Chemical & Environmental Engineering

2009 - 2010 Colloquium Series

Michael Doherty

Professor and Chair
Department of Chemical Engineering
University of California, Santa Barbara

Crystal Shape Engineering for Product and Process Design

Crystalline organic solids are ubiquitous as either final products or as intermediates in the fine chemical, pharmaceutical, and home & personal care industries. In most cases the properties of the crystalline solid (e.g., structure, shape, size) have a major impact on the functionality of the product as well as the design and operation of the manufacturing process, and in most cases the two cannot considered separately. Gibbs was the first to recognize that crystals rarely achieved their equilibrium (surface energy minimizing) shape but it took almost 100 years to discover how to identify their real growth shapes. In this seminar I will describe a novel, simple and accurate method for modeling the shape evolution of 3-dimensional faceted crystals from solution. The model is initialized from an arbitrary initial seed shape and size, but known polymorph. The growth and dissolution models for the crystal faces are based on the spiral screw dislocation model of Burton, Cabrera and Frank in which surface integration kinetics is the rate determining step. The model has been successfully applied to a selection of complex molecular crystals undergoing either dissolution or growth of interest in pharmaceutical applications. These insights lead to novel manufacturing strategies for engineering both crystal shape and size.

UC RIVERSIDE | UNIVERSITY OF CALIFORNIA | Bourns College of Engineering

Friday May 21, 2010
9:30 - 10:30 AM
Bourns A265
Refreshments at 9:15 AM