AnisoGNN: physics-informed graph neural networks that generalize to anisotropic properties of polycrystals

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Abstract

We present AnisoGNNs – graph neural networks (GNNs) that generalize predictions of anisotropic properties of polycrystals in arbitrary testing directions without the need in excessive training data. To this end, we develop GNNs with a physics-inspired combination of node attributes and aggregation function. We demonstrate the excellent generalization capabilities of AnisoGNNs in predicting anisotropic elastic and inelastic properties of two alloys.

1 Introduction

Structural materials (metals, alloys, ceramics) essential across multiple industries are predominantly used in their polycrystalline form constituted by numerous crystals known as *grains*. An interplay between the three-dimensional (3D) structure of grains and grain-level (*single-crystal*) properties of polycrystalline materials dictate their engineering performance. Single-crystal properties of metals and alloys are often directionally dependent, i.e. *anisotropic*. This grain-level, microscale anisotropy together with non-random distribution of grain orientations (*texture*) result in a macroscale anisotropy of overall (or *effective*) properties of polycrystals [8]. For example, most metals and alloys have anisotropic single-crystal elastic properties described by a stiffness or compliance tensor. A polycrystalline alloy with single-crystal anisotropy and non-random texture has therefore different values of effective Young's modulus if tested in different directions. Similarly, most alloys, beyond the elastic limit, plastically deform by dislocation glide on discrete slip systems, which results in the macroscale plastic anisotropy [1]. Non-random textures are ubiquitous in alloys as they arise as a result of thermomechanical processing (e.g., casting, rolling, annealing) [8]. Accordingly, the macroscale elastic and plastic anisotropies are common in commercial alloys and have significant effects on their behavior during processing, manufacturing, and service. As a classical example, "earing" during cup drawing of aluminum alloys is a manifestation of anisotropy of practical significance: ears are processing defects that need trimming, leading to material losses [5].

Models and simulations that predict effective anisotropic behavior of polycrystalline materials as a function of their microstructure are essential for process and performance optimization. Machine learning (ML) has recently emerged as a powerful strategy of establishing quantitative microstructure–property relationships [7]. ML models trained on data from numerical simulations offer an attractive combination of low computational cost and account for microstructure effects on properties. However,

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most ML models published to date do not systematically capture anisotropy of polycrystals. Capturing anisotropy in ML models is challenged by the need in training data for many directions. Generation of training data is time-consuming and expensive even with numerical simulations, not to mention experiments. It is for this reason, most ML models predict properties in only one (or three, at best) sample directions [12, 6, 2, 3]. In this contribution, we present a new ML strategy that generalizes property predictions to arbitrary sample directions without the need in significant additional training data thereby reducing the computational cost and time for ML model development.

2 Graph neural networks for polycrystals

2.1 Background and related work

Graph neural networks (GNNs) are a rapidly emerging ML approach to modeling polycrystals. GNNs rely on the graph representation of polycrystals, in which graph nodes represent grains, while graph edges connect nodes corresponding to neighboring grains that share a boundary [10]. Such graphs offer a reduced-order representation of polycrystals that is compact (as opposed to full-field 3D data), yet captures 3D grain connectivity. Capturing connectivity is essential for modeling properties determined by local interactions of neighboring grains [9]. The graph representation allows incorporating rich information about the microstructure beyond grain connectivity. Properties of grains, grain boundaries, and the polycrystal as a whole can be accounted as node-, edge-, and graph-level attributes. For example, node attributes can include grain centroid coordinates, crystallographic orientation, metrics of the grain size and shape [6], as well as local properties of individual grains [3, 11]. Graph-level attributes can in turn represent effective properties of polycrystals, which are of interest for learning and inference. Prior relevant work includes the following studies. Hestroffer et al. [6] trained a GNN on crystal plasticity finite element (CPFE) simulation data to predict yield strength and Young's modulus of titanium in a single loading direction. Pagan et al. [11] presented a GNN model of the elastic stress response of nickel and titanium alloys in one loading direction based on CPFE and 3D X-ray diffraction data. Dai et al. [2] trained a GNN model to phase field data to predict effective magnetostriction in one sample direction under applied magnetic field. Dai et al. [3] modeled effective ion conductivities and elastic moduli in three principal sample directions by GNNs trained on numerical data from the Fourier spectral iterative perturbation method.

