FM15L_10363

XXI International Congress of Theoretical and Applied Mechanics
Warsaw, Poland, August 15–21, 2004

Analysis of Flow-Induced, Step-Bunching Instabilities During the Growth of Crystal from Liquid Solutions

Bing Dail, Yong-Il Kwon, **Jeffrey J. Derby**

University of Minnesota, Minneapolis, USA

The growth of crystals from a supersaturated liquid is widely employed to produce large, single crystals or many crystals in crystallization separations processes. Crystal quality is often compromised by morphological instabilities, such as macrosteps, step bunches, and inclusions, which arise from the coupled effects of fluid dynamics, mass transport, and the growth of atomic layers (steps) across a vicinal crystal surface. We present a novel multi-scale model that couples bulk fluid dynamics with surface step growth to analyze these instabilities. The surface kinetic model rigorously accounts for the interactions of discrete growth steps through surface diffusion fields, adsorption and desorption events, solute incorporation, and surface convection due to step motion. This model is self-consistently coupled with a bulk model that describes the fluid flow and its effects on the convection and diffusion of solute to the surface. The governing equations are solved numerically by an efficient, moving-boundary, finite element method.

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