Automated generation of efficient scanning schemes for XRD pole figure measurements with area detectors

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Abstract

An automated method is presented to generate appropriate experimental designs to efficiently sample XRD pole intensities with area detectors. Considering X-ray wavelength, detector size and distance between the detector system and the specimen, the shape and position of the diffraction peaks on the detector vary from one crystal structure to another, and hence the mapping onto the pole hemisphere varies, too. Moreover, area detectors allow the simultaneous acquisition of pole intensities referring to several crystal forms, the total number of which equals the total number of diffraction peaks present at a unique detector position. According to these geometrical relationships, the method suggested here determines measurement grids and their measurement positions. In greater detail, detector positions are automatically selected to measure several diffraction peaks simultaneously. Then their $2\theta$ integration bounds and the mapping on the pole hemispheres are calculated. For any polar angle a locally almost uniform grid is constructed according to the resolution along the azimuthal angle. Automatically generated scanning schemes for several crystal structures and system setups will be shown and discussed. Corresponding measurement will be compared to conventional, i.e. manually designed scanning schemes. The method is available in a ready to use software package.

Keywords: