doi:10.1017/S1431927622011758
Microsc. Microanal. 28 (Suppl 1), 2022

Neural Architecture Search for Transmission Electron Microscopy: Rapid Automation of Phase and Orientation Determination in TEM images

Lies Hadjadj[1*], Alexis Deschamps[2], Edgar Rauch[2], Massih-Reza Amini[1], Muriel Veron[2], and Sana Louhichi[3]

[1.] Computer Science Laboratory (LIG), Grenoble, France.
[2.] Department of Physics (SIMaP), Grenoble, France.
[3.] Department of Statistics, Grenoble, France.
* Corresponding author: lies.hadjadj@univ-grenoble-alpes.fr

Transmission Electron Microscopy (TEM) has expanded the type of information obtained on nanocrystalline microstructures such as phase and orientation. Orientation microscopy refers to a technique which consists of solving spatially measurements of crystal orientations in a sample and reconstructing the microstructure from this information. Modern TEM experiments have also produced very large collections of datasets, which are often impossible to process manually. As a result, extensive research [1, 2] has proposed semi-automation approaches to analyze these datasets, these deterministic methods rely on classical computer vision techniques (e.g., Hough transform, Fourier filtering, segmentation and cross-correlation for similarity measure), which typically require manual hyperparameter tunning and a computation cost for each experiment. Deep neural networks (DNNs) have shown superior performance compared to classical computer vision techniques in most benchmark tasks [10], this led to the emergence of fully automated approaches [4, 5] and tools [6, 7] for various TEM tasks. In the context of orientation microscopy, ML-based approaches are still falling behind traditional techniques such as template matching [1] or Kikuchi technique [8] when it comes to generalization performance to unseen orientations and phases during training, this is due mainly to the limited amount of experimental data about the studied phenomena for training the models, it is a realistic and practical constraint specially for narrow domain applications where real data is not widely available. Some successful attempts have been made to use unsupervised learning techniques to gain more insight about the data [3, 9] but clustering information does not solve the orientation microscopy problem.

There is a clear need for automated and practical image analysis tools using the-state-of-the-art machine learning techniques for phase and orientation determination to complement the existing relatively slow, complex and hyperparameter-dependent approaches. To this end, we propose the design of a hybrid and generic multi-task ML pipeline with a double purpose of -i- boosting the existing slow TEM-based orientation microscopy techniques for better generalization accuracy but with higher computation cost and -ii- replacing them with a fully ML pipeline for fast real-time prediction during data acquisition but with lower generalization accuracy when training data is limited. The first stage of the proposed pipeline is a classification task to determine the phase from real diffraction diagrams given as input, to solve this first task we employ an extensive Neural Architecture Search (NAS) using AutoKeras [11] to find the best neural architecture for phase classification. In order to gain better generalization performance, we also used data augmentation for the NAS procedure as a form of random rotations of the diffraction diagrams. We solved the orientation microscopy task in the second stage, using a similar preprocessing proposed by [2] for the templates to extract intensity descriptors from their polar representation. We also used a blurring filter and a thresholding rule for the number of spots on the simulated templates in order to obtain similar descriptors to those extracted from real diffraction diagrams. Similar descriptors are often used for template matching techniques, their compact size allows us to efficiently simulate the orientation space for a given phase. Once the sequence of all template descriptors is simulated, we employed NAS to solve the problem of regressing Euler's angles from the sequence of descriptors knowing the phase class. At the end of this stage, we obtain one regressor model per class phase trained on all possible phase orientations, the last step consists of finetuning every regressor on intensity descriptors extracted from real diffraction diagrams. Figure 1 illustrates the first stage of classification for phase detection and the second stage of regression for orientation detection and fine tuning.

