IFPRI Project Abstract

Delivery of a Practical Tool for Predicting the Effect of Solvents and Growth Inhibitors on Crystal Morphology

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Project Objective:

The goal of this research is to develop a practical engineering tool for predicting the relative growth rates (growth kinetics) and morphology of solution-grown faceted crystals, including the effects of solvent, and impurities/additives. The methodology is being tested on a variety of systems including olanzapine, adipic acid, naphthalene, and a variety of drug substances, all grown from solution.
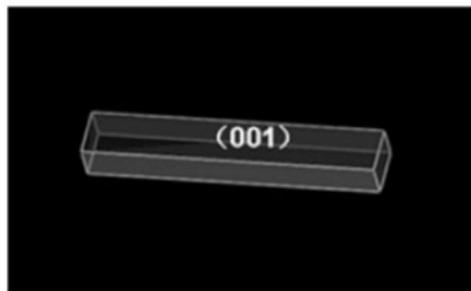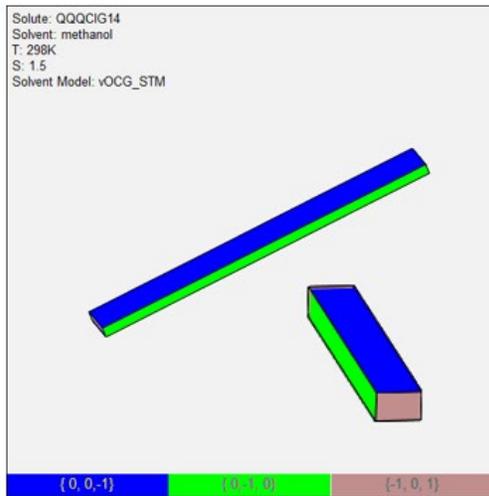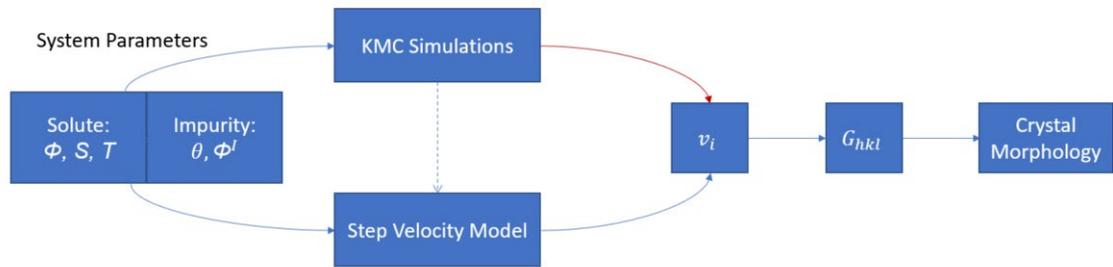
Approach:

Our approach is to leverage a decade of research & development building our crystal design software tool called ADDICT to develop (fast) mechanistic models of crystal growth validated by experiments, molecular simulations and kMC simulations. Kinetic Monte Carlo simulations are utilized for investigating impurity-mediated and noncentrosymmetric crystal growth in conjunction with novel kink density models. Solvent effects are incorporated into the modeling scheme via the use of COSMO-therm software that we have created ourselves based on literature information.
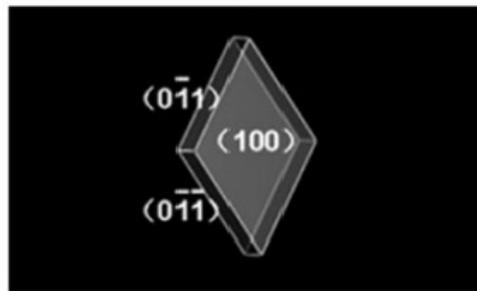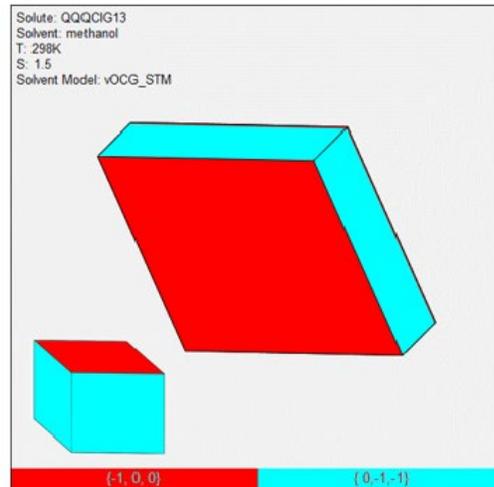
Recent Results:

We used kMC simulations to predict the crystal morphologies of various centrosymmetric molecules within ADDICT's architecture. We compare our predictions to experimental crystal habits from the literature and find very good agreement. In the figure we demonstrate the efficacy of kMC in predicting the morphologies of two distinct polymorphs of rubrene, a semiconductor used in the production of OLEDs. We additionally developed the framework for kMC simulations to extend to more complex cases such as impurity-mediated and noncentrosymmetric crystal growth systems. We demonstrate the potential of using such inputs to visualize the modified crystal morphology in real time via ADDICT.

Next Steps:

The project will continue to investigate more complex systems (i.e. noncentrosymmetric growth units) and corroborate novel model developments in the field of kink density and step velocity calculation with kMC simulations. These advances will be adopted within ADDICT to examine the spectrum of crystal morphologies for various growth conditions. morphology in real time via ADDICT.

System Parameters

KMC Simulations

Solute: Φ, S, T Impurity: θ, Φ^I

Step Velocity Model

v_i G_{hkl} Crystal Morphology

Solute: QQQCIG14
Solvent: methanol
T: 298K
S: 1.5
Solvent Model: vOCG_STM

{ 0, 0, -1}   {0,-1, 0}   {-1, 0, 1}

⟨001⟩

Solute: QQQCIG13
Solvent: methanol
T: 298K
S: 1.5
Solvent Model: vOCG_STM

{-1, 0, 0}   { 0,-1,-1}

⟨0$\bar{1}\bar{1}$⟩   ⟨100⟩   ⟨0$\bar{1}\bar{1}$⟩

Experimental ribbon morphology of triclinic crystals   Experimental rhombus morphology of monoclinic crystals