

A novel neutron texture diffractometer analyzing method with Convolutional Neural Networks for Face-Centered Cubic Material

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Abstract

In this study, we propose a convolutional neural network (CNN) model aimed at inferring texture types and their volume fractions from neutron diffractometer data. The model is trained using labeled texture data of face-centered cubic (FCC) materials, sourced from X-ray diffraction (XRD) measurements. The effectiveness of the model is evaluated using data obtained from neutron diffraction. Compared to traditional data analysis methods, the CNN model not only offers fast and accurate predictions of texture components and their volume fractions, but also demonstrates strong generalization ability. Even under a certain signal-to-noise ratio, the CNN model maintains high accuracy in inferring texture types and their volume fractions. This capability could facilitate the operation of neutron texture diffractometers at lower neutron beam intensities in the future, thus improving both the efficiency of texture analysis.

Full Text

Preamble

A Novel Neutron Texture Diffractometer Analyzing Method with Convolutional Neural Networks for Face-Centered Cubic Material

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In this study, we propose a convolutional neural network (CNN) model aimed at inferring texture types and their volume fractions from neutron diffractometer data. The model is trained using labeled texture data of face-centered cubic (FCC) materials, sourced from X-ray diffraction (XRD) measurements. The effectiveness of the model is evaluated using data obtained from neutron diffraction. Compared to traditional data analysis methods, the CNN model not only offers fast and accurate predictions of texture components and their volume fractions, but also demonstrates strong generalization ability. Even under low signal-to-noise ratio conditions, the CNN model maintains high accuracy in inferring texture types and their volume fractions. This capability could facilitate the operation of neutron texture diffractometers at lower neutron beam intensities in the future, thus improving the efficiency of texture analysis.

Keywords: convolutional neural networks, texture, neutron diffraction, X-ray diffraction, face-centered cubic material

Introduction

The crystallographic texture, defined as the preferred orientation distribution of grains in polycrystalline materials, induces anisotropy in material properties¹⁻³ and consequently affects both processing behavior and service performance. Moreover, texture serves as a critical diagnostic parameter in material failure analysis⁴. Therefore, precise texture characterization is fundamental for optimizing texture control strategies, refining processing parameters, and enhancing material performance. Current texture characterization methodologies employ multiple experimental techniques, including electron backscatter diffraction (EBSD)⁵, X-ray diffraction (XRD)⁶, synchrotron X-ray diffraction^{7,8}, and neutron diffraction (NuD)⁹, which provide complementary characterization capabilities for polycrystalline systems.

Quantitative analysis of texture distributions requires diffraction pattern acquisition across multiple crystallographic orientations and the utility of a neutron detector. Currently, a two-dimensional position-sensitive detector is usually used for improving the measurement efficiency of neutron texture diffractometers^{10,11}, and more data needs to be collected in a short period. Consequently, two main challenges arise in texture data processing. First, collecting a large amount of data slows down the processing speed and impedes real-time assessment of the texture information of the measured materials. This is because texture data processing involves multiple steps, including data acquisition, pre-processing to obtain the pole figure, orientation distribution function (ODF), and texture component analysis¹¹. Second, the accuracy of current texture

analysis methods is often compromised by significant errors in diffraction peak intensity fitting, particularly for polycrystalline materials that exhibit weak overall texture, a combination of strong and weak texture components, or strongly overlapping diffraction peaks. This naturally motivates the development of more powerful data analysis methods.

State-of-the-art machine learning (ML) technology has demonstrated remarkable capabilities for nuclear physics¹² and high energy physics¹³. In particular, ML has also shown remarkable capabilities in materials characterization, as evidenced by successful applications in various experimental techniques, including XRD^{14–16}, EBSD^{17–19}, and synchrotron X-ray diffraction^{20–22}. These achievements have motivated researchers at neutron scattering laboratories to explore the ML potential in related domains. Recent studies have documented ML implementations in neutron instrumentation, specifically single-crystal diffractometers²³, neutron reflectometers^{24, 25}, and imaging facilities^{26–28}. Nevertheless, ML deployment in neutron texture diffractometers remains uninvestigated.