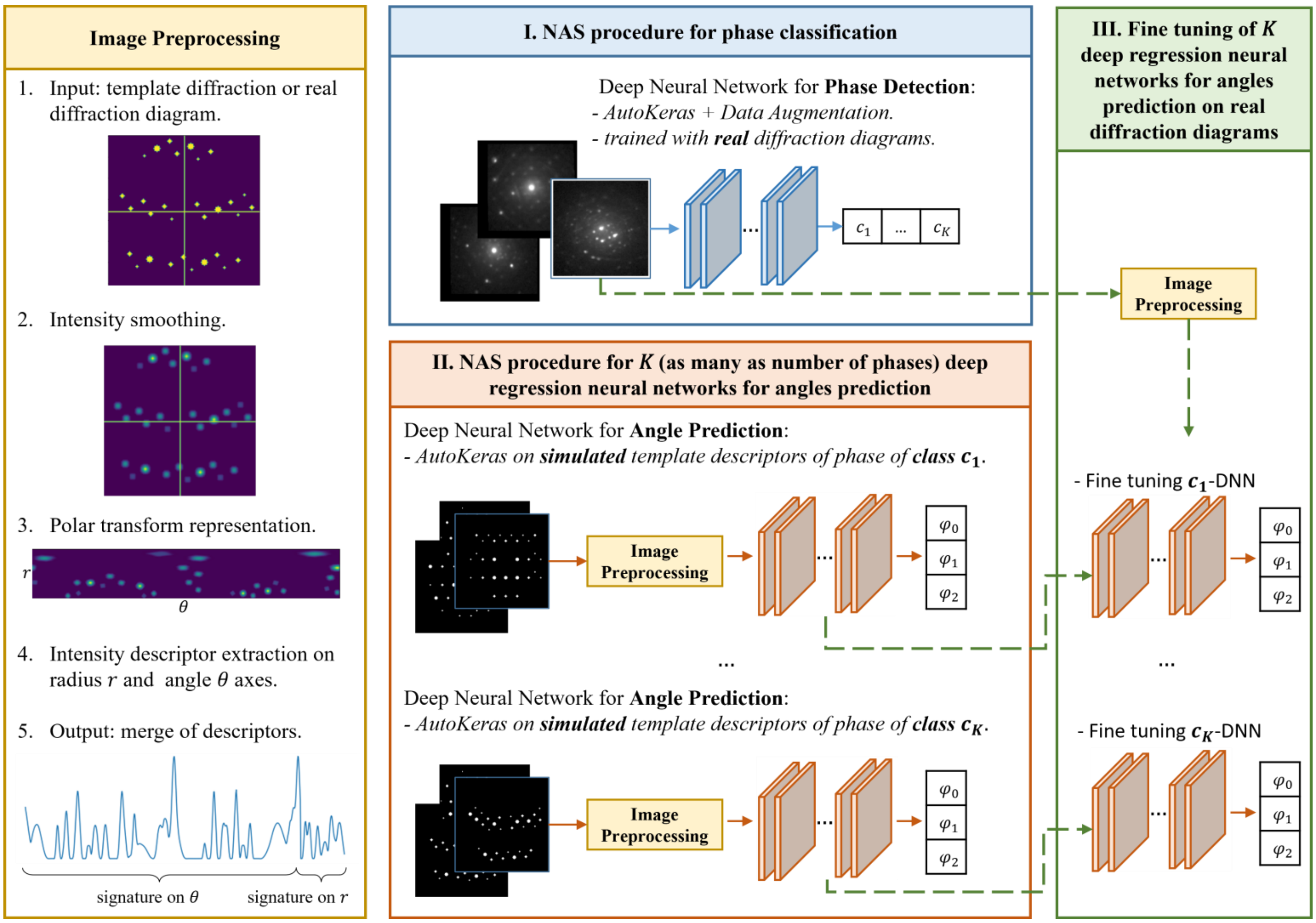

Figure 1. Offline procedure for training the ML pipeline for phase and orientation determination in TEM images.

In Figure 2, we show the prediction scheme ones the pipeline is trained. Note that every branch can use either the trained regressor model or a classical technique for angle prediction, we illustrate the figure with our python implementation of template matching using the intensity descriptors, but we can easily incorporate different techniques for every phase.

https://doi.org/10.1017/S1431927622011758 Published online by Cambridge University Press

