ABSTRACT

X-ray diffraction based microscopy techniques such as High Energy Diffraction Microscopy rely on knowledge of the position of diffraction peaks with high precision. These positions are typically computed by fitting the observed intensities in area detector data to a theoretical peak shape such as pseudo-Voigt. As experiments become more complex and detector technologies evolve, the computational cost of such peak detection and shape fitting becomes the biggest hurdle to the rapid analysis required for real-time feedback during in-situ experiments. To this end, we propose BraggNN, a deep learning-based method that can determine peak positions much more rapidly than conventional pseudo-Voigt peak fitting. When applied to a test dataset, BraggNN gives errors of less than 0.29 and 0.57 pixels, relative to the conventional method, for 75% and 95% of the peaks, respectively. When applied to a real experimental dataset, a 3D reconstruction that used peak positions determined using conventional 2D pseudo-Voigt fitting. Recent advances in deep learning method implementations and special-purpose model inference accelerators allow BraggNN to deliver enormous performance improvements relative to the conventional method, running, for example, more than 200 times faster than a conventional method on a consumer-class GPU card with out-of-the-box software.

Keywords Bragg Peak · High-Energy X-Ray Diffraction Microscopy · Deep Learning

1 Introduction

Advanced materials affect every aspect of our daily lives, including the generation, transmission and use of energy. Accelerating the pace of materials design promises to enhance economic activity and the transition to a cleaner energy future. However, current material design approaches rely heavily on intuition based on past experiences and empirical relationships. In order to qualify new materials for critical applications, several high-energy X-ray characterization methods have been developed over the past decade. One of the foremost is high-energy diffraction microscopy (HEDM).
Figure 1: A diffraction peak in X-ray diffraction (11 × 11 patch). The height denotes photon counts, and the red dots show the peak position computed by fitting a pseudo-Voigt profile.

[Park et al., 2017], which provides non-destructive 3D information on structure and its evolution within polycrystalline materials. HEDM techniques have enabled breakthroughs in understanding of various processes, through carefully designed experiments that are tractable for analysis by researchers [Naragani et al., 2017, Bernier et al., 2020, Wang et al., 2020]. These methods use diffraction and tomographic imaging of up to cm-sized objects with resolutions down to the micrometer level.

A conventional HEDM experiment involves four steps: (1) data acquisition, (2) transfer of full scan from detector to central storage, (3) offline Bragg peak analysis to determine precise peak characteristics, and (4) reconstruction of grain information from the peak positions generated in the third step [Sharma et al., 2012a]. A single typical HEDM scan involves illuminating the polycrystalline aggregate of interest and acquiring diffraction images (1440–3600 frames in total) while rotating the specimen at a constant speed. Data acquisition is increasingly fast: a single typical HEDM scan consisting of 1440–3600 frames takes about 6–15 minutes to acquire today at the Advanced Photon Source (APS) and projected to be 50–100 seconds after the planned upgraded APS (APS-U) [Streiffer et al., 2015] with faster detectors. Rotation of the specimen enables each grain to satisfy the Bragg-diffraction condition multiple times, resulting in multiple diffraction peaks from the grain. Reconstruction of Far-Field (FF) HEDM data depends on determination of the peak positions with sub-pixel accuracy, which can deviate significantly from the maxima as shown in Figure 1.

Peak positions are typically computed by (optionally) transforming the peaks to polar coordinates and then fitting the peaks to a pre-selected peak shape such as Gaussian, Lorentzian, Voigt, or Pseudo-Voigt [Sharma et al., 2012a].
The Voigt profile, a probability distribution given by a convolution of a Cauchy-Lorentz distribution and a Gaussian distribution, is often used in analyzing data from spectroscopy or diffraction. However, it is computationally expensive to fit a Voigt profile in 2D (or 3D) space for each Bragg peak, so the peak shape is approximated to a pseudo-Voigt profile. Depending on sample properties and the extent of the mechanical, thermal, electromagnetic, or chemical stimuli applied to the sample, processing time can range from 10 minutes to a few weeks for one typical HEDM dataset, even when using an HPC cluster with thousands of CPU cores. These long data analysis times are more than just an inconvenience: they prevent experimental modalities that depend on measurement-based feedback for experiment steering.

