Integrated intensities based on grain orientation distribution functions

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Measuring diffraction data using polycrystalline samples and handle these as a set of single crystal data – one of the major challenges is to extract the integrated diffraction intensities of the peaks. The reason for this is twofold: 1) The number of overlapping reflections grows with the number of crystalline grains in the sample, i.e. the intensity of the individual contributions from the overlapping peaks are difficult to separate. 2) the mosaicity of the grains can is often large, leading to spots which are far from spherical.

To overcome these problems we have adapted a new approach for extracting intensities of the overlapped reflections as well as the weak reflections by fitting the intensity using a peak profile. Our approach is to reconstruct the orientation distribution function (ODF) on a grid using the strong nonoverlapped reflections and from this the profile any reflection can be calculated. The algorithms for reconstructing the ODF and calculation of the reflection profiles are presented together with results obtained.