Deep Learning Based Inverse Modeling for Materials Design: From Microstructure and Property to Processing

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***Abstract*—Polycrystalline materials are crucial in various industries, necessitating a comprehensive understanding of the processing-structure-property-performance (PSPP) relationships. Traditional experimental methods are laborious and slow, while computational approaches predominantly address forward problems, deriving structures and properties from processing conditions. Conversely, inferring processing parameters from desired microstructures and properties remains a crucial yet challenging inverse problem due to the complex and nonlinear mappings involved. In this work, we propose a deep learning-based framework exploring non-sequential and sequential models to address two key inverse problems: predicting processing parameters from microstructures and from properties. Focusing on microstructural texture defined by the orientation distribution function (ODF), we apply our framework to copper, generating a dataset of 31,588 unique processing strain rates (s^{-1}) in $[0, 1]$ with corresponding ODFs and homogenized properties through simulations. Our inverse prediction results on processing parameters demonstrate high accuracy, with average test RMSEs of 0.0152 from microstructures and 0.0295 from properties. These findings validate the framework's efficacy as a tool for polycrystalline materials process design, enabling the precise determination of processing methods to achieve desired microstructures and properties.**

***Index Terms*—Inverse Modeling, Deep Learning, Polycrystalline Materials**

I. Introduction

Polycrystalline materials are crucial in various industries such as aerospace, automotive, and electronics due to their cost-effectiveness and mechanical properties [1]. Understanding the processing-structure-property-performance (PSPP) relationship enables the development of advanced materials with tailored properties, which is crucial for enhancing performance across multiple industrial domains [2]. However, analyzing this relationship is challenging due to the complex and heterogeneous microstructures, requiring advanced characterization and modeling techniques to optimize their behaviors [3].

While traditional experimental approaches have been the cornerstone for exploring PSPP relationships, they are often time-consuming and laborious. In recent years, computational methods have emerged as efficient alternatives. For instance, surrogate models have been developed for various materials, such as zirconia-toughened alumina ceramics [4] and nickel-titanium shape-memory alloys [5], accelerating the design of microstructures with desired properties.

Building on these advancements, a strain-rate independent crystal plasticity simulator has been developed to model microstructure evolution in polycrystalline materials under each elementary process [6]. This simulator employs the orientation distribution function (ODF) to represent microstructure texture and predicts future ODFs based on initial texture and processing parameters. This represents the forward problem in scientific modeling, predicting outcomes from known parameters. Conversely, the inverse problem, crucial for optimizing material design and manufacturing efficiency [7], involves determining the necessary processing parameters to achieve desired microstructures and properties [8]. However, forward simulations remain time-consuming due to intensive calculations and do not directly solve the inverse problem, which is particularly challenging due to the need to deduce exact processing parameters for specific material characteristics.

To address the challenges, machine learning (ML) techniques have been increasingly employed to understand material behavior and develop new materials with desired properties [9]. These methods have demonstrated considerable success in modeling microstructure evolution. For example, Farizhandi et al. [10] introduced a Predictive Recurrent Neural Network (PredRNN) model for rapid and accurate microstructure prediction. Montes et al. [11] developed a data-driven surrogate model combining phase-field and history-dependent machine learning techniques. Additionally, Mao et al. [12] proposed an AI-based framework to predict microstructural texture in polycrystalline materials, achieving less than 0.5% error rates. Despite these advances, most existing methods focus on the forward problem of polycrystalline materials rather than the inverse problem of predicting processing parameters from desired microstructures and properties.

