## **Carnegie Mellon** Materials Science and Engineering Seminar Series

Materials Research at Carnegie Mellon

## **Prof. Robert Sekerka**

Carnegie Mellon University Physics and Mathematics

## "Effects of Anisotrophy and Stability on Crystal Growth Morphology"

## Friday, October 27, 2006 11:00 A.M. Seminar in Doherty Hall 1212 Refreshments precede seminar at 10:30 A.M. in 2325 Wean Hall

Crystal growth morphology results from an interplay of crystallographic anisotropy and growth kinetics, the latter consisting of interfacial processes as well as long-range transport. The equilibrium shape results from minimizing the anisotropic surface free energy of a crystal under the constraint of constant volume and is given by the classical Wulff construction but can also be represented by an analytical formula based on the xi-vector formalism of Hoffman and Cahn. We give analytic criteria for missing orientations on the equilibrium shape in three dimensions. Crystals that grow under the control of interfacial kinetic processes tend asymptotically toward a "kinetic Wulff shape," based on the anisotropic interfacial kinetic coefficient. If capillarity is included, the sharp corners of this ``kinetic Wulff shape" become rounded, as shown by numerical computations of Yokoyama. If long-range transport were not an issue, crystals would presumably nucleate with their equilibrium shape and then proceed to evolve toward their 'kinetic Wulff shape," ultimately becoming bounded by surfaces of the more slowly growing orientations. But long-range transport of heat or solute is important during at least some stage of a crystal growth process and these transport processes themselves are unstable. This leads to shape (morphological) instabilities on the scale of the geometric mean of a transport length and a capillary length. The resulting shapes can be cellular or dendritic but can also exhibit corners and facets related to the underlying crystallographic anisotropy. Growth subsequent to morphological instability can be modeled by means of the phase field model, which is a diffuse interface model that eliminates interface tracking. Examples of computed cellular and dendritic morphologies show the transition from shallow to deep cells, liquid encapsulation, dendritic sidebranching, tip splitting, coarsening, solute microsegregation and many other phenomena that have been observed experimentally.

Robert F. Sekerka received his bachelor's degree in Physics (summa cum laude) from the University of Pittsburgh in 1960 and his AM (1961) and PhD (1965) degrees from Harvard University, where he was a Woodrow Wilson Fellow. His doctoral work was concerned with the theory of magnetic resonance and was directed by Nobel Laureate J.H. van Vleck. From 1965-68 he worked as a Senior Scientist in the Department of Theoretical Physics, Westinghouse Research Laboratories, and from 1968-69 he managed their Department of Materials Growth and Properties. In August 1969, he joined the faculty of Carnegie Mellon as Associate Professor of Metallurgy and Materials Science, was promoted to Professor in 1972, and served as Department Head from 1976-82. In 1982 he became Dean of the Mellon College of Science, which at that time consisted of the departments of Biological Sciences, Chemistry, Computer Science,

Mathematics and Physics, and served until 1991. In 1991 he was appointed University Professor of Physics and Mathematics and continues in that capacity today, with a courtesy appointment in Materials Science and Engineering. He is a fellow of the American Society for Metals, the American Physical Society and the Japanese Society for the Promotion of Science. Awards include the Phillip M. McKenna Award, the Frank Prize of the International Organization for Crystal Growth (IOCG) and the Bruce Chalmers Award of TMS. Most of his research is interdisciplinary and is concerned with theoretical problems in materials science that lead to challenging problems in physics and mathematics. Examples are the thermodynamics of stressed solids, transport phenomena, surfaces and interfaces, phase transformations, the precise definition of chemical potentials in stressed solids, the fundamental basis of the Onsager reciprocal relations in multi-component diffusion and heat flow, the influence of anisotropic surface tension on crystal shape, the theory of morphological stability (with his long-standing colleague William Mullins), phase field theory, and Lattice Boltzmann modeling of fluid dynamical phenomena. He is a consultant to NIST and currently serves as President of IOCG. Please see http://sekerkaweb.phys.cmu.edu and http://www.iocg.org for further information and publications.