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xrdfit: A Python package for fitting synchrotron X-ray diffraction spectra

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Software

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Summary

The evolution of peak profiles in synchrotron X-ray diffraction (SXRD) data can tell us how the internal crystallographic structures of metals change during applied heating, high temperature straining and cooling cycles (Canelo-Yubero et al., 2016; Daniel, Nguyen, Atkinson, & Quinta da Fonseca, 2019; Hu, Sun, Hector, & Ren, 2017; Stark et al., 2015), which is invaluable information used to improve industrial processing routes (Salem, Glavicic, & Semiatin, 2008). The experiment requires a beamline, at a synchrotron radiation facility such as Diamond Light Source (Diamond Light Source Ltd, 2020), to produce a high energy X-ray beam and illuminate a polycrystalline sample (Daniel et al., 2019). The results are recorded in the form of time-resolved diffraction pattern rings, which are converted into a spectra of intensity peaks versus two-theta angle for a given direction (Ashiotis et al., 2015; Filik et al., 2017; Hammersley, Svensson, Hanfland, Fitch, & Hausermann, 1996). However, since many intensity profiles are collected during each experiment, with detectors recording at speeds greater than 250 Hz (DECTRIS - detecting the future, 2020; Loeliger et al., 2012), fitting each of the individual lattice plane peaks can take a long time using current available software (Basham et al., 2015; Hammersley, 2016; Merkel & Hilairet, 2015).

There are existing packages which can be used to fit peaks in SXRD spectra, examples include DAWN (Basham et al., 2015), Multifit/Polydefix (Merkel & Hilairet, 2015) and Fit2d (Hammersley, 2016). In these cases, the software are compiled packages with a graphical user interface. Setting up the peak fits usually involves a point and click method to select the peak bounds, meaning it is unlikely to create a repeatable analysis. These packages also struggle to distinguish any peaks that overlap, which is important for capturing changes in multi-phase materials (Daniel et al., 2019). MAUD (Lutterotti, Vasin, & Wenk, 2014) is a software package that approaches fitting in a different way. MAUD uses the Rietveld refinement method (Rietveld, 1969) to match a model of the beamline setup and material properties to the data. This method allows determination of additional material properties, such as crystallographic texture, but applies an averaging over the peak positions and intensities to fit the model, meaning individual peak shifts cannot be accurately determined.

`xrdfit` is a Python package we have developed for a faster fitting of diffraction peaks in SXRD (and XRD) spectra, which can be used for datasets containing many thousands of patterns. It is intended as an easy to use tool which enables automated, repeatable identification of peak positions and profiles in spectra with multiple individual or overlapping lattice plane peaks. The features of `xrdfit` are shown schematically in Figure 1. `xrdfit` uses the Python package `lmfit` (Newville, Stensitzki, Allen, & Ingargiola, 2014) for the underlying fitting. Features are included for selecting different 'cakes' of data and automating fitting over many spectra, to enable tracking of peaks as they shift throughout the experiment. By analysing how different lattice plane peaks change during simulated processing, as can be seen in Figure 2, the transformation and micromechanical behaviour of the material can be understood.

