

## **Crystal shape – Evolution and characterization**

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In the recent years, the shape of crystals has moved into the academic focus. There is a strong interplay between crystal shape and process conditions. In the one direction, process conditions (e.g. shape modifying additives, face-specific growth or dissolution rates or stirrer induced attrition) obviously govern the evolution of the particle shape. However, the shape also has significant impact on the further processing or usage. Undesired crystal shape may e.g. cause filtration problems (platelets or needles) or result in low dissolution kinetics of pharmaceuticals hindering bioavailability. A detailed understanding of the shape evolution fundamentals and their model based representation can support the solution of these problems.

As an objective one needs to develop concepts capable of dealing with the large variety of different crystal geometries. A optimal crystal characterization should be both suitable for experimental characterization and capable of providing a framework for mathematical modeling. In the presentation a crystal representation will be presented that is based on concepts from the mathematical field of convex geometry. This representation will be applied to exemplary experimental and simulation technological cases.

Besides the characterization of crystal shape, obviously also the monitoring and model-based assessment of shape evolution is of primary interest. The major reason the development of different crystal shapes is the difference in the rates processes occurring on the different crystallographic faces. In the past molecular dynamics simulations have proven useful to probe the crystal growth and dissolution behavior on a molecular level. By exemplary cases it will be shown how molecular dynamics simulations can be used to determine the rate processes (growth or dissolution) at the crystal-solvent-interface.