In this paper, we propose a novel deep learning based framework exploring both sequential models and non-sequential models to address the inverse modeling of processing-structure and processing-property linkages in polycrystalline materi-

als. This framework predicts processing parameters based on changes in the orientation distribution function (ODF) or desired properties. Our framework employs a two-step simulation process: first, simulating microstructures represented by ODFs using processing parameters through crystal plasticity simulation, then generating material properties through homogenization. The ODF, a statistical representation of the crystallographic orientations within a polycrystalline material, directly impacts its overall properties. Our study generates a dataset comprising 31,588 unique combinations of processing parameters for Copper, represented as strain rate values (s^{-1}) between $[0, 1]$. Each combination generates a sequence of ODFs and their corresponding homogenized properties. Our framework is designed to predict the original processing parameters from either sequential or single ODFs or properties, providing a powerful tool for optimizing material design and manufacturing processes.

To evaluate our framework, we conducted extensive testing on the Copper dataset, achieving promising results with an average RMSE as low as 0.0152 from microstructures and 0.0295 from properties. These results demonstrate the efficacy of our framework in providing a fast, accurate method for inverse modeling. Compared to computational simulation methods, our approach significantly reduces computation time while maintaining negligible accuracy loss, addressing the challenging inverse problem of efficiently processing materials to achieve desired microstructures and properties.

II. Background and related works

A. Orientation Distribution Function (ODF) and Crystal Plasticity Simulation

Polycrystalline materials consist of numerous crystals, each with distinct crystallographic orientations that define the material's microstructural texture. This microstructural texture is quantified by the Orientation Distribution Function (ODF), denoted as $A(\mathbf{r}, t)$, which represents the volume density of each distinct crystal orientation. Here, $\mathbf{r}$ signifies the Rodrigues orientation of the crystals in the orientation space and t indicates time. The ODF can be used to calculate homogenized properties through the Taylor approximation [13] and allows for efficient modeling of deformation processes, enabling the prediction of microstructural evolution under various processing parameters.

Given an initial ODF $A(\mathbf{r}, 0)$, the crystal plasticity simulation, influenced by processing parameters, can be used to model the evolution of the current texture $A(\mathbf{r}, t)$. This evolution is governed by the ODF conservation equation. The ODFs always adhere to the volume normalization constraint. The Eulerian rate form of this conservation equation in the crystallographic orientation space is expressed as [14]:

$$\frac{\partial A(\mathbf{r}, t)}{\partial t} + \nabla A(\mathbf{r}, t) \cdot \mathbf{v}(\mathbf{r}, t) + A(\mathbf{r}, t) \nabla \cdot \mathbf{v}(\mathbf{r}, t) = 0 \quad (1)$$

where $\mathbf{v}(\mathbf{r}, t)$ is the reorientation velocity, derived from the velocity gradient ($\mathbf{L}$), a macroscopic measure of the deformation applied to the material [15]. Consequently, different deformation processes, such as tension/compression and shear, result in different ODFs as outputs after applying a load for a specific amount of time. Our study aims to conduct inverse modeling to deduce the processing methods from the ODFs or corresponding homogenized properties.

B. Homogenized Polycrystal Property

The volume-averaged (homogenized) properties of polycrystalline materials are calculated using the Taylor approximation, which utilizes single-crystal properties and microstructural texture. Representing averaging with the symbol $\langle \cdot \rangle$, the homogenized polycrystal property $\langle \chi \rangle$ can be calculated by averaging over the ODF with single-crystal material properties in the orientation space. This relationship is expressed by the equation:

$$\langle \chi \rangle = \int_{\Omega} \chi(\mathbf{r}) A(\mathbf{r}) \, d\mathbf{v} \quad (2)$$

where $A(\mathbf{r})$ is the ODF, $\chi(\mathbf{r})$ represents the single-crystal material properties depending on the crystal orientation, and Ω is the orientation space. The can also be expressed in linear form as:

$$\langle \chi \rangle = \mathbf{P}^T \mathbf{A} \quad (3)$$

where $\mathbf{P}$ encapsulates the integration weights, Jacobian determinants, Rodrigues parameterization metric, and other factors. Our study focuses on elastic properties, including the stiffness tensor $\mathbf{C}$ and the compliance tensor $\mathbf{S}$. The volume-averaged properties can be calculated through equations such as $\mathbf{C}^{\text{avg}} = \langle \mathbf{C} \rangle$.

