

## **CRYSTALLITE VOLUME, AREA, SPECIFIC AREA AND MORPHOLOGY OBTAINED VIA RIETVELD REFINEMENT**

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When a drug substance is crystalline and the associated crystallography is known, it is possible to refine its crystalline structure by analyzing its X-ray powder diffraction pattern with the Rietveld method. This pattern contains also information about the microstructure, crystallite size and lattice deformation, of the sample. The information obtained for the microstructure depends on the correct modeling of all the contributions to the diffraction pattern: the crystallography of the phases, the background and the instrumental aberrations. These aberrations are irrelevant when the drug substance is nanocrystalline, because the peak broadening of the diffraction pattern is mainly determined by crystallite size and lattice deformations. Modeling the crystallite size with a basis of spherical harmonics during the refinement provides information about the crystallite morphology and dimensions, which are used to generate the crystallite surface area by approximating it with a three-dimensional boundary conforming Delaunay triangular mesh. In a similar way, the crystallite volume is also obtained by approximating it with a tetragonal mesh. The information about the microstructure could be of interest to understand solubility, dissolution and bioavailability of the drug substances.