2.2 New GNN approach

We propose a new GNN approach that captures anisotropic properties in a wide range of directions *without the need in training data in those directions*. The key idea of our approach is to rotate the microstructure in respect to a fixed sample direction rather than simulate (or experimentally test) the material along different sample directions to obtain properties in those directions. While the difference is subtle, this "rotation trick" offers advantages for the GNN model development. For example, property in the x direction of the sample for a microstructure rotated 90° around the z axis is equivalent to the property in the y direction. At the same time, to the GNN (or other ML) model, the rotated microstructure appears as yet another microstructure for inference. This trick of predicting property in a fixed sample direction for rotated microstructures allows us to focus on the property in a single direction. The approach is beneficial because it requires less training data compared to ML models targeting properties in multiple directions relying on data for each individual direction.

To strengthen the generalization of our GNN approach to anisotropic behavior, we further propose the use of most relevant local properties of grains as node attributes together with a physics-inspired aggregator function. While prior studies used the crystallographic orientation as a key attribute for the grain-nodes [6], crystallographic orientation may not be most compatible with aggregator functions commonly used in GNNs. For example, consider a cluster of neighboring grains represented by a set of graph nodes connected by graph edges. A mean or max aggregator function applied to Euler angles (or other orientation representation) of these graph nodes would result in a new crystallographic orientation that is not representative of any of the grains in the cluster. In our GNN approach, we propose to use a tensor property most relevant to the effective property being modeled. For example, for effective *elastic* properties, e.g., Young's modulus, we propose to use the local stiffness tensors as the most relevant attributes of grain-nodes. For modeling an effective *plastic* property, we propose the local Schmid tensors as the most relevant attributes. These property tensors are typically known at the grain level as single-crystal elastic constants in the case of the stiffness tensor and as a tensor

product of the slip plane normal and slip direction vectors in the case of the Schmid tensor. Relevant single-crystal tensors can be identified for other (e.g., non-mechanical) effective properties as well. Upon selecting the relevant single-crystal tensor, we propose to rotate it to the macroscopic, sample frame using the known crystallographic orientation for each grain. These local properties of the grains expressed in respect to the sample frame ultimately define the response of the grains upon loading (or other stimulus) and thus serve as excellent candidates for attributes of grain nodes. With these attributes, a simple mean aggregator function often used in GNNs gains a physical meaning: the mean of the local tensor properties of the neighboring grains in a cluster represents their average tensor property consistent with simple micromechanics models [4].

3 Case studies and results

We demonstrate our new GNN approach in the following case studies: (i) effective anisotropic Young's modulus of a polycrystalline Ni-base superalloy, René 88DT, and (ii) effective anisotropic yield strength of polycrystalline aluminum. For both case studies, we used a set of 300 digitally generated microstructure volume elements (MVEs). The MVEs represented equiaxed microstructures with 12 distinct *initial* textures. Four initial textures were obtained by polycrystal plasticity simulations of uniaxial tension, uniaxial compression, plain strain compression, and simple shear, which provide deformation textures common in commercial alloys after thermomechanical processing. To generalize the GNN model to different loading directions, the microstructure dataset further included MVEs with rigidly rotated instances of these four textures. Four textures were obtained by rotation to 45° and four additional textures were obtained by rotation to 90° – both about the z axis. We used the MVE dataset (and their effective properties from simulations) to train GNN models and test their ability to predict anisotropic properties under different training/testing scenarios: (a) random split of the 300 dataset with $70\,\%$ used for training and $30\,\%$ used for testing; (b) MVEs with 45° rotated textures used for testing; (c) MVEs with 90° rotated textures used for testing; (d) MVEs with textures rotated to both 45° and 90° as the testing set. For all four scenarios, we trained two types of GNN models: (i) GNN with architecture from [6] with crystallographic orientations and grain size as graph node attributes; (ii) GNN with simplified architecture having elements of a relevant property tensor of individual grains and grain size as graph node attributes. Our new simplified architecture has a single message passing layer with the mean aggregation function and a linear layer.