Although we describe BraggNN framework as applied to FF-HEDM, it is also useful for other diffraction techniques dealing with single or polycrystal diffraction. The data and source code that support the findings of this study are openly available at [https://github.com/lzhengchun/BraggNN](https://github.com/lzhengchun/BraggNN).

## 2 BraggNN and its Training

A significant fraction of HEDM data analysis time is spent on determining peak positions, motivating us to seek methods for accelerating this operation. Artificial neural networks are known for their universal approximation capability that allows them to represent complex and abstract functions and relationships [Hornik, 1991]. Thus, a promising solution to the Bragg peak localization challenge is to train a deep learning model to directly approximate the position of Bragg peaks. Advances in both machine learning (ML) methods and AI inference accelerators allow such a model to run far faster than conventional methods, making it feasible to extract peak information from streaming data in real-time, enabling rapid feedback and reducing downstream transfer, storage, and computation costs.

### 2.1 Model Design

Deep learning (DL) is part of a broader family of machine learning methods based on artificial neural networks to progressively extract higher level features from the pixel-level input through a hierarchical multi-layer framework. The convolutional neural network (CNN), a widely used building block of DL models for visual image analysis, is parameter efficient due to the translation-invariant property of its representations, which is the key to the success of training deep models without severe over-fitting. Although a strong theory is currently missing, much empirical evidence supports the notion that both the translation-invariant property and convolutional weight sharing (whereby the same weights are shared across an entire image) are important for good predictive performance [Cheng et al., 2017].

In this work, we express this task as a regression problem using supervised machine learning and present BraggNN, a deep neural network-based model, for precisely localizing Bragg peaks far more rapidly than that can be achieved by applying conventional fitting methods to peak shape profiles. Note that we are not concerned here with the problem of locating within an image a patch that contains a peak (the object localization problem) because Bragg peaks are easily separated from background by using a heuristic thresholding value, and from neighbor peaks by using a connected-component labeling algorithm (overlapped peaks and fitting in 3D will be studied in future work) [Fiorio and Gustedt, 1998; Wu et al., 2005]. Our problem rather is to determine, with sub-pixel precision, the center-of-mass of a diffraction peak in a supplied patch: the peak localization problem.

The BraggNN network architecture, shown in Fig. 2, comprises series of CNN layers (four in the figure) acting as feature extractors are followed by a series of fully connected layers (three in the figure) that generate a regression prediction. Each CNN kernel/filter is an artificial neuron that, in contrast to traditional algorithms in which kernels are hand-engineered, learns to extract a type of feature (e.g., various oriented edges, or blobs of color) from its input. Each 2D CNN neuron has $3 \times 3 \times c$ learn-able weights plus one learn-able bias to convolve a feature map (a 3D volume shaped as height $\times$ width $\times$ depth/channel) with $c$ channels (e.g., the input patch has one channel as shown in the figure).

Here we use the first layer, which takes a Bragg peak in a patch with $11 \times 11 \times 1$ ($c = 1$) pixels as input and outputs 64 feature maps (each has $9 \times 9$ pixels), as an example to explain the convolution operation. At every convolution position, for example the one shown as a dotted line in the figure, the dot product between the weights and the input entry ($3 \times 3 \times c$ centered at the convolution position) is computed and added to the learn-able bias. This convolution result, called the activation, is then passed through a rectified linear unit (ReLU, $f_{\text{relu}}(x) = \max (x, 0)$) activation function to yield a feature. Each kernel is convolved (vertically and horizontally) across the input image, producing a $9 \times 9$ feature map. Thus, although the operation is colloquially referred to as a convolution, mathematically, it is a sliding dot product or cross-correlation. Each layer has multiple independent neurons that result in multiple feature maps. All feature maps are stacked along the depth dimension and then passed to the next layer as input. For example,
Figure 2: Application of the BraggNN deep neural network to an input patch yields a peak center position (y, z). All convolutions are 2D of size 3 × 3, with rectifier as activation function. Each fully connected layer, except for the output layer, also has a rectifier activation function.

as the first layer has 64 neurons, it turns a 11 × 11 × 1 input patch to a 9 × 9 × 64 volume. Multiple convolutions layers are chained to encode the input image into a representation in latent space.