C. Related Works

Inverse modeling has emerged as a crucial approach in materials informatics. Several studies have demonstrated the effectiveness of machine learning techniques in solving complex inverse problems. For instance, Tran et al. [16] developed an active learning framework for optimizing microstructure properties in additive manufacturing and grain growth. Liu et al. [17] presented a machine learning methodology for microstructure optimization in Fe-Ga alloy, addressing the inversion of property-microstructure relationships. Additionally, Pei et al. [18] introduced a neural network-based approach for alloy inverse design, focusing on complex microstructure images in martensitic and ferritic steels. Despite these advances in machine learning for inverse modeling, there remains a lack of attention on inverse modeling for polycrystalline materials.

Recent years have seen increased attention to deep learning techniques for analyzing polycrystalline materials. For instance, Mao et al. [7] proposed an AI-driven framework that optimizes microstructures for elastic properties, discovering multiple solutions faster without compromising optimality. A deep learning augmented genetic algorithm [19] was proposed to investigate polycrystalline 2D material fracture, demonstrating the model's capability to predict fracture paths. Hsu et al. [20] developed a deep generative framework to design polycrystalline materials with specific mechanical properties. While several prior works on inverse modeling in materials

science have explored the application of ML for structure-property optimization, here we focus on inverse modeling for process design of polycrystalline materials, inferring processing parameters from microstructures and properties.

III. Methods

In our study, we introduce an inverse modeling framework designed to enhance traditional deformation process simulation technology. As illustrated in Figure 1, it conducts data generation through simulation as forward modeling and addresses two primary inverse modeling tasks: predicting the processing parameters from microstructure evolution (ODFs) and from homogenized properties of these microstructures.

For the first task, we use either the ODF sequence or the final ODF, emphasizing the latter as it reflects the accumulated effects of the deformation process and relates closely to final material properties. The second task utilizes either the properties of the entire ODF sequence or only the final ODF. We explore both non-sequential and sequential modeling methods to address these challenges. Non-sequential approaches, including machine learning methods as baselines and autoML techniques, are applied to both the ODF sequence and the final ODF. Sequential modeling methods are employed to capture temporal dynamics in time-series data like the ODF sequence and corresponding properties. These predictions guide the generation of desired microstructures and properties for enhanced material performance.

A. Data Generation from Simulation

To generate datasets for our inverse modeling tasks, we employ a strain-rate independent crystal plasticity simulation, as depicted in the upper left portion of Figure 1. This simulation models deformation under tension/compression and shear forces in the XY, YZ, and XZ planes, with varying strain rates for each scenario. The resulting data capture the material's microstructure evolution over p steps, represented by Orientation Distribution Functions (ODFs). Let ODF_i denote the ODF at the i-th step of the deformation process, where $i \in \{1, 2, \ldots, p\}$. The sequence of ODFs is represented as: $(\text{ODF}_1, \text{ODF}_2, \ldots, \text{ODF}_p)$. This sequence includes both intermediate ODFs and the final ODF, reflecting the accumulated effects of the deformation process.

For the second task of inferring processing parameters from homogenized material properties, we derive the stiffness tensor $\mathbf{C}$ and the compliance tensor $\mathbf{S}$ for each generated ODF through homogenization, as shown in the upper right portion of Figure 1. The property sequences are expressed as:$(\mathbf{C}_1, \mathbf{C}_2, \ldots, \mathbf{C}_p)$ and $(\mathbf{S}_1, \mathbf{S}_2, \ldots, \mathbf{S}_p)$, where $\mathbf{C}_i$ and $\mathbf{S}_i$ represents the tensors at the i-th step. These tensors provide critical information about the material's elastic properties at each step of the deformation process. Both ODF sequences and their corresponding properties serve as foundational inputs for our non-sequential and sequential modeling methods to predict processing parameters.

