EasyDiffraction: Making diffraction data analysis and modelling easier

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Diffraction is a key tool for structure analysis. However, currently available software for modelling and analysis of diffraction data may be, on the one hand, difficult for new users looking to apply diffraction to their field of expertise and, on the other hand, not flexible enough for domain experts.

EasyDiffraction (https://easydiffraction.org) is a new project aimed at lowering the barrier of entry to diffraction data analysis by providing a simple graphical interface (see Fig. 1) allowing for the calculation of powder diffraction patterns based on structural models and refinement of their parameters against experimental data. The software is distributed as an all-in-one package that includes all dependencies and can be installed with just a few clicks on different operating systems. For more complex problems and increased flexibility the Python library behind EasyDiffraction can be used through Jupyter notebooks and scripting.

EasyDiffraction relies on existing crystallographic libraries as calculation engines to cover the necessary functionality. This software is still in beta and has only some basic features of the CrysFML (https://code.ill.fr/scientific-software/crysfml) and CrysPy (https://github.com/ikibalin/cryspy) libraries, such as support for one-dimensional constant wavelength and time-of-flight powder diffraction data. We are collaborating with the Institut Laue-Langevin (https://www.ill.eu) and Leon Brillouin Laboratory (https://www-llb.cea.fr/en) regarding the CrysFML and CrysPy, respectively. More functionality and support of other libraries will become available as the project matures.

EasyDiffraction evolved from the mock-up of the graphical interface for diffraction and has a strong focus on user experience and interaction. An intuitive and user-friendly interface of EasyDiffraction (see Fig. 1) can thus help improve the user experience in the field of diffraction and thereby make it easier to train users and students, as well as be better prepared for experiments. At the European Spallation Source (https://ess.eu), we plan to integrate EasyDiffraction into the full data processing workflow to increase experiment automation and make better use of beam time.

EasyDiffraction is built on the EasyScience framework (https://easyscience.software), a platform aimed at unifying data analysis and reduction software. In addition to diffraction, this framework has been successfully applied to reflectometry (https://easyreflectometry.org). Quasielastic neutron scattering and neutron imaging are also considered to be targeted in the future.

EasyDiffraction is being developed free and open source (https://github.com/easyscience/EasyDiffraction) and we hope to attract interested people to jointly contribute to this project and help us, for the benefit of everyone, in making diffraction data analysis and modelling easier.

Figure 1. Intuitive and user-friendly interface of EasyDiffraction.