The fully connected (FC) neural network layer takes the encoded representation produced by the CNN layer as input, estimates the center of the input Bragg peak, and produces the (x, y) coordinates as output. In a similar manner to the CNN layer, each FC layer has multiple artificial neurons, each of which has the same number of learnable weights as its input plus one learnable bias. The 3D feature map (e.g., 5 × 5 × 4) produced by the last CNN layer is reshaped into a 1D vector before feeding it into the first FC layer. The dot product between the neuron’s weights and input is computed and added to the bias. Thus, n neurons in a given FC layer generate an output vector of dimension n, which are passed into the ReLU activation function and then serve as the input of the next layer. As one can see, unlike the CNN neurons that receive input from only a restricted subarea of the previous layer for each convolution point, each neuron in a FC layer is connected to all neurons in the previous layer. The output layer in our design has no activation function (or, equivalently, it applies a linear activation).

The whole process that turns an input Bragg peak patch into two floating point numbers (the coordinates of the peak center) is called a feed forward pass. The ℓ2-norm is computed between the model output and ground truth (estimated by using pseudo-Voigt fitting) as the model loss. Training then proceeds as follows. We compute the gradient of each neuron’s weights with respect to the loss function by using the chain rule (implemented via automatic differentiation in deep learning frameworks such as PyTorch [Paszke et al. 2019]). This process of computing the gradient of learnable weights is called back propagation. The neuron’s weights are then updated by using the gradient descent optimization algorithm [Kingma and Ba 2014]. Training iterates the feed-forward and back-propagation process on different (Bragg peak patch, ground truth center) pairs many times, until the model no longer makes noticeable progress in minimizing the ℓ2-norm.

We train the BraggNN model with a collection of input-output pairs, each with a peak patch as input and the peak center position obtained from pseudo-Voigt fitting as output. Once the BraggNN model is trained, we can then apply it to patches obtained from new diffraction data as follows: (1) We use the connected-component labeling algorithm [Fiorio and Gustedt 1996; Wu et al. 2005] to detect connected regions (i.e., peaks) in binary digital images. If the region has multiple maxima, indicating the presence of overlapping peaks, the region is discarded. Overlapping peaks will be investigated in a later study. (2) For each region detected in the previous step, we determine the coordinate (row and column index of the image matrix) of its peak (maxima), and crop a patch with a pre-defined size (an odd number, must be the same as that used for training BraggNN) with the peak coordinate as the geometric center. Application of the trained BraggNN model to such a patch then yields an estimate of the peak position. Given this center of mass, we then map the position of the peak in the patch back to the diffraction frame based on the location of the patch in the diffraction frame. Each diffraction frame is processed independently, focusing only on 2D shapes of the peaks. In case of heavily deformed materials, where orientation changes within grains cause diffraction signal to be present in multiple frames, 3D peak processing would be required and will be investigated in a future study.
The performance of a deep neural network depends heavily on the quantity, quality, and diversity of the data used to train the model. If data are not sufficiently diverse, it is easy to experience overfitting, whereby a network learns a function with very high variance that models the training data perfectly but performs badly on other data. Many application domains, including ours, lack access to large (in terms of both quantity and diversity) and high-quality (accurately annotated) labelled data. Data augmentation is a strategy that enables practitioners to significantly increase the diversity of data available to train their DL models, without actually collecting new data. Data augmentation techniques such as cropping, padding, and horizontal flipping are commonly used to train large neural networks for image classification [Cubuk et al., 2018, Shorten and Khoshgoftaar, 2019] such as CIFAR-10 [Krizhevsky, 2009] and ImageNet [Deng et al., 2009].

While some existing data augmentation techniques may be useful in the Bragg peak context to avoid overfitting, none are useful for training a more generic model (e.g., one that generalizes to data outside the training set, or that handles unseen peaks cropped from noisy diffraction frames) because the augmented samples used in the above mentioned techniques will not be found in practice.

Thus, we introduce a novel physics-inspired data augmentation method that can both avoid overfitting and help to train a more generic model able to deal with imperfect peak cropping from noisy diffraction frames. Specifically, when cropping patches for model training we deviate the peak center from the geometric center randomly by up to ±2 pixels in horizontal and vertical directions. Fig. 3 demonstrates a batch of 10 patches with (Fig. 3(a)) and without (Fig. 3(b)) data augmentation.

