SimSetup: An Integrated Digital Workflow for Planning and Analysing Residual Stress Measurements on Engin-X

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Abstract

Residual stress measurements using neutron diffraction require careful planning to ensure accurate sample alignment, reliable coordinate transformation, and efficient use of limited beamtime. This presentation introduces a new software application being developed for Engin-X [1] users to support experiment planning, diffraction peak fitting, and residual stress analysis. The app enables users to import or define sample geometry, align it with the instrument stage, visualise measurement accessibility, calculate neutron path lengths, and estimate acquisition times. By integrating planning, GSAS-style peak fitting, lattice-parameter extraction, and stress calculation in one workflow, the software improves experimental efficiency and supports more realistic beamtime proposals.

Functions of the software

The app provides an integrated digital workflow for setting up Engin-X residual stress measurements. Users can import or define sample geometry, align the sample model to the experimental stage, and calculate measurement-point coordinates within the instrument coordinate system. The software also provides clear 3D visualisation of the sample, stage, beam position, theodolite view, and detector geometry, helping users to check whether proposed measurement locations are experimentally accessible, as shown in Figure 1.

A key feature of the experiment-planning workflow is that, once the sample alignment has been determined, the app can calculate neutron path lengths for each proposed measurement point and provide an estimate of the required acquisition time. This allows users to assess the trade-off between data quality and measurement duration before the experiment. Since neutron beamtime is limited, this capability is particularly valuable for optimising measurement strategies, prioritising critical locations, and avoiding unrealistic or inefficient scan plans, which are critical in preparing a beamtime application proposal.

In addition to experiment planning, diffraction peak fitting is being integrated into the same software environment. The fitting functions are adopted from GSAS-style peak descriptions, while the workflow is designed to be similar to the current OpenGenie-based fitting approach used for Engin-X data reduction and analysis. This allows users to fit diffraction peaks and obtain lattice parameters within the same software, as illustrated in Figure 2. A further residual-stress calculation tab then allows stresses to be calculated once lattice parameters are available.

