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

Peter Crowther[1] **and Christopher S. Daniel**[1]

1 Univeristy of Manchester, UK

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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, such as Diamond Light Source (Diamond Light Source Ltd, 2020a), 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 of up to 250 Hz (Diamond Light Source Ltd, 2020b), fitting each of the individual lattice plane peaks can take a long time using current available software (Basham et al., 2015; Merkel & Hilairet, 2015). Distinguishing the evolution of any overlapping peaks, for multi-phase materials, can also be difficult and time-consuming. Therefore, a faster and more robust Python package has been developed to fit the evolution of multiple and overlapping peaks for datasets containing many thousands of SXRD patterns.

`xrdfit` is a Python package for fitting the diffraction peaks in SXRD (and XRD) spectra. It is intended as an easy to use tool for the quick analysis of individual and overlapping lattice plane peaks, to discern the peak position and profile. 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.

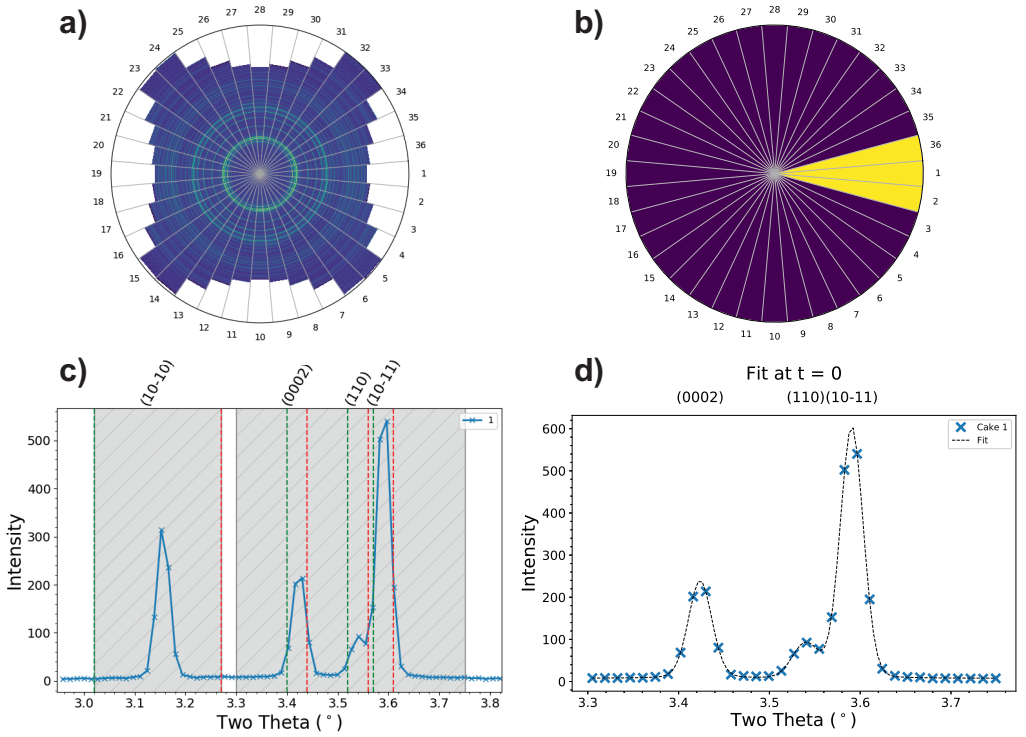

Figure 1: A schematic representing the features of xrdfit and the analysis of a synchrotron X-ray diffraction (SXRD) pattern, showing: (a) a polar plot of the caked intensity data; (b) an option for selecting different cakes and merging caked datasets; (c) adjustable peak bounds (grey) and adjustable maxima and maxima 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, reducing the effort required to analyse their experimental data.

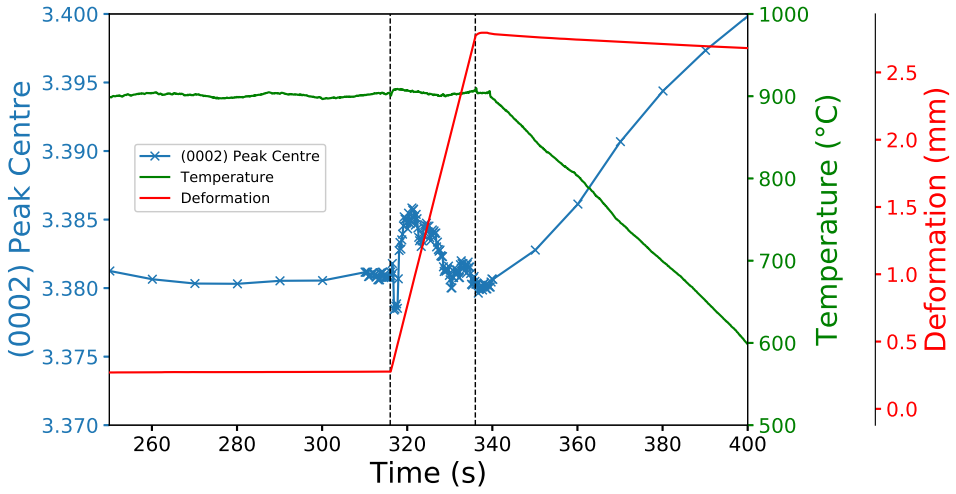

Figure 2: An example analysis of a two-phase titanium (Ti-6Al-4V) alloy during high temperature and high strain rate deformation, showing characteristic shifts of the α (0002) peak centre. The shifts of the peak can be used to calculate elastic lattice straining in the hexagonal close-packed (hcp) lattice,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

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