This data augmentation approach helps to train a more general model because, like regularization, [Zhang et al., 2016] it adds prior knowledge (the center-of-mass is not always near the geometric center) to a model training and increases training data. It also helps to make the testing dataset statistically more similar to the peak patches that will be encountered during inference in production. The ablation evaluation in Appendix 4.2 shows the effectiveness of this novel data augmentation method.

2.3 Model Training

An important tunable parameter when training a model is the input patch size, as shown in Fig. 2. The appropriate patch size depends on the pixel size of the detector and size of the diffraction peaks. Best practice is to choose a patch size that can fully cover all valid peaks and still leave 2–4 pixels from peak edge to patch edge for data augmentation. Since
the input patch size will determine the size of the neurons in the first fully connected layer, a model trained with one patch size cannot work with another patch size in practice. Another tunable parameter is for data augmentation, i.e., the interval of $m$ and $n$. We typically choose the same interval size for $m$ and $n$. During training, we independently sample (with replacement) a number from the interval for $m$ and $n$ separately in order to prepare each sample of each mini-batch online.

We implemented our model by using the PyTorch [Paszke et al., 2019] machine learning framework. We train the model for a maximum of 80,000 iterations with a mini-batch size of 512, with validation-based early stopping applied to avoid using an over-fitted model for testing and production use. Training takes about two hours using one NVIDIA V100 GPU, and only a few minutes using the Cerebras CS-1 artificial intelligence computer.

In the experimental studies reported in this paper we train and evaluate BraggNN on a diffraction scan dataset collected using an undeformed bi-crystal Gold sample [Shade et al., 2016] with 1440 frames (0.25° steps over 360°) totaling 69,447 valid peaks. We use 80% of these peaks (55,478) as our training set, 6,000 peaks (~9%) as our validation set for early stopping [Goodfellow et al., 2016] and the remaining 7,869 peaks (~11%) as a test dataset for model evaluation.

3 Results Analysis and Discussion

Once the model is trained, we evaluate its performance from two perspectives: 1) we measure distance (i.e., error) between each BraggNN-estimated center and the corresponding center obtained via conventional pseudo-Voigt profile (conventional method); 2) we apply BraggNN to an experiment of a different sample, reconstruct grains using peak information by BraggNN, and compare reconstructed grain size and position with those reconstructed using conventional method Sharma et al. [2012a].

3.1 Model Performance

We start with quantitatively evaluating BraggNN by looking at the accuracy of Bragg positions estimated by it. Fig. 4 shows the distribution of difference between position of diffraction peaks determined using BraggNN (a-c) or peak Maxima (d) and conventional pseudo-Voigt fit. Fig. 4(a-b) show that BraggNN tends to underestimate the positions more often than overestimating them. As quantified using Euclidean distance in Fig. 4(c), most peaks deviate little (e.g., 75% of peaks deviate less than 0.3 pixels) from the position identified by conventional method. The difference between position of the maximum intensity of Bragg peaks (with resolution of up to 0.5 pixels) and conventional method results, shown in Fig. 4(d), are much higher than differences between BraggNN and conventional method results Fig. 4(c).

3.2 Reconstruction Error Analysis

Since the reconstruction of grain positions is our final goal, we also evaluate the trained BraggNN on a different dataset [Turner et al., 2016] and compare with results from the conventional method. The dataset consists of Far-Field (FF) and Near-Field (NF) HEDM data acquired in-situ during deformation of a Ti-7Al sample. FF-HEDM data was acquired using the same beam configuration at the same location in the sample as NF-HEDM data, thus enabling a one-to-one comparison of Center-Of-Mass (COM) position of grains. FF-HEDM directly outputs COM position of grains, whereas COM positions were calculated from NF-HEDM reconstructions using the voxelized information. A single 2D slice of the specimen was reconstructed using the MIDAS software package [Sharma, 2020] Sharma et al. 2012b[a] in three different configurations: FF-HEDM reconstruction using BraggNN, FF-HEDM reconstruction using conventional pseudo-Voigt fitting and NF-HEDM reconstruction.