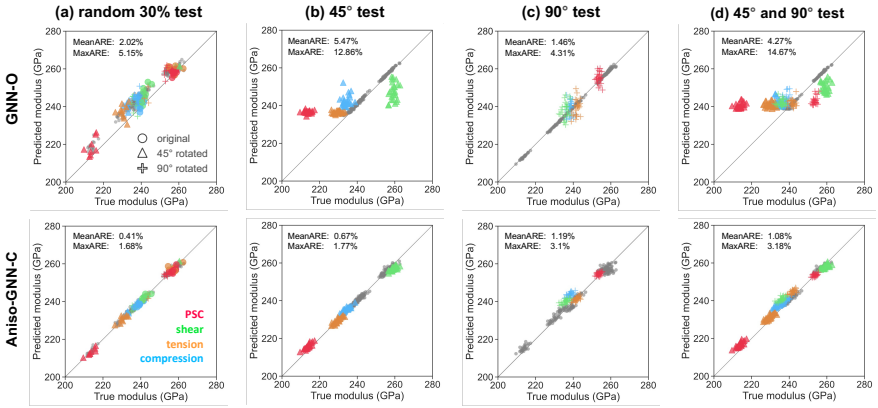

Figure 1: Modeling Young's modulus of René 88DT: parity plots comparing fits to training data (gray markers) and predictions for testing data (colorful markers) of two GNN models: GNN-O (quaternions as node attributes) and AnisoGNN-C (rotated stiffness tensor as attributes). Marker colors represent the initial textures, the marker shapes represent the rigid rotations of the texture.

Fig. 1 compares the accuracy of the two GNN models in the four training/testing scenarios by parity plots (GNN predictions vs. ground truth). Our new GNN model (AnisoGNN-C) demonstrates superior performance in all four scenarios compared to the previously published GNN architecture with orientation quaterniors as node attributes (GNN-O). The GNN-O model shows good agreement with ground truth in the case of the random split between training (gray markers) and testing (colorful markers) subsets of the data with mean absolute relative error (meanARE) of $2\,\%$. However, the accuracy of the GNN-O model drops as soon as it attempts to predict the Young's modulus for the

rotated textures not included in training. The performance is worst in Scenario (b), where the GNN-O model predicts the Young's modulus for the MVEs with textures rotated 45° unseen during training (Fig. 1b). The performance is equally poor in Scenario (d), where the GNN-O model is trained on the original four textures only and predicts the Young's modulus for MVEs with eight rotated textures (Fig. 1d). We expect Scenarios (b,d) are challenging for the GNN-O model because the model needs to *extrapolate* the Young's modulus values outside of its training range. The Young's modulus varies in the range between 235 and $265\,\mathrm{GPa}$ in the training set and in the range from 210 to $240\,\mathrm{GPa}$ in the testing set for Scenario (b). The GNN-O model tends to predict values in the range it has "seen" during training and thus overestimates the Young's modulus for MVEs with the plain-strain compression textures (PSC, red markers in Fig. 1) that have low true elastic modulus values.

The superior accuracy of the AnisoGNN-C model for the challenging Scenarios (b,d) testifies to strong generalization abilities of our proposed GNN approach. Indeed, with the rotated stiffness tensor as node attributes instead of orientations, the AnisoGNN-C model predicts the Young's modulus of MVEs with rotated textures to both 45° and 90° with remarkable accuracy (within $1\,\%$ meanARE) even though it was trained only on MVEs with four original, unrotated textures.

