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STRESSFIT –software for analysis of residual stress distributions

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Mapping of residual stresses in polycrystalline materials by neutron diffraction employs relatively large sampling volumes, which helps to smooth out stochastic noise due to limited number of contributing grains, but also causes a number of undesired effects commonly called as pseudo-strains. These include smearing of measured strain distributions, as well as false strains observed due to non-uniform sampling occurring at the sample surface or inner phase boundaries, and due to steep composition or texture gradients and variation of beam attenuation. STRESSFIT is a Python package developed with the aim to address this kind of problems. On the input, it employs a list of sampling events, which can be generated by neutron ray-tracing simulation of the instrument at given experimental geometry. STRESSFIT then provides tools for making convolution of this sampling distribution with the probed material properties, yielding “as measured” peak positions, widths and intensities suitable for evaluation of the pseudo-strains and for fitting of experimental data using free intrinsic strain and scattering intensity distributions as the model functions. As a result, the intrinsic (deconvoluted) strain distributions can be partially recovered. Apart of the package API, STRESSFIT also provides a user-friendly interface using Jupyter notebook widgets to facilitate usual workflow of neutron strain mapping data analysis. The package is available at <https://github.com/NPLtools/stressfit>.

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