MONTY: An Algorithm for Predicting Growth Rates for any Crystal Structure in any Orientation

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A crystal growth simulation program, based on the Monte Carlo algorithm, is presented. The experimental crystal structure is input for the algorithm. It is modeled by a set of molecular interactions, which are obtained from molecular mechanics calculations. The mother phase is parameterized by its bulk thermodynamic properties. As a result, besides the growth rate, the microscopic surface structure can be studied under various growth conditions. [1].

Two examples are presented. The program was used to simulate the growth of two polymorphs of aspartame; the extreme aspect ratio of the experimental needle crystals is well-predicted [2]. The second example involves naphthalene. There it is shown, using the spiral growth option in the algorithm, that it is impossible to grow crystals of naphthalene at moderate supersaturations without the presence of screw dislocations. This is supported by using AFM [3].

The results show the importance of the details of the crystal structure, its energetics and the actual growth conditions, for the crystal morphology. In contrast to established morphology prediction models the algorithm can deal with parameters like supersaturation, temperature, concentration and dissolution free energy. In particular, surface roughening effects can be studied for real crystal structures.

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