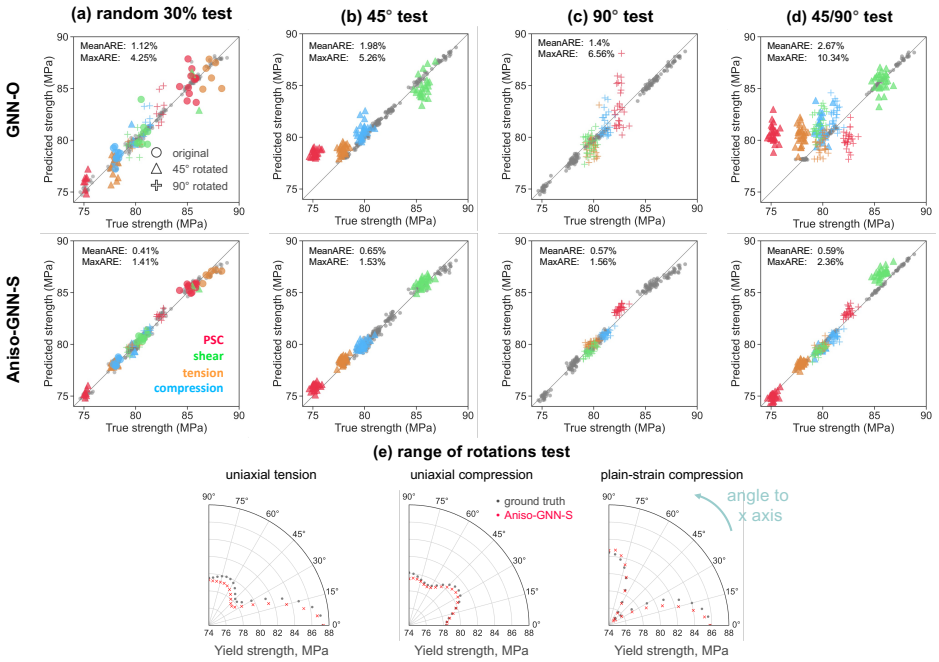

Figure 2: Modeling yield strength of aluminum: (a–d) parity plots comparing fits to training data and predictions for testing data for two GNN models: GNN-O (quaternions as node attributes) and AnisoGNN-S (rotated Schmid tensor as attributes); (e) AnisoGNN-S predictions for textures rotated for a wide range of angles about the sample z axis.

We further test the predictive power of our GNN approach on yield strength as an inelastic property of a different material – aluminum. We used the grain size and the Schmid tensor rotated to the sample frame as node attributes (AnisoGNN-S). The parity plots comparing the GNN-O and the AnisoGNN-S models for the yield strength in aluminum (Fig. 2) lead to the same conclusions as for the Young's modulus of the Ni-base superalloy. The AnisoGNN-S model exhibits better accuracy in all training/testing scenarios, while the GNN-O model struggles to accurately predict yield strength for MVEs with unseen rotated textures (Fig. 2(b,d)). These results confirm the generalization abilities of our GNN approach for anisotropic yield strength – a non-linear plastic property. We finally demonstrate the application of the AnisoGNN-S model for predicting the yield strength of aluminum microstructures with textures rotated to a wide range of angles around the sample z axis (Fig. 2e). The AnisoGNN-S model was trained only on yield strengh of MVEs with original four unrotated textures yet demonstrates excellent generalization to properties in an arbitrary loading direction.

4 Conclusion

We presented a new GNN approach to modeling anisotropic elastic and plastic properties of polycrystalline materials. Our GNN models generalize to properties in new sample directions by accurately predicting properties for rigidly rotated microstructures (textures in case of equiaxed grains). To ensure generalization abilities we train GNNs on graphs with physics-based node attributes: tensorial properties of grains relevant to the effective property of interest. We obtain these attributes by rotating the single-crystal property tensors to the sample frame using the crystallographic orientation of each grain. We demonstrated the predictive power and generalization of our GNN models in two case studies: the Young's modulus of Ni-base superalloy and the yield strength of aluminum.

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