In this work, we propose a machine learning-based framework for texture analysis in crystalline materials. The paper is organized as follows. First, a face-centered cubic (FCC) material texture dataset, derived from high-resolution XRD measurements, is established. Subsequently, a customized convolutional neural network (CNN) architecture is developed and optimized using this dataset. Finally, the model is validated for accuracy and noise immunity.

II. Methods

A. Flow Chart of the Texture Analyzing and the Texture Distributions

As shown in Fig. 1 [Figure 1: see original paper], the traditional texture analysis process typically comprises four key stages: First, acquisition of pole figure data for different crystallographic planes through XRD or NuD experiments, recorded using a two-dimensional position-sensitive detector. Subsequently, raw pole figure data undergo background correction and normalization to obtain the normalized pole density distribution. The spherical harmonic expansion method is then applied to calculate the three-dimensional ODF. Finally, texture components are identified and their volume fractions quantified through ODF interpretation.

Due to the highly symmetric close-packed configuration of $\{111\}$ crystallographic planes in FCC structured materials, which provides 12 equivalent slip systems, these materials exhibit unique advantages in ductility, toughness, and resistance to irradiation damage. Consequently, FCC materials are widely used in various industrial sectors, including automotive, aerospace, marine, and nuclear reactor industries. The comprehensive research foundation and extensive experimental data available for texture studies of FCC materials make investigations into their crystallographic texture particularly valuable.

Given this research background, the present study focuses specifically on analyzing the texture characteristics of FCC structured materials, where the (111), (200), and (220) pole figures serve as fundamental inputs for texture characterization. Six representative FCC texture components were selected for analysis: Goss²⁹, Brass^{30–32}, Cube³³, Copper³², S³¹, and R³⁴ orientations. Fig. 2 [Figure 2: see original paper] illustrates the characteristic pole figures of these six texture components, demonstrating their distinct distribution patterns in the (111), (200), and (220) crystallographic planes. This conventional texture analysis requires approximately 5 minutes per sample.

ML approaches offer significant potential for workflow optimization. As illustrated in Fig. 1, establishing direct mappings between pole figures and texture components could substantially enhance analysis efficiency.

B. CNN Texture Analyzing Method

1. CNN Architecture CNN³⁵, a deep learning architecture specialized for processing grid-structured data (e.g., images, time-series signals), has demonstrated remarkable success in computer vision and materials informatics applications^{36–38}. In this study, we employ a CNN architecture to establish an efficient mapping relationship between pole figure data and corresponding texture components with their volume fractions. Fig. 3 [Figure 3: see original paper] shows the architecture of the CNN model which consists of input, extraction, fully connected, and output layers. In our case, the input data for the input layer is $x^{(0)} = \{I^{(111)}(\chi, \phi), I^{(200)}(\chi, \phi), I^{(220)}(\chi, \phi)\}$, where $I^{(hkl)}(\chi, \phi)$ is the intensity distribution on χ (the polar angle between the (hkl) crystallographic plane normal and the sample normal direction) and ϕ (the azimuthal rotation angle about the sample normal axis). The final output is $y_i = \{V_{frac}^{(1)}, V_{frac}^{(2)}, V_{frac}^{(3)}, V_{frac}^{(4)}, V_{frac}^{(5)}, V_{frac}^{(6)}\}$, where $V_{frac}^{(j)}$ denotes the volume fractions of the j -th texture components.

The feature extraction module comprises sequential processing through Conv_{Before}, Inception_1, Inception_2, Inception_3, and Conv_{After} sub-structures. Initial feature extraction occurs through Conv_{Before}, followed by multi-scale feature learning via three Inception modules. The Conv_{After} sub-structure finalizes the feature extraction process, preparing high-level representations for subsequent layers. Architectural details are provided in Appendix Fig. 10 [Figure 10: see original paper].

The fully connected layer consists of six parallel hidden layers (32 neurons each) with independent parameters. These layers integrate high-dimensional features from the extraction module and perform dimensionality reduction through linear transformations, ultimately predicting the volume fractions $V_{frac}^{(j)}$ for the six texture components via output layers. In our work, the CNN model is implemented using the PyTorch framework³⁹.

2. Data Set Preparation To facilitate ML implementation, we established a dataset comprising 137 experimentally measured pole figures: 121 collected via XRD from silver-, nickel-, and copper-based alloys, with an additional 16 aluminum alloy pole figures acquired through neutron diffraction experiments at the China Advanced Research Reactor (CARR).

