Enhanced analysis beyond macroscopic strain for engineering diffraction experiments

Science and Technology Facilities Council

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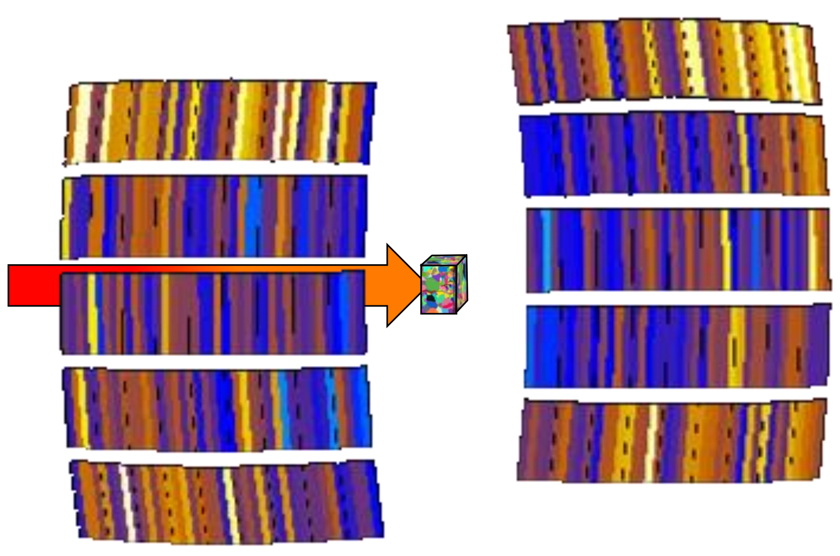
Introduction

Time-of-flight neutron diffraction instruments generally employ a significant detector solid angle coverage, subdivided into pixels small enough to give good resolution in 2θ angle. However, data analysis typically reduces this to a single diffraction spectrum. While different *hkl* peaks in this spectrum may be analysed separately to study intergranular strains, so far generally no attempt is made to exploit e.g. the per-pixel variation in recorded spectra or the incoherent background.

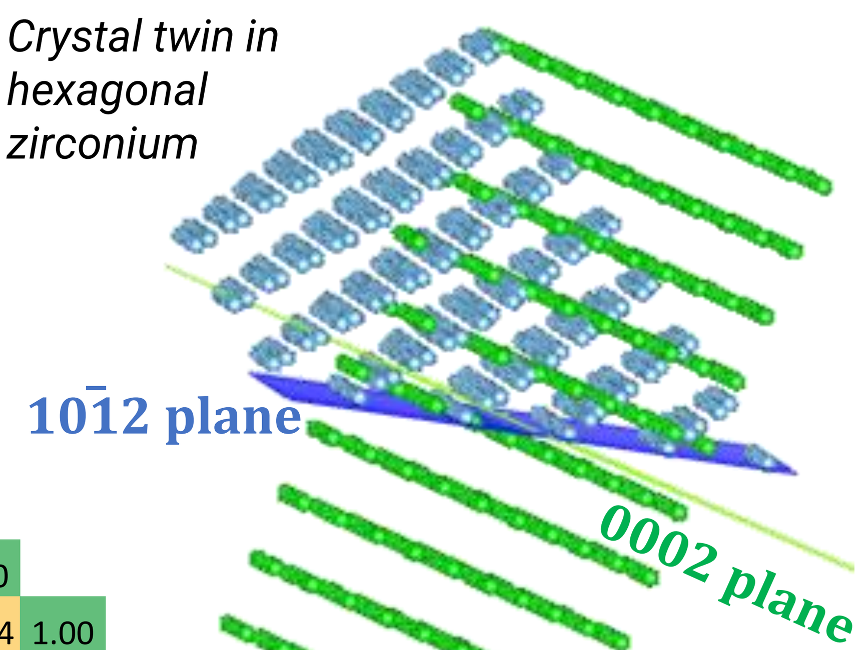
This work seeks to use this extra data to analyse other parameters of interest to the engineering community. Here, we show examples of measuring hydrogen levels and crystal orientation relationships.

Example 1: Orientation relations

Each *hkl* diffraction peak illuminates the detector bank in a non-uniform way, based on how many grains happen to have an *hkl* oriented for diffraction towards a specific pixel. Individually these patterns are random – but where an orientation relationship tends to be present between neighbouring grains (as e.g. from twinning), there will be a statistical correlation in the intensity patterns for pairs of *hkl* planes in the two orientation variants that are near-parallel.



