{Z}, \boldsymbol{X}, G, -O_{x_1}(\alpha_j) O_{x_2}(\beta_j) O_{x_3}(\gamma_j)) \tag{5}$$

In this approximation, SymGNN can learn from a variety of orthogonal transformations of the graph, Moreover, a distribution of the most effective orthogonal transformation that benefits the energy barrier prediction can be learned. The exact distribution we learned in our experiments is the von Mises (Tikhonov) distribution [20].

Taking the invariant representations output from the symmertization module, the second prediction module performs message passing to predict energy barriers. To model the complexity, we also compute attention of edge features with decreasing attention heads and skip connections. In contrast to regular shallow GNNs on homophily graphs, we set the number of layers to four to capture the physical influence of both close-by and far-away nodes as suggested by material science literature. As we show in our experiments in Section 5, our design can significantly outperform other baseline models for predicting energy barriers of MGs.

4.4 Explanation for Structure-Property Relationship

To make the best use the SymGNN model and truly bolster the scientific research of MGs and disordered materials in general, we generate explanations to better reveal the structure-property relationship. We pick the GNNExplainer approach as a starting point for selecting a subgraph G_S with important edges. Since GNNExplainer was developed for classification problems, the cross-entropy-based objective does not generalize to the regression problem of energy barrier prediction. Therefore, we modify the objective in Equation 2 by replacing entropy mean squared error (MSE) as below,

$$\min_{\mathcal{G}} \mathbb{E}_{G_S \sim \mathcal{G}} \text{MSE}(Y \mid G = G_S, X = X_S) \tag{6}$$

Empirically, we demonstrate that this regression explainer is capable of selecting meaningful edges that verify the hypothesis by material scientists and bring new insights.

5 Experiments

We conduct experiments on an MG dataset to evaluate SymGNN and compare its performance with other baseline models. We then perform an ablation study of the symmetrization module. Finally, we generate and analyze explanations for energy barrier predictions.

5.1 Dataset

In this investigation, we employ molecular dynamics to simulate the behavior of a representative Cu64Zr36 metallic glass (MG) subjected to shear deformation. The simulated MG system comprises 8000 atoms, generated through the conventional melting-quenching procedure with varied cooling rates spanning from 10^{14} to 10^{10} K/s. To evaluate the influence of system size, we also simulate small system (i.e., 3000 atoms). To initiate the simulation, the sample is initially melted at 2000K under zero pressure for 1ns, facilitating the erasure of its initial configuration memory. Temperature and pressure control are maintained through the isothermal-isobaric (NPT) ensemble, employing a Nosé-Hoover thermostat [22, 13]. Subsequently, the liquified state is rapidly quenched to 1K, with cooling rates ranging from 10^{14} to 10^{10} K/s. The resulting glassy structure is further relaxed to its local energy minimum through energy minimization, utilizing the conjugate gradient algorithm. The interatomic interactions within the system are described using the embedded-atom method (EAM) potential [21]. To ensure the statistical robustness of our findings, 11 independent metallic glass samples are generated for each cooling rate. A timestep of 1fs is adopted for all simulations, and the entire set of simulations is carried out using the LAMMPS package [24]. To obtain the energy

Table 1: Training and testing scores of the best model on the validation set.

	Methods	Training Scores	Testing Scores
Non Invariant	GCN	0.1322 ± 0.0060	0.3063 ± 0.0084
	GCN with Edge Features	0.8142 ± 0.0161	0.5123 ± 0.0507
	E(n) Equivariant GNN	0.4526 ± 0.0005	0.2588 ± 0.0077
	MLP	0.2569 ± 0.0096	0.0575 ± 0.0127
	SymGNN w/o symmetrization	0.8736 ± 0.0007	0.2669 ± 0.0371
Invariant	SymGNN	0.8368 ± 0.0027	$\mathbf{0.7859 \pm 0.0056}$
	Non Invariant model + edge length	0.7221 ± 0.0049	0.7264 ± 0.0063

barriers of atoms, we employ the activation-relaxation technique nouveau (ARTn) [2, 5] to calculate the energy barriers within metallic glasses (MGs). Specifically, starting from a local energy minimum in the landscape, initial perturbations are introduced to a chosen atom and its nearest neighbors. This perturbation allows exploration along a direction of negative curvature, increasing the likelihood of locating a saddle point in the energy landscape. The Lanczos algorithm [2] is then applied to guide the system to the saddle point by following the direction of negative curvature. A force tolerance of $0.05eV/\text{Å}^{-2}$ is chosen to ensure convergence of the saddle points. In accordance with previous investigations [10, 11, 34], 20 searches for saddle points are conducted for each atom. Consequently, the ARTn exploration focuses on determining the average energy barrier associated with atoms. This parameter is recognized as a key factor influencing the propensity for plastic rearrangement in disordered materials [31, 30].

