Measuring the elastic strain of individual grains in polycrystalline materials

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3DXRD is not only an excellent tool when it comes to non-destructively determining the positions and orientations of individual grains within the bulk of a polycrystalline material, the experiment can also provide grain resolved elastic strain tensors. To extract this information the program FitAllB, which fits centre-of-mass grain positions, orientations and strain tensors from the experimental far-field 3DXRD data, was developed. The program builds on peaksearch, ImageD11 and GrainSpotter and will eventually be implemented in the Fable GUI.

By the use of simulated data the presentation will focus on some of the important aspects you have to take into account in order to determine the strain tensors of the individual grains to the desired accuracy of 10^{-4}. The first thing is how to handle the peak overlaps that will inevitably occur, especially for textured and/or deformed materials. Secondly a careful calibration of the global parameters relating to the experiment (sample-to-detector distance, tilts of detector and sample and beam centre on detector) must be performed. For this purpose the option of fitting the global parameters simultaneously for any number of indexed grains is included in FitAllB.

Finally some examples of applying FitAllB to analyze experimental 3DXRD data will be shown. These will include an experiment performed using both a near- and a far-field detector, thus making it possible to improve the grain positions by fitting these against the near-field data. Again this can be done within FitAllB. In addition to the centre-of-mass grain positions, orientations and strain tensors, FitAllB also calculates the relative volumes of the grains based on the peak intensities, so using a tessellation routine a crude 3D map of the elastic strain in the polycrystal can be obtained.