All data were acquired using the equal-angle step method with χ and ϕ sampling intervals of $5^\circ \times 5^\circ$ (Fig. 4 [Figure 4: see original paper]). This angular resolution ensures sufficient accuracy for spherical harmonic reconstruction while minimizing experimental data requirements, as evidenced by the resultant dataset dimensions of $3 \times 19 \times 72$, where the first dimension corresponds to the three crystallographic planes [(111), (200), (220)], the second dimension represents the angular sampling points along χ (0° to 90° in 5° steps), and the third dimension represents the angular sampling points along ϕ (0° to 355° in 5° steps). Diffraction intensities I_{hkl} were recorded at each measurement position and processed through LaboTex software (v3.0)⁴⁰ for ODF calculation. The extracted volume fractions V_{frac} of the six texture components served as labels of the dataset for subsequent ML analysis.

The limited size of the raw dataset ($N = 121$) is insufficient to train deep learning models effectively. To overcome this data scarcity, we propose a symmetry-based data expansion strategy leveraging crystallographic pole figure symmetries.

The data expansion is done by considering the symmetry properties of pole figure. Ideally, the pole figures on the (111), (200), and (220) planes exhibit mirror symmetry with the transverse direction (TD, the direction perpendicular to the main deformation direction during the processing of the material) and the rolling direction (RD, the direction along which the material is rolled during processing) as the axes of symmetry due to the geometric symmetry of the cubic sample. Thus, only 1/4 of the pole figure is useful for determining the texture in material, which means the effective data matrix will be $3 \times 19 \times 18$ rather than the whole pole figure data, i.e., $3 \times 19 \times 72$. However, due to the statistical and systematic uncertainties in the measurements, the experimental results of the pole figures do not strictly satisfy this symmetry requirement. This property suggests that we can split one pole figure into four different sub-pole figures to increase the number of training datasets with minimal influence on the identification of the texture type and its volume fraction. To verify the accuracy of texture identification using 1/4 pole figure, we examined the results of texture identification using the 1/4 pole figure shown in Fig. 5 Figure 5: see original paper. Our calculations show that the predicted results are consistent with those obtained using the complete pole figures.

The following process was designed and is shown in Fig. 5. First, three pole figures are divided into four parts according to the mirror symmetry axis as shown in Fig. 5(a), yielding 12 effective pole figures. Then, we randomly select a part from each pole figure and format it into matrix format, reducing the ϕ direction data from 72 to 18. Similar selection operations are applied to the

remaining two pole figures. Finally, the three selected matrices are stacked to form a pole figure data represented in a three-dimensional matrix format (i.e., $3 \times 19 \times 18$). Through this procedure, a dataset with $121 \times 4 \times 4 \times 4 = 7744$ samples was formed.

In order to facilitate a reliable model, the data set has been divided into a training set and a validation set according to a ratio of 8:2. The model parameters are updated according to the training set during the learning process, and the validation set is employed to fine-tune the model parameters.

3. Data Preprocessing Before training the CNN model, the data have to be preprocessed due to the following two reasons. One is that the differences in the physical properties of X-rays and neutron rays give rise to a considerable intensity range, from 10^2 to 10^5 , as observed in the pole figure data obtained from various material tests. This large range of intensity poses challenges for CNN model training. In order to ensure that the model trained using the XRD dataset can also perform effectively in the NuD prediction task, it is necessary to normalize the measurement intensity of the sample according to the following steps:

$$x(\chi, \phi) = \frac{I(\chi, \phi) - I_{min}(\chi, \phi)}{I_{max}(\chi, \phi) - I_{min}(\chi, \phi)}$$

where x is the reduced measured signal intensity, and $I_{min}(\chi, \phi)$ and $I_{max}(\chi, \phi)$ are the minimum and maximum measured signal intensities, respectively.

