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Machine Learning Approaches on X-ray Scattering Beamline: First results and perspectives

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To face the ever growing massive and complex data collected on real materials during samples mapping and screening or in situ measurements at synchrotron beamline, fast software assistance with a minimum user input is nowadays required before, during and after the experiments.
On the french CRG IF BM32 beamline at the European Synchrotron (ESRF) X-ray scattering experiments are carried out for the study of surfaces and interfaces. Recently, we designed a Neural Network (NN) for the recognition of hkl Miller indices of Laue spots in Laue patterns produced by the microbeam illumination of polycrystals. During the training, the NN learned a very large number of possible configurations of Laue spot neighborhoods from simulated data. Compared to usual indexing technique applied to several crystals superimposed Laue patterns, we achieved a general speed up, even to a factor 100 in the low unit cell symmetry [1], allowing the online analysis of data.
In the framework of the french national DIADEM project aiming at the acceleration of materials design, the beamline is starting developments using machine learning approach to increase the throughput of the beamline. First we intend to build automatic systems for the beamline optics alignement and correction. Then we plan to optimize the acquisition by detecting region of interest and adapting the motors scan parameters (velocity, exposure, trajectory). Finally for the data analysis to determine the structural properties of the specimen, we focus on one hand on the automation of the inversion of the X-ray reflectivity spectra, and on the other hand the classification of Laue spots by their 2D shape and the recognition of possible corresponding extended defaults (dislocations).

References:

[1] R.R.P. Purushottam Raj Purohit et al, J. Appl. Cryst. (2022). 55, 737–750

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