B. Non-sequential Modeling Methods

Our proposed framework utilizes non-sequential modeling methods to predict processing parameters from both time-series and final ODF or property data. Non-sequential models treat each input independently and ignore temporal dependencies. For time-series data, we concatenate the ODF sequence $(\text{ODF}_1, \text{ODF}_2, \ldots, \text{ODF}_p)$ into a single feature vector of size $p \times d$, where d denotes the ODF dimensionality. Similarly, the sequences of stiffness tensors $(\mathbf{C}_1, \mathbf{C}_2, \ldots, \mathbf{C}_p)$ and compliance tensors $(\mathbf{S}_1, \mathbf{S}_2, \ldots, \mathbf{S}_p)$ are concatenated and flattened into feature vectors. Given that the final step of the microstructure and its properties encapsulate its ultimate state, we specifically select and flatten the last step ODF (ODF_p) and its homogenized properties $(\mathbf{C}_p, \mathbf{S}_p)$ as inputs for our non-sequential modeling methods. These representations serve as inputs for various non-sequential models.

To establish baseline performance, we employ established machine learning techniques, including Ridge regression and random forest, capturing relationships from linear to complex non-linear interactions. Additionally, we employ AutoKeras, an advanced AutoML tool, to automate model selection and hyperparameter tuning for Densely Connected Neural Networks (DCNNs). AutoKeras explores a wide range of neural network architectures and configurations, ensuring the selection of well-tuned and effective models. This approach efficiently identifies optimal model structures and parameters, enhancing our framework's predictive performance.

C. Sequential Modeling Methods

Considering the time-series nature of the evolved microstructures and their homogenized properties, we utilize several sequential modeling methods. Our proposed model architecture leverages time-series layers to capture the temporal dependencies inherent in the data. We use Long Short-Term Memory (LSTM) networks, a type of recurrent neural network (RNN) designed for sequential data. LSTMs address the vanishing gradient problem through a gating mechanism, enabling the network to maintain and update information over long sequences. This makes them well-suited for capturing temporal changes in microstructure evolution and predicting processing parameters. Gated Recurrent Units (GRUs), as another type of RNN optimized for sequential data, simplify the LSTM architecture by combining gates and merging the cell state with the hidden state.

Our proposed model architecture incorporates either LSTM or GRU layers combined with fully connected layers to process the time-series data. We use the sigmoid activation function in the output layer to bound predictions between 0 and 1, appropriate for our processing parameter values. This combination of sequential and dense layers allows the model to effectively learn the temporal patterns and relationships within the data, leading to more accurate and reliable predictions.

We further explore a transformer architecture to capture complex temporal dependencies. This model includes an input embedding layer that projects the input features into a higher-dimensional space, followed by a positional encoding layer to

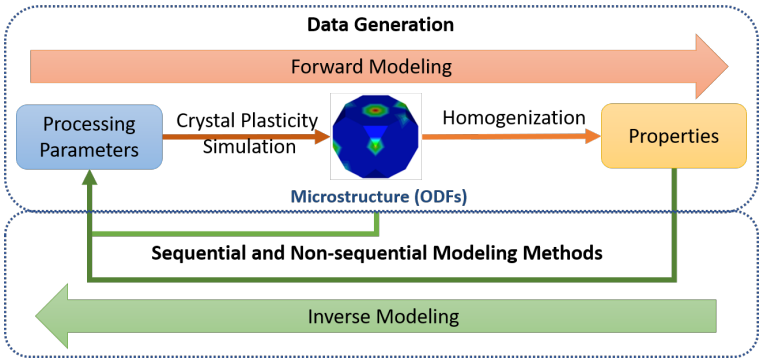

Fig. 1. Overview of Deep Learning-based Inverse Modeling Framework. The figure's top shows data generation via forward modeling, where processing parameters drive crystal plasticity simulation to produce microstructure sequences ($\text{ODF}_1, \ldots, \text{ODF}_p$), followed by homogenization to generate property sequences: stiffness tensors ($\mathbf{C}_1, \ldots, \mathbf{C}_p$) and compliance tensors ($\mathbf{S}_1, \ldots, \mathbf{S}_p$). The figure's bottom depicts two primary inverse modeling tasks addressed by our framework: predicting processing parameters from microstructures and properties using both non-sequential and sequential deep learning methods.

