

SIMULATING SURFACE KINETICS AND BULK TRANSPORT IN SOLUTION CRYSTAL GROWTH

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Solution crystal growth processes can be thought of as novel chemical reactors, whose behaviors are governed by complex interactions of bulk transport phenomena, surface diffusion, and growth kinetics. Of critical practical importance is the stable growth of discrete facets of large crystals at fast rates. However, crystal quality is often compromised during fast solution growth by a host of morphological flaws including macrosteps, step bunches, and inclusions. These instabilities arise from the complex interplay between transport and kinetic factors.

We present a novel model for the growth of a vicinal facet from solution, which couples surface phenomena and bulk effects. The surface kinetic model, based on the theory of Burton, Cabrera, and Frank (BCF), rigorously accounts for the interactions of discrete growth steps through surface diffusion fields, adsorption and desorption events, ledge growth kinetics with Schwoebel effects, and convective transport due to step motion. This model is self-consistently coupled with a bulk transport model that describes bulk diffusion to terraces, direct bulk diffusion to growth steps, and bulk convective transport due to step motion and applied flow fields. No analytical approximations are made; rather, the simultaneous governing equations are solved numerically by an efficient, moving-boundary finite element method. The coupled transport-kinetic model is applied to elucidate mechanisms responsible for step growth dynamics that occur during solution crystal growth. Of particular interest are nonlinear dynamical states, which may exhibit chaotic behavior.