The other reason is that significant differences exist in the volume fraction V_{frac} values across different labels. As illustrated in Fig. 6, the brass component exhibits a volume fraction of 6.02%, whereas the cube component demonstrates only 0.44%. This 5.58% discrepancy between component fractions significantly impacts the model's predictive accuracy. To address this issue and improve model performance, we apply a logarithmic transformation, which can be mathematically represented as:

$$y = \ln(V_{frac} + 1)$$

As shown in Fig. 6, this nonlinear mapping is capable of suppressing considerable distinctions between volume fraction values while simultaneously preserving subtle differences between such values. Once the trained CNN model has been employed to calculate the normalized pole figure data, the predicted value can be utilized to ascertain the volume fraction of the texture in the material through:

$$V_{frac} = e^y - 1$$

4. Model Training In this network architecture, the parameters are optimized using the stochastic gradient descent (SGD) algorithm. Due to our data augmentation procedure, which generates 64 pseudo-samples from each original sample, there is a risk of data leakage where the model might prematurely learn patterns from the validation set during training. Since this work focuses on the applications of the CNN method to identify the type of texture and their volume fractions, we assumed the trained CNN model is adequate when the value of the loss function is less than 10^{-2} . Furthermore, to check the capability of the built CNN model, we also tested the model with neutron texture diffraction data which will be discussed in the following section.

The parameter update rule is defined as:

$$\theta_{new} = \theta_{old} - \eta \nabla L$$

where η is the learning rate, and L is the loss function.

In order to ensure that the model exhibits effective predictive capabilities, it is essential to set a small learning rate. However, this approach can lead to the model falling into a local minimum. Therefore, the CyclicLR learning rate scheduling strategy⁴¹ is employed to avoid this issue and ensure the model's optimal performance. The characteristic of this strategy is that the learning rate exhibits a periodic decay throughout the training epochs. The learning rate varies cyclically between 3×10^{-5} and 3×10^{-3} , with each 120-epoch cycle reducing its maximum rate by 50% while maintaining a constant minimum rate of 3×10^{-5} . Fig. 7 [Figure 7: see original paper] illustrates the adjustment of the learning rate with the number of epochs.

For the CNN model predicting volume fractions of six texture components, we define the composite loss function L as:

$$L = \sum_{j=1}^{N_t} MSE_j$$

where N_t is the number of texture components and MSE_j is the mean square error for the j -th texture component. In this work, $N_t = 6$. The MSE_j is given by:

$$MSE_j = \frac{1}{N_j} \sum_{i=1}^{N_j} (V_{frac,j}(i) - V_{frac,j}^{CNN})^2$$

Fig. 8 [Figure 8: see original paper] shows the loss function value as a function of epoch for the training set and validation set. The loss reaches about 5.0×10^{-3} after approximately 150 epochs under the proposed optimization strategy. After

being tuned by the validation sets, the value of the validation loss is about 2.0×10^{-3} , which is less than that for the training loss.

5. Generalization Ability Under Noise In order to test and verify the generalization ability of the CNN model, we aimed to demonstrate its capacity to predict the volume fraction of textures in materials measured by neutron diffraction. We utilized 16 sets of pole figure data obtained from neutron diffraction measurements to test the trained CNN model.

To quantify the generalization ability of the model, we analyzed the differences between the prediction results of the CNN model, i.e., $V_{frac,j}^{CNN}$, and the traditional analysis results, i.e., $V_{frac,j}$. The coefficient of determination R^2 is employed to quantify the discrepancies between these two sets of results:

$$R^2 = 1 - \frac{\sum_i (V_{frac}^{CNN}(i) - V_{frac}(i))^2}{\sum_i (\bar{V}_{frac}^{CNN} - V_{frac}(i))^2}$$

where \bar{V}_{frac}^{CNN} represents the mean predicted value. If the prediction can well reproduce the true data, the value of R^2 is closer to 1. The results of R^2 calculations are displayed in the yellow part of Fig. 9 [Figure 9: see original paper], where the minimum value of R^2 is 0.98805. This shows that the model can well predict the volume fraction of a certain texture from the data of neutron diffraction measurement.