retain sequence order information. Its core comprises multiple transformer encoder layers with self-attention mechanisms and feedforward neural networks to model intricate relationships within the data. The final output is passed through a fully connected layer and a sigmoid activation function to ensure the predictions are within the range of [0, 1]. This transformer-based model complements our LSTM and GRU architectures, providing a robust framework for capturing temporal patterns in microstructure evolution or its properties.

IV. Evaluation

A. Dataset

We evaluated our framework on two inverse modeling tasks, each with a distinct dataset. The first task involves predicting processing parameters from the microstructure inputs. We employed the strain-rate independent crystal plasticity simulation with randomly sampled strain rate values (s^{-1}) between $[0, 1]$ to create 31,588 unique parameter combinations. For each combination, we simulated 10 steps ($p = 10$), starting from a uniform initial ODF and producing the final deformed ODF along with nine intermediate steps. Each ODF is represented as a 76-dimensional vector, resulting in an input size of 10×76.

In our second task, our framework predicts the processing parameters from properties. The second dataset was derived from the first through homogenization as described in Section II-B. For each ODF, we calculated two elastic properties: the stiffness tensor $\mathbf{C}$ and the compliance tensor $\mathbf{S}$, both sized 6×6. These tensors were concatenated to form the input data with a size of $10 \times 6 \times 6 \times 2$, using the same processing parameters as the first dataset for labels. For both datasets, we divided the data into 70% for training and 30% for testing.

B. Evaluation Metrics

We use the Root Mean Squared Error (RMSE) as the primary evaluation metric, aligning with the Mean Squared Error (MSE) loss used during training. RMSE provides an interpretable measure of the average prediction error in the same units as the output variable. We calculate RMSE for each individual processing parameter to gain detailed insights into the model's performance:

$$\text{RMSE} = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(\text{Process\_actual}_i - \text{Process\_pred}_i)^2} \quad (4)$$

where n is the number of samples, Process_actual_i is the actual value and Process_pred_i is the predicted value of the processing parameter for the i-th sample. The processing parameters (strain rates) range between $[0, 1]$. We calculate the average RMSE across all 5 processing parameters for a comprehensive assessment of overall prediction accuracy.

C. Experimental Settings

We employed distinct configurations for non-sequential and sequential models. For non-sequential models, we utilized AutoKeras to explore various architectures and used the AdamW optimizer with a Mean Squared Error (MSE) loss function. The learning rate for these models was set to 0.001. Sequential models used the Adam optimizer with an MSE loss function, with learning rates of 0.001 for ODF-based models and 0.0001 for property-only models. The training dataset was further split into 70% training and 30% validation sets. The best models, selected based on validation performance, were then evaluated on the unseen test dataset. In the following sections, we compare the results of non-sequential and sequential models on our two primary inverse modeling tasks.

D. Evaluation on Predicting Processing from Microstructure

To assess the performance of our framework on the first task, we compared it with several baseline machine learning methods. The dataset consists of sequences of 10 ODFs (size 10×76) as inputs and 5 processing parameters as labels. Additionally, we assessed the framework using only the final ODF (size 76) as inputs, allowing us to compare the predictive results of the complete ODF sequence versus the final microstructural state.

TABLE I
TEST RMSE FOR PREDICTING 5 PROCESSING PARAMETERS FROM 10 ODFS USING NON-SEQUENTIAL BASELINES, NON-SEQUENTIAL DEEP LEARNING MODELS, AND SEQUENTIAL DEEP LEARNING MODELS.