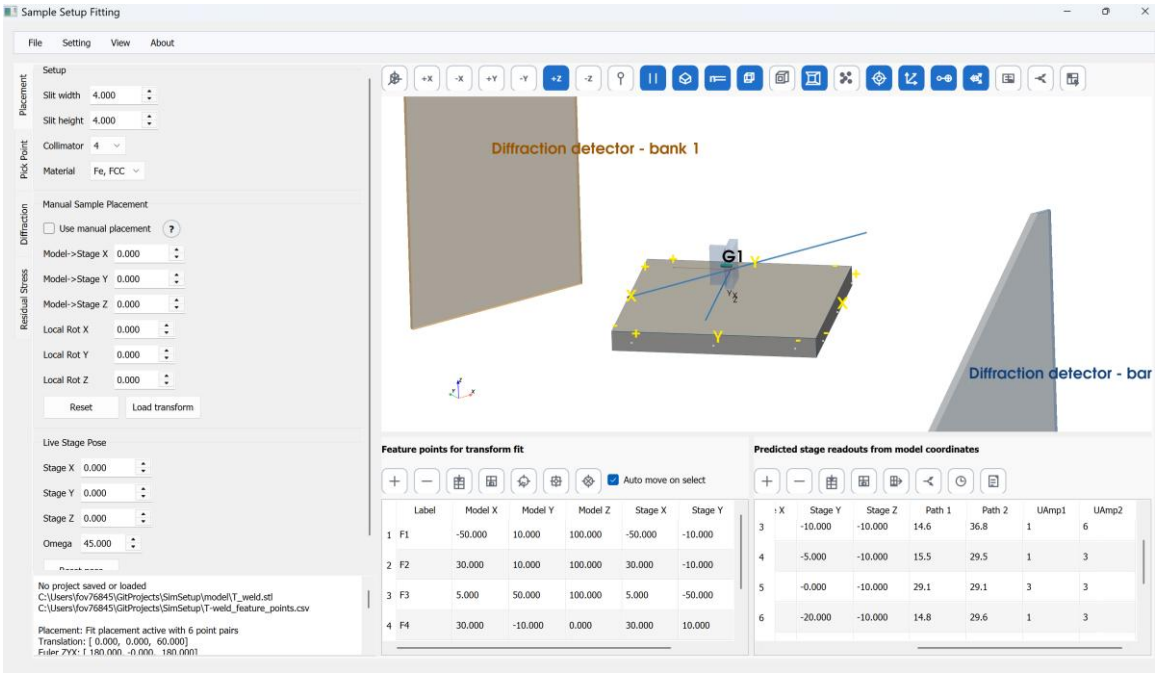

Figure 1. UI of the experiment planning tab.

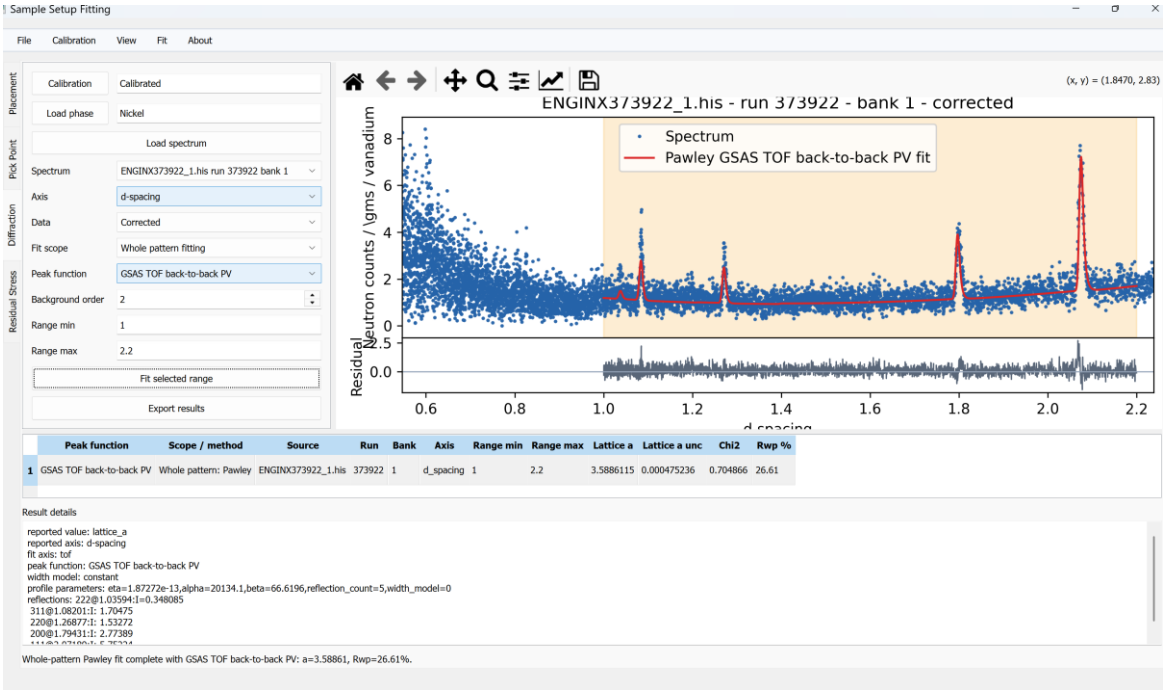

Figure 2. UI of the diffraction fitting tab.

Summary

By combining experiment setup, coordinate calculation, acquisition-time estimation, diffraction fitting, and residual stress calculation in a single application, the software aims to provide a more transparent and user-friendly workflow for Engin-X users. The tool is expected to help users prepare experiments more effectively, reduce setup errors, improve beamtime efficiency, and support more consistent residual stress analysis for users from both academia and industry.

Reference

[1] Santisteban, J. R., Daymond, M. R., James, J. A. & Edwards, L. (2006). J. Appl. Cryst. 39, 812-8