# 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 advent 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 maps the lattice orientation and distortion from the 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 have a better angular resolution.

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 subgrain structure and the elongation of Laue spot the presence of geometrically necessary dislocation.

coupled with a wire profiler can resolve subsurface, 3D information non-destructively thanks to the microscale penetration depth of X-ray, namely the differential-aperture X-ray microscopy (DAXM) technique (Larson *et al.*, 2002, Yang *et al.*, 2004, Barabash *et al.*, 2009).

Despite the wealth of information provided by the Laue microdiffraction pattern, the interpretation of Laue microdiffraction pattern is not straightforward as the wavelength 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, and any additional information concerning the scanned microstructure would noticeably facilitate the interpretation process, for example, Örs *et al.* (2018) used the orientation obtained by EBSD to overcome the difficulty of indexing the Laue microdiffraction patterns.

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