# Processing scanning Laue microdiffraction patterns with machine learning algorithms: A case-study with fatigued polycrystalline copper

## Introduction

Laue diffraction, that may occur when a polychromatic X-ray beam illuminated a crystal, was first discovered in 1912, and has revealed both the electromagnetic nature of X-ray and the periodic ordering of atoms in crystal (Eckert, 2012). Thanks to the polychromaticity of the employed X-ray, multiple diffraction peaks can be recorded in a single exposure without any rotation that might lead to the ambiguity of the illuminated volume (Chung & Ice, 1999). With the development of polychromatic beam focusing optics, notably Kirkpatrick–Baez mirrors, micron-sized high-brilliance polychromatic X-ray beam can be produced at synchrotron radiation sources and directed to probe inside materials with submicrometric spatial resolution, i.e. Laue microdiffraction. In analogy to EBSD (electron backscatter diffraction) technique, Laue microdiffraction technique serves by raster scanning the sample to generate the lattice orientation and distortion maps from the one-by-one analysis of the diffraction pattern emanating from each scanned spot (Spolenak *et al.*, 2003, Tamura *et al.*, 2003, Zhou *et al.*, 2018). The two techniques are comparable (Plancher *et al.*, 2016) and complementary to each other (Örs *et al.*, 2018). It is generally accepted that EBSD has an edge on finer spatial resolution of nanoscale, whilst Laue microdiffraction can have a much better accuracy on the lattice orientation and distortion with an attainable order of 10-9 (Zhang, Bieler*, et al.*, 2018).

A salient feature of Laue microdiffraction is its sensitivity to the local misorientation in the illuminated volume (Barabash *et al.*, 2001, Barabash *et al.*, 2003), more specifically, the fragmentation of Laue spot may indicate the presence of geometrically necessary boundaries and the elongation of Laue spot the presence of geometrically necessary dislocations. Although a critical aspect of the spot shape analysis lies on the assumption that the dislocations were dominantly edge-type in the illuminated volume, a recent study with focused ion beam transmission electron microscopy confirmed that this analysis stood still if the dislocations had predominately screw-type (Zhang, Balachandran*, et al.*, 2018). With the aid of a wire profiler (typically Pt), the shape of spot can be spatially resolved to yield subsurface, 3D mapping of lattice orientation and distortion non-destructively (Yang *et al.*, 2004, Barabash *et al.*, 2009, Das *et al.*, 2018), namely the differential-aperture X-ray microscopy (DAXM) technique (Larson *et al.*, 2002).

Despite the wealth of information behind Laue microdiffraction pattern, the interpretation of Laue microdiffraction pattern is not straightforward since the wavelength or indexation pertaining to each diffraction peak is unknown. Standard treatment involves modulating the orientation and calibration parameters to minimize the discrepancy between the simulated and experimental diffraction pattern, and has been implemented in software such as *XMAS* (Tamura, 2014) and *LaueTools* (<https://gitlab.esrf.fr/micha/lauetools>). The standard treatment is in essence a trial-and-error process that usually suffers from inefficiency, especially for the raster scanned diffraction patterns which has to be treated one by one. Therefore, any additional information concerning the scanned microstructure would facilitate the process, for example, Örs *et al.* (2018) used the orientation obtained by EBSD to overcome the difficulty in indexing the Laue microdiffraction patterns; Kou *et al.* (2018) suggested indexing one Laue microdiffraction pattern per grain as the reference with which the rest patterns of the grain could be analyzed without indexation.

Concurrently, the emerging image processing techniques have demonstrated their potential in the interpretation of Laue microdiffraction patterns: Petit *et al.* (2015) introduced the digital image correlation (DIC) technique to have a better measurement of relative lattice distortion with reference to an assumed stress-free position, i.e. Laue-DIC method, Zhang *et al.* (2015) later extended the framework of Laue-DIC to get rid of the dependence on the stress-free reference; Zhang *et al.* (2019) used DIC to correct the misalignment of the investigated volume in the experiments of DXAM;

In a word, the indexation of diffraction peaks is the key to full interpretation of diffraction pattern. However, in certain circumstances, full interpretation of diffraction patterns is unnecessary or fast parallel computing capabilities are unavailable, thereby necessitating the development of indexation-free approach towards on-the-fly analysis of raster scanned diffraction patterns. Zhou *et al.* (2018) proposed using the distribution of average recorded intensities and average filtered intensities of the raster scanned diffraction patterns to visualize the characteristics microstructural features. The recently emerging convolutional neural networks (CNN) has been used to extract features from diffraction patterns for further clustering and labeling the raster scanned diffraction patterns (Song *et al.*, 2019).

In the present work, we demonstrated the application of machine learning algorithms to the raster scanned diffraction patterns of the fatigued polycrystalline copper. Substantial dislocation structures will grow in copper after the cyclic loading (Mughrabi, 2009), leading to blurred diffraction patterns even with almost indiscernable diffraction peaks. Although template matching schemes have been shown applicable to the indexation and misorientation analysis of blurred diffraction patterns, huge amount of calculation was still inevitable (Gupta & Agnew, 2009) and the reliability of outcome would be degraded in line with the formation of dislocation structures. On the other hand, machine learning algorithms, which were developed to handle big data, were possible to circumvent the difficulty of indexation and segment raster scanned diffraction patterns according to their features, thereby mapping phases, grains, or grain substructures. Since the microstructure of the scanned area was not known *a priori*, unsupervised labeling algorithms had to be adopted. The objective of this paper is to: (i) outline the computational pipeline from the raw data to the clustering of diffraction patterns; (ii) compare the performance of several algorithms; and (iii) discuss the influence of the diffraction patterns on the results of clustering.

## Experiment

The diffraction patterns were collected from raster scanning of fatigued polycrystalline copper. The sample was cyclically loaded in stress-control mode with the stress varying sinusoidally within the range . The sample was fatigued up to cycles with a frequency of .

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