This simulation is used to construct a dataset consists of nine graphs. Among them, six graphs are used for training, one graph for validation, and two graphs for testing. Each training/validation graph has 8,000 nodes and roughly 260,000 edges, and each test graph has 3,000 nodes and roughly 100,000 egdes. The raw dataset is gathered with nodes only, and edges are constructed between two nodes if their Euclidean distance is smaller than a threshold, which is chosen to be $5\text{Å} = 10^{-10}m$ for better prediction performance. As suggested by the material scientists, these nine graphs already have a good coverage of a wide range of MGs.

5.2 Experiment Setting

Baselines: We evaluate our model by comparing the test performance on the MG dataset to a variety of other ML models including Graph Convolutional Network (GCN) [15], E(n) Equivariant GNN (EGNN) [27] that are designed to handle equivariant features, and a non-graph based multi-layer perceptron (MLP) model. As GCN is inherently not designed for rich edge features, we also implemented a graph convolution type network that can handle edge features. Furthermore, we perform an ablation study named SymGNN w/o symmetrization where we remove the symmtrization layer, and in addition we have include a simple baseline in which we use the absolute length of edge instead of its 3d coordinates as an input edge feature to achieve invariance.

Evaluation: The predicted energy barriers are evaluated by the Pearson product-moment correlation coefficient against the true values following from previous work in material science literature [1]. We run each experiment 4 times with different random initializations, we run the experiment four times with different random initialization. For each experiment, we use the validation set to determine the best model, and compute the score with the best model on the test set. The final is the mean and standard deviation of these scores on the test/train set from different runs, and is reported in table 1.

Implementation: We train the 4-layer SymGNN for 20,000 epochs using an Amsgrad optimizer [25] with a learning rate of 0.0001. For SymGNN, the distribution over the angles α, β, and γ is parameterized by the von Mises (Tikhonov) distribution [20], which is a wrapped-around normal distribution on the circle.

5.3 Evaluation Results

We report the results of SymGNN and other baselines in Table 1. It can be seen from the table that SymGNN outperforms the baselines by a large amount and exhibits a much stronger generalization

power. When we remove the symmetrization module, (i.e. SymGNN w/o symmetrization), the ablated model cannot generalize well. Also we observe that models capable of handling invariance can lead to much better result compared to the ones that cannot, which again highlights the importance of symmetrization module in achieving good prediction performance.

For a time comparison with traditional molecular dynamics simulation, our ML-based approach needs much fewer computation resources and is much more efficient. In traditional physical simulation, the calculation of the energy barrier for each atom takes around 20 minutes in a supercomputer with 16 parallel threads. Therefore, for a graph that has a similar size to our test graph, the computation will take $\frac{20\times3000}{60\times24} \approx 41$ days. On the other hand, SymGNN only takes around 3.5 hours to train on a single chip NVIDIA A10G GPU, and the inference time on the test graph is almost negligible.

5.4 Explanation Case Study

Finally we apply the extended version of GNNExplainer to our trained models to select the most important edges during the prediction of one specific node. First, we perform a global analysis in which we show all the top-k selected edges, and observe the special properties of edges being selected. Next, we zoom in the explanation and plot the local version of the explanation, where only the closet nodes to a given node are considered, and we would like to investigate how frequent will edge being selected among these closer atoms.

Explanation Visualization We show our visualizations for a randomly sampled node in this graph. In Figures 2 and 3, all atoms are drawn in their actual 3D coordinates. For the global version of explanation 2, we visualize the top 50 edges selected by GNNExplainer. For the local version of explanation 3, we display only the top 10 closet nodes to the node being explained.