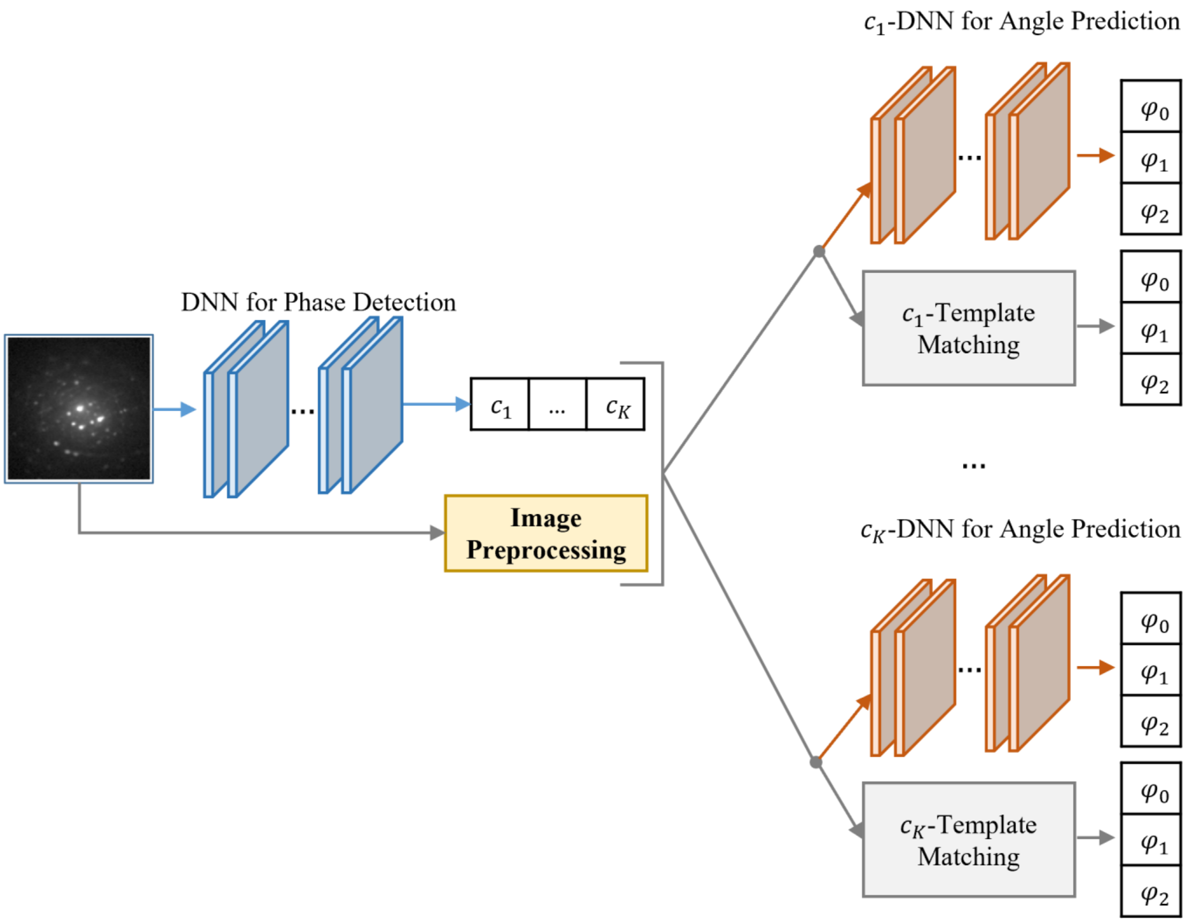

Figure 2. Online procedure of the proposed ML-pipeline for the prediction of phase and orientation in TEM images.

Experiments. We conduct our experiments using three different experimental sets of data on the same steel sample, each collected map consists of 500 × 500 diffraction images of size 144 × 144 pixels each. They all contain three main phases namely ferrite (Fe BCC), Niobiume Crabine (NbC) and cementite (Fe3C). The data were collected on a JEOL 2100F TEM instrument, using a Stingray camera recording the phosphorus screen. We employed two maps for training and selected one map which contains new orientations for testing. For the classification task, we noticed that the performance of the found NAS architecture on the validation set is not an indicator of how well the model will be able to generalize to new orientations, we were able to achieve 99.9% accuracy without data augmentation on 30% ratio size for the validation set and still poorly predict the test map. Data augmentation greatly helped improving the results in test map with a slight decrease to 95% in the validation set during training. The quality of the similarity between simulated and real descriptors heavily depends on the preprocessing steps, which has a direct implication on the final regression performance. Fine tuning allows to reduce this bias when training with real descriptors, and we are currently investigating better ways of solving the orientation problem with ML techniques.

References:

[1] E.F. Rauch, L. Dupuy, Rapid Spot Diffraction Pattern Identification Through Template Matching, Archives of Metallurgy and Materials 50 (2005), 87-99.
[2] S. Zaefferer, and G. Wu, Development of a TEM-based Orientation Microscopy System. Applications of Texture Analysis (2008), 221-228.
[3] B. Martineau et al., Unsupervised machine learning applied to scanning precession electron diffraction data. Advanced Structural and Chemical Imaging (2019), doi:10.1186/s40679-019-0063-3.
[4] Z. Alexander et al., Blind Source Separation in SPED datasets: Machine learning assisted phase and orientation determination in multilayer oxide electronic thin film devices (2020).
[5] J. A. Aguiar et al, Decoding crystallography from high-resolution electron imaging and diffraction datasets with deep learning, Science Advances (2019), doi:10.1126/sciadv.aaw1949.
[6] M. Xu, A. Kumar, and J. LeBeau, Automating Electron Microscopy through Machine Learning and USETEM, Microsc. Microanal. 27 (2021), p. 2988. doi:10.1017/S143192762110103394.
[7] J. Munshi et al., 4D >Crystal: Deep Learning Crystallographic Information from Electron Diffraction Images, Microsc. Microanal. 27 (2021), p. 2774. doi:10.1017/S1431927621009739.
[8] Kikuchi, J.-i. and Yasuhara, K. (2012). Transmission Electron Microscopy (TEM). In Supramolecular Chemistry (eds P.A. Gale and J.W. Steed). doi:10.1002/9780470661345.smc022.
[9] C. Shi et al., Rapid and Semi-Automated Analysis of 4D-STEM data via Unsupervised Learning, Microsc. Microanal. 27 (2021), p. 58. doi:10.1017/S1431927621000805.
[10] Papers with Code, https://paperswithcode.com/area/computer-vision (accessed February 17, 2022).
[11] H. Jin, Q. Song, and Xi Hu. Auto-keras: An efficient neural architecture search system. Proceedings of the 25^{th} SIGKDD International Conference on Knowledge Discovery & Data Mining. ACM, 2019.