Example intensity over diffraction banks



	Zr$10\bar{1}0$	Zr0002	Zr$10\bar{1}1$	Zr$10\bar{1}2$	Zr$11\bar{2}0$	Zr$10\bar{1}3$	Zr$20\bar{2}0$	Zr0004
Zr$10\bar{1}0$	1.00							
Zr0002	-0.04	1.00						
Zr$10\bar{1}1$	-0.01	0.08	1.00					
Zr$10\bar{1}2$	-0.08	0.28	-0.07	1.00				
Zr$11\bar{2}0$	0.22	0.09	-0.07	0.06	1.00			
Zr$10\bar{1}3$	-0.06	0.07	0.00	0.02	0.01	1.00		
Zr$20\bar{2}0$	-0.07	-0.15	-0.05	0.01	0.10	0.04	1.00	
Zr0004	0.03	0.27	0.02	-0.08	-0.09	0.13	0.09	1.00

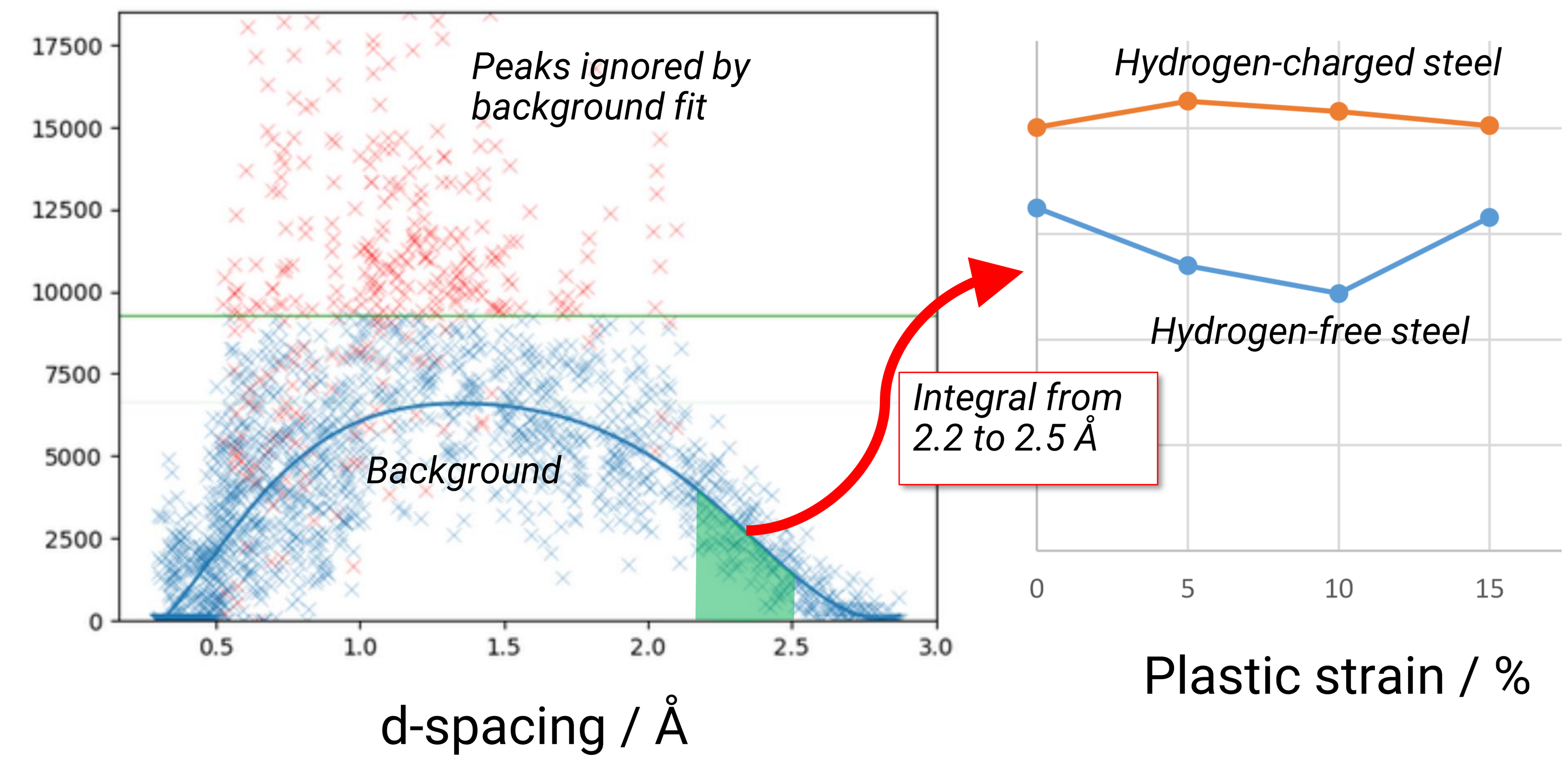
Pearson correlation R for intensities of different diffraction peaks

Methods

Numerical methods were implemented in Mantid Workbench, a Python framework and GUI for working with neutron time-of-flight data. A key resource in this work was the large back archive of data (~4TB) acquired on the ENGIN-X beamline over 20 years of operation.

Example 2: Hydrogen in steels

Hydrogen scatters neutrons incoherently, adding to the background of neutron diffraction spectra. By fitting a Chebyshev polynomial to the background, we can find a parameter that could help quantify the amount of hydrogen present.



Further work

These techniques may be useful for future automated data mining projects at neutron or synchrotron facilities. Practical problems arise though from missing or inconsistently structured metadata. Going forward, it is urged that some scheme to improve capture of this metadata is needed, ideally by getting the original experimenters to “buy in” to the process (e.g. using their submitted metadata to help automate their later analysis) rather than just enforcing requirements by facility policy.

MANTID

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