



Contribution ID: 53

Type: **Poster**

## Tackling Laue pattern solving using neural networks

*Tuesday, 9 April 2024 18:30 (20 minutes)*

Traditionally, the analysis of Laue diffraction pattern, crucial for determining the crystal orientation, has been a time-consuming process, requiring manual input of a **skilled user**. The development of an fully autonomous recognition tools aims to streamline this procedure, enhance accuracy, and to enable automation of various tasks such as crystal coalignment [1].

Existing Laue orienting software (for example OrientExpress, QLaue [2], LauePt [3] or LaueTools [4]) requires manual input and cannot solve Laue patterns automatically. In the recent years, problem is approached via machine learning. A paper by Purohit, et al. (LaueNN [5]) explores a use of a perceptron architecture. Another possibility is the use of **reinforced learning**. On the other hand, images from x-ray detector itself could be directly processed using convolutional networks or **generative models**. The spatial correlation of data, the reflection spots, suggests a potential use of **graph convolutional networks**. We will discuss all these approaches and show our proposals for general problem of automatic Laue pattern solving.

[1] see contribution “ALSA: Automatic Laue Sample Aligner”, <https://mambaproject.cz/alsa>

[2] <https://github.com/stuwilkins/QLaue>

[3] <https://github.com/yafeiliu/LauePt4>

[4] <https://gitlab.esrf.fr/micha/lauetools/>

[5] Purushottam Raj Purohit, Ravi Raj Purohit, et al., Journal of Applied Crystallography 55.4 (2022).

**Primary author:** ČERVENĚ, Tomáš (Charles University)

**Co-authors:** BITZAN, Filip (Charles University); LUKEŠ, Petr (Charles University); ČERMÁK, Petr (MGML, Charles University); VENCLÍK, Štěpán (Charles University)

**Presenter:** ČERVENĚ, Tomáš (Charles University)

**Session Classification:** Posters

**Track Classification:** MLC