Fast Quantitative Determination of Crystallite Size Distributions from 2D X-ray Diffraction Data

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Crystallite sizes and crystallite size distributions (CSDs) of polycrystalline materials are of primary importance for their physical properties. Particularly important are the CSDs for the mechanical behaviour, e.g. the dependency of yield strength on the grain diameter via the Hall-Petch equation. Moreover, many transport properties depend on the grain-boundary network (GBN) which is determined also by the CSDs. As the manufacturing process strongly influences the CSDs (and GBNs) it is often necessary to control these quantities in fields reaching from metallurgy over ceramics to pharmaceutical products. Likewise, in natural samples much can be learned from CSDs about the formation process. Optical and electron microscopy on polished and etched surfaces are routinely used methods to measure CSDs. However, the latter methods are time-consuming (and generally only give 2D information), and in certain cases are unsuitable, in particular for unstable samples or *in-situ* investigations of changing CSDs. Here we propose a new fast diffractometric method for establishing CSDs of powders or polycrystalline aggregates using a 2D detector, a method which we like to call *fast diffraction CSD analysis*.

Our method uses 2D diffraction data with spotty Debye-Scherrer rings, usually (but not necessarily) measured in transmission. The individual Bragg spots are identified and their intensity is extracted from the diffraction data by a program written in the interpreter language Python. We demonstrate the capabilities of our *fast quantitative diffraction CSD analysis* in a study of the CSD of cryogenic polycrystalline materials (gas hydrates, ice), which are inaccessible to standard (electron-) optical methods. Information on the growth mechanism of these materials are obtained from the CSD analysis. The determination of CSDs using our fast quantitative method was also applied for time-resolved work with a resolution of a few minutes at synchrotron sources.