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LaueNN: Neural network based hkl recognition of Laue spots and its application to polycrystalline materials

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Abstract

A feedforward neural network (FFNN) model is introduced for efficient and accurate prediction of Laue spots hkl in single/multi-grain/multiphase Laue images. Laue micro-diffraction is an X-ray scattering technique for the determination of local structural parameters (strain, stress and orientation) in materials from microstructure mapping (2D and 3D). The use of a polychromatic beam offers many experimental advantages (no rotation of the sample, many diffraction spots, signal that can be used even in the presence of strong orientation disorder). However, in the case of polycrystalline microstructures, the determination of the structural parameters (lattice parameters) from the fine analysis of the relative position of the spots requires identifying unambiguously all the spots forming the Laue pattern corresponding to an individual crystal among all other spots. The indexation step of the data analysis must be reliable to input unambiguous experimental dataset to the structural model refinement (final step in analysis) and rapid; since production rate of data on the synchrotron line can amount to several 10000s diffraction images per hour, each Laue image being able to contain contribution from multi-grain/ multi-phase present in the probed volume of the material.

Several approaches have been carried out by different groups allowing to index single crystals [1, 2] and polycrystals (for example: XMAS, LaueTools [3-5]). In the latter case, the most time consuming, in the whole data analysis workflow, is the indexation step i.e., determination of Laue spot hkl Miller indices from sets of spots related to the probed crystal. To this effect, we propose [6] employing a FFNN based model to tackle the bottleneck of indexation thereby providing considerable speed over the classical indexation techniques for complex Laue patterns. The model is completely trained on the relative angular distribution of spots present in simulated Laue patterns. With the feature engineering and an optimized FFNN model, accuracies of at-least 90% is easily achieved irrespective of crystal system. The training and validation accuracies and losses that define the metrics of the model learning is presented in Figure 1(a,b). While Figure 1(c,d) shows the ground truth and prediction results for a copper Laue pattern. The present model is also validated on several experimental campaigns performed at the French CRG-IF beamline BM32 at the European Synchtrotron (ESRF). Real-time/ on-the-fly HKL indexation of polycrystalline or complex Laue patterns is now possible with the proposed FFNN architecture, thereby providing users valuable and rapid feedback during data collection on the beamline and accelerate the data treatment from raw data to reliable and interpretable structural parameters.

References

[1] Dejoie, C., Tamura, N. (2020). J. Appl. Cryst., 53, 824-836
[2] Gupta, V.K., Agnew, S.R. (2009). J. Appl. Cryst., 42, 116-124
[3] Kou, K., Chen, K., Tamura, T. (2018). Scripta Materialia, 143 (2018) 19-53
[4] Song, Y., Tamura, N., Zhang, C., Karami, M., Chen, X. (2019). Acta Crysta, A75, 876-888
[5] Micha, J.-S., Robach, O., Tardif, S. https://gitlab.esrf.fr/micha/lauetools
[6] Purushottam Raj Purohit, R.R.P. , et al., accepted for publication in J. Appl. Cryst., (2022)

LaueNN model accuracy and losses with evaluation