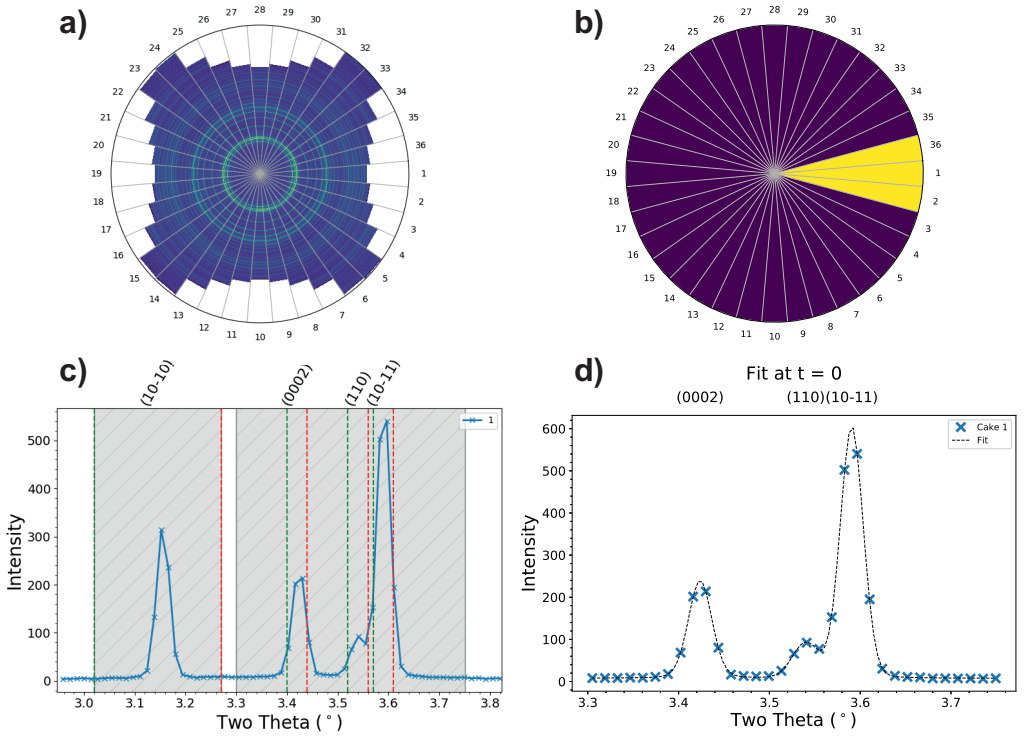

Figure 1: A schematic representing the features of `xrdfit` and the analysis of a synchrotron X-ray diffraction (SXRD) pattern, showing: (a) a polar plot of the caked intensity data; (b) an option for selecting different cakes and merging caked datasets; (c) adjustable peak bounds (grey) and adjustable maxima and minima bounds (red and green) for constraining the peak fit; (d) an example fit of multiple and overlapping peaks.

`xrdfit` is designed to be accessible for all researchers who need to process SXRD (and XRD) spectra and so does not require a detailed knowledge of programming or fitting. The package has been used for the analysis of data taken during the hot deformation of a two-phase titanium alloy, which is presented in an article currently in press (Daniel et al., 2019), and will be used for future studies investigating the high temperature processing of metals in our research group. We hope that its public release will allow other researchers to benefit from fast data fitting (up to 40 times faster than the current software), reducing the effort required to analyse their experimental data.

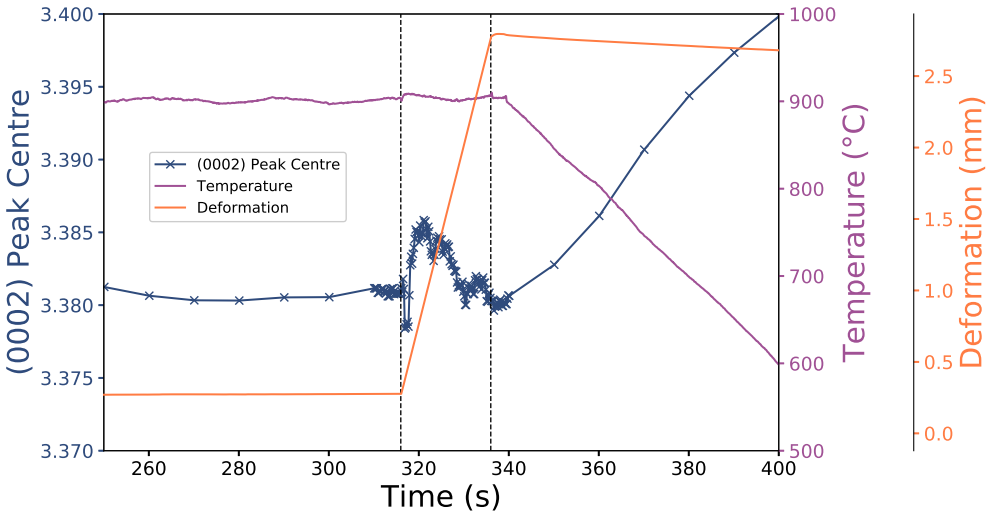

Figure 2: An example analysis of a two-phase titanium (Ti-6Al-4V) alloy during high temperature and high strain rate deformation, showing characteristic shifts of the α (0002) peak centre. The shifts of the peak can be used to calculate elastic lattice straining in the hexagonal close-packed (hcp) lattice, as well as measure the thermal contraction on cooling.

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