In order to ascertain the capacity of the CNN to precisely predict data at low signal-to-noise ratio, random noise $\delta I(\chi, \phi)$ obeying a uniform distribution was added to the entire measurement region. The intensity of the noise is set to 10% of the maximum value of the pole figure data, i.e., $\delta I(\chi, \phi) = 10\% \times I_{max}(\chi, \phi)$. Subsequently, the model was employed to predict texture components and their fractions according to the data $I(\chi, \phi) + \delta I(\chi, \phi)$. The green part of Fig. 9 shows the R^2 metric predicted by the model after adding noise with intensity of 10% of maximum strength. Compared to the R^2 metric predicted by the model with noise-free data, the results with 10% noise show a slight decrease in the accuracy of the model's predictions. However, the minimum value of R^2 at this point is 0.94233, indicating that the model still has high prediction accuracy. This result demonstrates that the prediction using CNN retains high anti-interference ability. In cases where the intensity of the noise is greater than 10% of the maximum value of the pole figure data, the identifications become much worse.

Finally, we also check the time consumption for texture identification from the pole figure data. When using the trained CNN model, the analysis time for a single sample is less than 1 second, which is 300 times faster than the traditional method.

III. Summary and Outlook

In summary, we present a CNN model that is suitable for multi-objective prediction from pole figure data obtained by XRD measurements of FCC materials. The model was trained using the SGD algorithm and subsequently tested on pole figure data obtained from neutron diffraction measurements. The analysis results demonstrate that the model retains a high degree of predictive capability on the neutron diffraction measurement data, even though the dataset originates from XRD measurements. This is attributed to latent parameters learned in the CNN model containing the correct texture component information, which enables the CNN model to arrive at the correct conclusion on the texture component regardless of whether the input data comes from XRD or NuD.

Furthermore, the application of the CNN model to analyze pole figure data not only enables rapid prediction of material texture information but also exhibits considerable potential for utilization in specific scenarios. For example, the robust data anti-interference capacity enables the delivery of precise texture information even under high-noise conditions, which may come from lower intensity or short measuring time. In the future, further exploration of the potential applications of the CNN model in neutron texture diffractometers, such as processing raw data into texture components, will be conducted.

Appendix A: Details of the Extraction Layers in the CNN Model

Fig. 10(a)-(f) present the detailed structure of the extraction layers in the CNN model.

Panel (a) shows the CNN feature extraction layer employs Conv2dBlock (abbreviated as CB) as its fundamental building unit. Each CB sequentially integrates a convolutional layer, batch-normalization (BN) layer, and ReLU activation function in series.

The input data first enters the Conv_{Before} module. As shown in Panel (b), the initial input dimensions of $3 \times 19 \times 18$ (channels \times height \times width) are expanded to $3 \times 21 \times 21$ through zero-padding. This is subsequently processed by three cascaded CB units: the first CB utilizes a 1×1 convolutional kernel to expand the channel dimension to 32, the second CB employs a 3×3 kernel for spatial feature extraction while keeping the channel count unchanged, and the third CB further extends the channels to 64 using another 1×1 kernel. A 3×3 max-pooling layer with stride 2 then performs spatial down-sampling, ultimately yielding feature maps of dimensions $64 \times 10 \times 10$.

The Inception series modules achieve multi-scale feature fusion through differentiated architectures. Specifically, the Inception_1 module processes input features through four parallel branches (see Panel (c)): 1) a single CB with 1×1 kernel (32 output channels), 2) a branch combining a 1×1 CB and a

3×3 CB (64 output channels), 3) a pathway consisting of a 1×1 CB followed by two 3×3 CBs (16 output channels), and 4) a branch incorporating a 3×3 max-pooling layer with stride 1 and a 1×1 CB (16 output channels). Channel-wise concatenation of these branches generates $128 \times 10 \times 10$ feature maps. The Inception_2 module (see Panel (d)) follows similar architectural principles with branch outputs of 32, 64, 16, and 16 channels (from left to right). Inception_3 (see Panel (e)) employs six parallel branches producing 32, 32, 32, 4, 4, and 8 channels respectively, ultimately outputting high-dimensional features of size $112 \times 10 \times 10$.

The Conv_{After} (see Panel (f)) module executes spatial compression and channel reduction on the $112 \times 10 \times 10$ input features. This process compresses the tensor into a 512-dimensional vector through sequential operations: spatial reduction via max-pooling, channel-wise compression via large-kernel convolutions, and final flattening. These condensed features are then propagated through fully connected layers to generate quantitative predictions for six distinct texture volume fractions.

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Note: Figure translations are in progress. See original paper for figures.

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