Crystal Shape and Topography: Prediction and Optimisation with the CrystalGrower Model

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Particle or crystal shape engineering represents a fundamental aspect of any industry that produces or handles solid matter, including fields such as, pharmaceuticals, agrochemicals, energy, and electronics. Numerous important physical properties, such as mechanical strength, dissolution/sublimation rates, agglomeration, and compressibility are influenced by the crystal shape. Therefore, understanding the effects of intermolecular interactions on the shape and size of a crystal becomes crucial in determining how these physical properties can be controlled.

The CrystalGrower software developed by Anderson *et al*. [1,2] provides a generalised Monte Carlo (MC) model for crystal growth, introducing an improved 3D approach based on the MONTY approach by Meekes and co-workers. [3] The model can be utilised to simultaneously model both the crystal shape and surface features. Those which are automatically generated and governed by the input (free) energy parameters for specified intermolecular interactions within a nearest neighbour model, obtained from a crystal structure.

The general workflow for CrystalGrower to date has involved fitting of the nearest neighbour interaction energy parameters to an experimentally observed crystal shape and information from atomic force microscopy. In this work, a powerful new automated protocol will be presented that rapidly predicts the free energies of interaction for use within such a MC model for a wide range of molecular crystalline solids and solvents, thereby removing a major bottleneck to the study of new materials. Furthermore, it will be shown how global search algorithms can also be utilised along with a robust shape descriptor and a reference (experimental) crystal shape to optimise the aforementioned interaction energies. In combination, the above methods create a powerful tool that can aid crystal shape engineering across a wide array of fields.

References

[1] Anderson MA et al. Predicting crystal growth via a unified kinetic three-dimensional partition model. Nature. 2017;544:456-459.
[2] Hill AR et al. CrystalGrower: a generic computer program for Monte Carlo modelling of crystal growth. Chem. Sci. 2021;12:1126-1146.
[3] Boerrigter SXM et al. MONTY: Monte Carlo Crystal Growth on Any Crystal Structure in Any Crystallographic Orientation; Application to Fats. J. Phys. Chem. A. 2004;108:5894-5902.