

ImageD11: software for peaksearch, calibration and other adventures in reciprocal space

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ImageD11 is a software package for analysis of x-ray diffraction data from 2D images. It has been developed principally in the python programming language and uses compiled C modules for time consuming computations. The peaksearch and transformation modules have been connected to the fable gui already, while other parts of the program are available directly from python, or a command line.

The peaksearching algorithm is a 3D connected components labelling of pixels which are above a simple threshold value. Multiple thresholds can be specified and this can sometimes help to deal with cases of overlapping peaks. Python threads are used to allow some degree of parallelism to be exploited to help to speed up the program. In practice the data throughput is often limited by network or disk access time and not by the CPU.

In order to be confident whether a specific peak should be indexed by a particular grain or not, it helps to be as accurate as possible in measuring the peak position and comparing this to the computed position from a grain. These computations rely on a precise knowledge of the sample to detector distance, detector tilts and diffractometer geometry. The basic transformation module from ImageD11 allows many of the parameters to be fitted from a powder style dataset. There is also a refinegrains module which fits individual grains as well as the geometry of the diffraction experiment, to give grain positions, lattice parameters etc.

There are some algorithms for indexing in ImageD11. They seem to work for reasonable numbers of grains with known unit cells, or relatively few (<10) with unknown cells. In the unknown case the program works either in reciprocal space by combining g-vectors, or somewhat better, in real space using the output of a Fourier transform of the peak positions. Peaks found in the output of the latter give the real space lattice vectors which are easier to match individually with the observed data in reciprocal space. Very recently a new module was added to ImageD11 for making a reconstruction of a volume of reciprocal space from a series of diffraction images. This can be used for looking at diffuse scattering from single crystals.