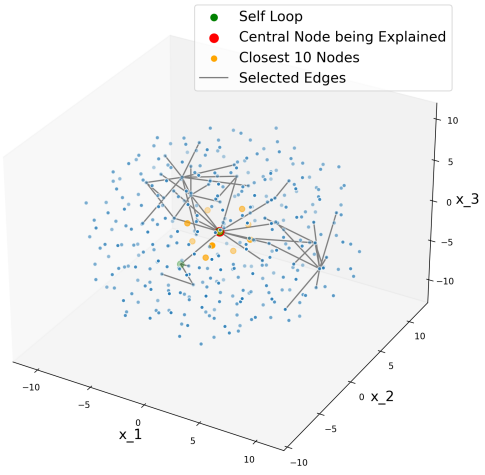

Figure 2: Global Version of the Explanation

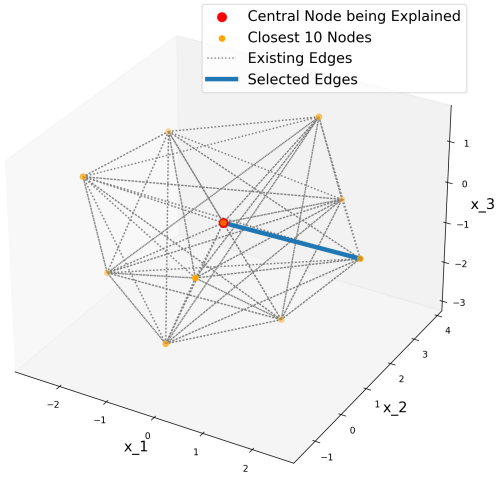

Figure 3: Local Version of the Explanation

From the visualizations, it can be noted that most of the selected edges lie relatively close to the central node being explained. However, from the global version, we see that edges close to the central node or far away from the central node may both be selected. Also, as we can see from the local version of the explanation, only one edge within the top 10 closet edges is selected by GNNExplainer. These observations confirm the material scientists' physical intuition that atoms that are in middle-range of distance to the central atom should play a more important role in determining its energy barriers.

6 Conclusion and Future Work

In this paper, we study the connection between the local atomic structures of metallic glasses and their energy barrier of the energy landscape. We formalize this problem as node regression on graphs and propose Symmetrized GNN (SymGNN) to solve the problem by effectively capturing the invariance

of orthogonal transformations of the graph. We compare SymGNN with several baseline models and demonstrate that SymGNN performs the best across all models being evaluated. In addition, we extend the GNNExplainer for regression tasks and generate explanations to verify the hypothesis proposed by material scientists and potentially benefit new scientific discoveries.

For the prediction model, we plan to further examine and compared SymGNN with more geometric deep learning models that can achieve invariance. For the explanation, the future work we plan to conduct includes more explorations in terms of various across-node statistics in order to achieve statistically significant and physics informed result. From physical intuitions, the edge that plays an important role in the prediction should exhibit some unusual behavior. For example, the edge being selected may have a higher-than-usual length compared to other edges that connect to the same node, or it may exhibit a more skewed angle compared to the other edges. By evaluating the statistics of the distance/angle distribution across different nodes, we can better examine the coherence between physical intuition and the actual selected edges by explainer.

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A Proofs

A.1 Proof of Corollary 4.4

Proof. We know by elementary linear algebra that an orthogonal matrix $A \in \mathbb{R}^{3\times 3}$ satisfies $A^{-1} = A^T$. Therefore, the determinant satisfies

$$\det(A)^{-1} = \det(A^{-1}) = \det(A^T) = \det(A) \tag{7}$$

This implies that $\det(A)^2 = 1$. As A has real entries, $\det(A) \in \mathbb{R}$. So the only two possibilities for the determinant is $\det(A) = \pm 1$. By definition, a non-rotation is thus any orthogonal matrix that has determinant -1. Let $T : \mathbb{R}^3 \to \mathbb{R}^3$ be an arbitrary non-rotation orthogonal transformation. As $-T$ satisfies $\det(-T) = (-1)^3 \det(T) = 1$, by definition $-T \in SO(3)$. By theorem 4.3, there exists angles α, β, γ so that $-T = O_{x_1}(\alpha)O_{x_2}(\beta)O_{x_3}(\gamma)$. Negate it, we obtain the desired angles that satisfy $T = -O_{x_1}(\alpha)O_{x_2}(\beta)O_{x_3}(\gamma)$. □