Models	Test RMSE Values	Average Test RMSE
Ridge Regression	[0.0455, 0.0418, 0.0373, 0.0418, 0.0391]	0.0411
Random Forest	[0.0356, 0.0329, 0.0329, 0.0330, 0.0330]	0.0335
AutoKeras	[0.0161, 0.0164, 0.0138, 0.0148, 0.0170]	0.0156
LSTM	[0.0167, 0.0184, 0.0158, 0.0158, 0.0173]	0.0168
Transformer	[0.0255, 0.0283, 0.0226, 0.0224, 0.0241]	0.0246
GRU	[0.0148, 0.0176, 0.0141, 0.0134, 0.0161]	**0.0152**

TABLE II
TEST RMSE FOR PREDICTING 5 PROCESSING PARAMETERS FROM LAST ODF USING NON-SEQUENTIAL MACHINE LEARNING BASELINES AND NON-SEQUENTIAL DEEP LEARNING MODELS.

Models	Test RMSE Values	Average Test RMSE
Ridge Regression	[0.0612 0.0587 0.0504 0.0612 0.0571]	0.0577
Random Forest	[0.0417 0.0421 0.0400 0.0406 0.0400]	0.0409
AutoKeras	[0.0268 0.0295 0.0237 0.0245 0.0257]	**0.0260**

TABLE III
TEST RMSE FOR PREDICTING 5 PROCESSING PARAMETERS FROM 10 ODFS PROPERTIES USING NON-SEQUENTIAL BASELINES, NON-SEQUENTIAL DEEP LEARNING MODELS, AND SEQUENTIAL DEEP LEARNING MODELS.

Models	Test RMSE Values	Average Test RMSE
Ridge Regression	[0.1182, 0.1015, 0.1166, 0.1119, 0.1312]	0.1159
Random Forest	[0.0862, 0.0526, 0.0597, 0.0564, 0.0531]	0.0616
AutoKeras	[0.0326, 0.0288, 0.0281, 0.0300, 0.0281]	**0.0295**
LSTM	[0.0716, 0.0563, 0.0632, 0.0547, 0.0524]	0.0596
Transformer	[0.0495, 0.0446, 0.0473, 0.0420, 0.0399]	0.0447
GRU	[0.0523, 0.0354, 0.0412, 0.0359, 0.0361]	0.0402

TABLE IV
TEST RMSE FOR PREDICTING 5 PROCESSING PARAMETERS FROM PROPERTIES OF THE LAST ODF USING NON-SEQUENTIAL MACHINE LEARNING BASELINES AND NON-SEQUENTIAL DEEP LEARNING MODELS.

Models	Test RMSE Values	Average Test RMSE
Ridge Regression	[0.1673, 0.1447, 0.1707, 0.1902, 0.1372]	0.1620
Random Forest	[0.1155, 0.0893, 0.0989, 0.1282, 0.0677]	0.0999
AutoKeras	[0.0784, 0.0573, 0.0592, 0.0791, 0.0506]	**0.0649**

1) Using Evolution of 10 ODFs: Table I presents the RMSE for each of the five processing parameters and the average RMSE, comparing baseline machine learning methods, non-sequential deep learning models (AutoKeras), and sequential deep learning models. Among the baselines, Random Forest performs best with an average RMSE of 0.0335, outperforming ridge regression. The optimal AutoKeras model uses four dense layers (1024, 512, 128, 5) with ReLU activations. The input sequences were flattened into a 760-dimensional vector.

Given that the ODFs are time-series data reflecting microstructure evolution, we evaluated sequential models using LSTM, GRU, and transformer layers. A grid search was conducted to optimize the hyperparameters, selecting the model with the minimum validation loss for testing. The results show that the GRU model achieved a significant reduction in the average RMSE, lowering it from 0.0335 (Random Forest) to 0.0152, a reduction of 54.62%. As anticipated, the GRU model, designed for sequential data, slightly outperformed the non-sequential model from AutoKeras, which achieved 0.0156. These improvements over baselines underscore our framework's effectiveness in learning from sequence data, enabling accurate predictions of processing parameters based on microstructural evolution.

