New Tools for Microstructure Analyses of Polycrystalline Materials using an X-ray Area Detector

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X-ray diffractometers equipped with an area detector are very powerful tool for polycrystalline material characterization. From the 2D diffraction patterns of a polycrystalline samples, collected using an adequate exploration procedure, important microstructure information (grain crystal size and crystallographic texture) can be extracted. Here, we present some hardware and software tools for automatic microstructure analyses. For instance, XtalSizer automatically determines a set of parameters from a single 2D diffraction pattern that characterize the sample crystal size in the micrometric range. Real crystal sizes can be determined after proper calibration with standards samples with known sizes. This technique is independent of the aggregation state of crystals in the sample; It can be used in powder samples as well as in densely packed samples (i.e., ceramics). Also, the range of size determined (tens to hundreds of microns) are complementary to crystallite size determined from the broadening of Bragg peaks (0.1 micron and below) increasing the potential of X-ray diffraction techniques to characterise polycrystalline materials. We have also developed another software tool, XTexture, that calculate and plots the pole figures from a set of 2D diffraction patterns. This software tools allow fast determination of microstructural information that using other traditional techniques (i.e, optical microscopy, X-ray texture diffractometer) would be very tedious to acquire.

Keywords: CCD area detector, crystallographic texture, grain size