First we compare the FF-HEDM reconstructions using peak positions obtained from BraggNN to the FF-HEDM reconstructions using conventional pseudo-Voigt fitting, shown in Fig. 5. The difference in position in the $x$-axis (along the x-ray beam, Fig. 5(a)), $y$-axis (horizontal direction perpendicular to the $x$-axis, Fig. 5(b)) and $z$-axis (vertical direction coincident with the rotation axis, Fig. 5(c)) are centered around 0, implying there is no systematic bias between the two reconstructions. The euclidean distance between grains reconstructed using BraggNN and conventional pseudo-Voigt fitting (Fig. 5(d)) is less than 15 $\mu$m for 50% of the grains.

We note that, although we compare BraggNN with conventional pseudo-Voigt fitting, the ill-posed inverse problem means that conventional pseudo-Voigt is not the ground truth. Therefore, we use and compare the grain COMs estimated from NF-HEDM, which results in higher resolution reconstructions by providing a space-filling orientation map, to grain COMs obtained using the FF-HEDM reconstruction technique that is the focus of this paper. A total of 68 grains were identified using NF-HEDM, out of which all the grains could be matched using conventional pseudo-Voigt fitting,
but 6 grains were not detected using BraggNN because BraggNN ignored overlapping peaks. Fig. 6(a) shows the position of grains imaged using the three different reconstruction methods (NF-HEDM, pseudo-Voigt FF-HEDM and BraggNN FF-HEDM) overlaid on grain shapes obtained using NF-HEDM. It can be seen that most of centroids can be detected using BraggNN.

Quantitatively, Fig. 6(b) shows the distance between grains imaged using pseudo-Voigt FF-HEDM and NF-HEDM; the mean and median distances are 19.9 µm and 15.3 µm, respectively. Similarly, Fig. 6(c) shows the distance between grains imaged using BraggNN and NF-HEDM. The mean and median distances are 17.0 µm and 13.2 µm. It can be seen that the results from BraggNN are, on average, 15% better than pseudo-Voigt fitting. The markers in Fig. 6(b-c) are colored according to mean of the difference in position of expected and observed diffraction spots for each grain. Here too, BraggNN performs better than pseudo-Voigt fitting by 28.6%.

Internal Angle, another measure of quality of reconstructions, is mean of the angle between expected and observed diffraction-vectors for each grain. The size of markers in Fig. 6(b-c) is directly proportional to Internal Angle of the respective grain with BraggNN performing better than pseudo-Voigt fitting by 13%.

### 3.3 Computational Efficiency

Comparison of the reconstructed grain characteristics obtained with BraggNN with those obtained with conventional methods reveals no noticeable difference. However, BraggNN is much faster. Our highly optimized implementation of 2D pseudo-Voigt fitting, coded in the C programming language, takes about 400 core-seconds to process a dataset of 800,000 peaks on an 2.6 GHz, four-core, Intel Xeon server processor. On the same platform, BraggNN takes less
than 7 core-seconds to process the dataset, a speedup of $57 \times$. As it is an out-of-the-box solution to run BraggNN on a GPU with any deep learning framework (i.e., no extra efforts needed to program BraggNN for GPU), we also evaluate BraggNN on a NVIDIA V100 GPU.

Analysis of the dataset takes only 280ms, for a speedup of more than $350 \times$ relative to the pseudo-Voigt fitting code on a quad-core server CPU (to the best of our knowledge, there is no GPU-accelerated 2D pseudo-Voigt fitting implementation available so far). If no server-class GPU is available near the experiment facility, BraggNN on a desktop with an affordable gaming NVIDIA RTX 2080Ti card only takes about 400ms, a speedup of $250 \times$ relative to running conventional pseudo-Voigt fitting on a high-end workstation CPU. We note that the dataset that we used for our evaluation is small, having been collected at only every 0.25° ($1440$ images for $360°$). If we collect with step size of 0.01° ($36000$ images for $360°$) to assure better angular resolution in peak coordinates, the conventional method will take hundreds of hours to process all peaks while BraggNN can do it within an hour.

4 Ablation Study

We describe experiments that we used to study the effectiveness of the data augmentation method described in §2.2 and the non-local self-attention block in our BraggNN architecture design.