2) Using the Last ODF: Given the significance of the final microstructural state, we evaluated non-sequential models using only the last ODF from the sequence. Table II shows that Random Forest achieved the best baseline test RMSE of 0.0409. In contrast, the AutoKeras-optimized neural networks achieved a significantly lower test RMSE of 0.0260, a 36.43% reduction. The optimal model comprises three fully connected layers (512, 64, 5) with ReLU activation. Using only the last ODF results in slightly worse prediction accuracy compared to the full 10 ODF sequence (best RMSE 0.0152) due to less information on microstructure evolution. Despite this, the results demonstrate our framework's ability to make reasonably accurate predictions from the final microstructural state.

E. Evaluation on Predicting Processing Parameters from Properties

For the second inverse modeling task, we used a dataset consisting of time-series properties derived from 10 ODFs, represented by a tensor of size $10\times6\times6\times2$, calculated through homogenization. Both non-sequential and sequential modeling methods are assessed on this dataset. To specifically examine the final microstructure properties, we assessed non-sequential models using the last ODF properties of size $6 \times 6 \times 2$.

1) Using 10 ODFs Properties: Table III compares the prediction accuracy of non-sequential modeling methods, including machine learning baselines, dense networks explored with AutoKeras, and sequential modeling methods using LSTM, GRU, or Transformer layers. Random Forest performs best among baselines with an average test RMSE of 0.0616. The AutoKeras-optimized dense networks achieve the lowest RMSE of 0.0295, representing a significant reduction of 52.11% from the best baseline. The optimal model uses four 1024-unit dense layers with batch normalization.

Despite the time-series nature of the data, sequential models perform slightly worse, unlike with ODF sequences. This suggests that sequential models may not fully capture relevant information from property tensors as effectively as from ODFs. Additionally, the best average RMSE from predicting with 10 ODFs is 0.0152, compared to 0.0295 from properties. This indicates that predicting processing parameters from

properties is more challenging, as structures might contain more information directly related to the processing methods, making prediction easier than using properties alone.

2) Using last ODF Properties: Similar to the first task, we evaluate our framework using the properties derived from the last ODF to predict the processing strain rates. Table IV shows that Random Forest achieves the best baseline average RMSE of 0.0999, worse than previous evaluations. This result is expected since microstructures are simulated from processing parameters, while properties are then derived from these microstructures. Properties from only the last ODF contain less information than the full ODF sequence.

Following this trend, the best model optimized by AutoKeras achieves a test RMSE of 0.0649, which is also inferior to predictions from microstructures or the sequence of properties. This model contains four dense layers with 32, 1024, 256, and 5 units with ReLU activation and batch normalization layers in between. Furthermore, the first processing parameter consistently shows large test RMSE values among the five across predictions, indicating a potential area for future refinement.

V. Conclusion

In this paper, we present a deep learning-based framework exploring both non-sequential and sequential models to address the inverse problem of predicting processing parameters from microstructures and properties in polycrystalline materials. Our framework achieves high accuracy with RMSE as low as 0.0152 for microstructures and 0.0295 for properties. While our framework shows promise as a powerful tool for material design, it currently predicts only a single combination of processing parameters. Future work could extend to generating multiple viable parameter combinations and incorporate simulations for comprehensive evaluation. Moreover, given our framework's high accuracy in predicting processing parameters from microstructures, it could be integrated with approaches that predict microstructures from properties (e.g., Mao et al. [7]) to potentially enhance predictions from properties to processing parameters. In conclusion, our framework represents a significant advancement in addressing the inverse problem in materials science, providing a promising pathway for optimizing the design and manufacturing of polycrystalline materials.

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