4.1 Non-local Attention

We used a non-local self-attention block on the feature maps of the first CNN layer for BraggNN in order to capture global information on the input patch of peak. The intuition behind this is that a global view at the early layer can help
Figure 6: A comparison of BraggNN, pseudo-Voigt FF-HEDM and NF-HEDM. (a) Grain positions from NF-HEDM (black squares), pseudo-Voigt FF-HEDM (red circles) and BraggNN FF-HEDM (blue triangles) overlaid on NF-HEDM confidence map. (b-c) Difference in position of grains between pseudo-Voigt FF-HEDM (b), BraggNN (c) and NF-HEDM as a function of Grain Size. Color of markers in (b-c) represent the mean difference in position of expected and observed diffraction spots. Size of markers in (b-c) represent the mean Internal Angle (see text).

CNN layers better extract feature representation in the latent space for fully-connected layers to better approximate its center [Wang et al., 2018]. Here, we conduct an ablation study to show its effectiveness. We train two models, one with attention block one without, using the same datasets, i.e., attention block is the only difference, and then we evaluate their estimation accuracy. Fig. 7 shows the distribution of deviations. It is clear that both the 50th and 75th percentile deviations are more than 20% worse than Fig. 4(c) where BraggNN has the non-local self-attention block, the 95th percentile is about 15% worse.

4.2 Data Augmentation

We presented a novel data augmentation method to prevent model over-fitting and to address inaccurate patch cropping using the connect component in the model inference phase. In order to study its effectiveness, we trained BraggNN on a simulation dataset with and without augmentation. When trained with augmentation, we use an interval of $[-1, 1]$ for both $m$ and $n$. Fig. 8 demonstrates three arbitrarily selected cases in our test dataset where the computed peak location deviated from the corresponding patch’s geometric center (i.e., $(5, 5)$ for a $11 \times 11$ pixel patch) in different directions. We can see from the demonstration that BraggNN is able to locate the peak values precisely even when the peak is deviated from the geometric center.

In order to quantitatively evaluate the effectiveness of data augmentation, we sample $m$ and $n$ independently from {-1, 0, 1} when preparing our test dataset to mimic imperfect patch cropping. That is, only $1/3 \times 1/3 = 1/9$ of the patches have maxima at the geometric center.

Fig. 9 compares the prediction error on the test dataset in a statistical way. Comparing Fig. 9(a) with Fig. 9(b), we see clear improvement when augmentation is applied for model training. The 50th, 75th, and 95th percentile errors are all reduced to about 20% of those obtained when BraggNN is trained without data augmentation: a five times improvement.

5 Conclusions and Future work

We have described BraggNN, the first machine learning-based method for precisely characterizing Bragg diffraction peaks in HEDM images. When compared with conventional 2D pseudo-Voigt fitting and higher resolution nf-HEDM,
Figure 7: Distribution of difference between peak positions located by BraggNN without the self-non-local self-attention block and conventional pseudo-Voigt fitting.

Figure 8: Peaks located by BraggNN when peaks is deviated from geometric center. The error is the Euclidean distance ($\ell_2$) between truth (solid line cross) and BraggNN prediction (dotted line cross). Upper row: using BraggNN trained without data augmentation. Bottom row: using BraggNN trained with data augmentation for the same peaks as the upper row.
Figure 9: Distribution of difference between peak position located by BraggNN (right: with \((m, n) \in \{-1, 0, 1\}\) or \(\text{left: without data augmentation}\) and conventional pseudo-Voigt fitting. \(P_{n}\text{th}\) denotes the \(n\text{th}\) percentile.

BraggNN-localized peak-based reconstruction is within acceptable deviation while running more than 50\(\times\) faster on a CPU and up to 1000\(\times\) faster on a GPU. The speedup is important for high-resolution, high-throughput, and latency-sensitive applications, including real-time analysis and experiment steering (e.g., searching area of interest for multi-scale image).

As for future work, we plan to extend BraggNN and apply a deep learning-based object localization technique directly to diffraction frames to (1) avoid labelling the connection component, (2) deal with dense peak diffraction where peaks are partially overlapped — a problem for which the conventional methods have exponential complexity, while the deep learning-based method has sub-linear complexity, and (3) generalize the model to work with 3D peaks for deformed grains.

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