COMPUTATIONAL MODELING OF GROWTH AND PROCESSING OF SINGLE-CRYSTAL MATERIALS
1000 – MANUFACTURING AND MATERIALS PROCESSING

JEFFREY J. DERBY*, JOCHEN FRIEDRICH†, AND KOICHI KAKIMOTO‡

* Department of Chemical Engineering and Materials Science, University of Minnesota
        421 Washington Ave, SE, Minneapolis, MN 55455 USA
        derby@umn.edu

† Fraunhofer IISB
        Schottkysstr. 10, 91058 Erlangen, Germany
        Jochen.Friedrich@iisb.fraunhofer.de

‡ Research Institute for Applied Mechanics, Kyushu University
        6-1, Kasuga-koen, Kasuga 816-8580
        kakimoto@riam.kyushu-u.ac.jp

Key words: Crystal growth, Fluid mechanics, Continuum transport, Phase change, Solid-state structure

ABSTRACT

This Minisymposium will focus on computational models that are applied to understand the growth and processing of single-crystal materials. Crystal growth itself is an exquisite materials synthesis process, and the industrial production of single-crystal products and devices of high quality and low cost embodies enormous challenges. Modeling provides a multidisciplinary and fundamental tool for understanding, controlling, and optimizing crystal growth and related manufacturing processes. Advances in these areas will impact advanced manufacturing processes that affect electronic and photonic devices for information, energy, defense, and detector systems, the production of fine chemicals and pharmaceuticals, and more. Improvements in these crystal-based systems will favorably impact wide-ranging domains relevant to worldwide prosperity, security, and health.

Papers will be solicited in following topical areas.

Modeling of fluid mechanics, transport, and phase change in crystal growth. This includes topics such as the growth of bulk and substrate crystals from the melt by Czochralski, Bridgman, vertical gradient freeze, floating zone, edge-defined film-fed growth, and other methods; the growth of crystals from fluxes, such as the traveling solvent or traveling heater method, and liquid solution growth processes, including the growth of organic materials by crystallization; and the vapor growth of epitaxial layers and thin films via chemical vapor transport, chemical vapor deposition, molecular-beam epitaxy, and other methods

Modeling of defect and microstructure formation in crystal growth. This session will focus on processes responsible for defect formation and evolution during the growth of single crystals, such as point defects,
defect complexes, dislocations, grain boundaries, precipitates, inclusions, and cracking. Continuum and microscopic approaches to these issues are of interest.

**Modeling of manufacturing processes involving single-crystal materials.** Topics for this session will focus on the modeling of the fundamental physical aspects involved in a variety of manufacturing steps for single crystal products devices, such as cutting, slicing, grinding, polishing, annealing, and others.

In all of these areas, we seek papers that present modeling advances, such as multi-scale, multi-physics coupling; model-based control, optimization, and design; bifurcation and stability analyses; phase-field, level-set, and fixed-mesh methods; cellular automata and Lattice-Boltzmann methods; and advanced numerical techniques, including parallel computation and GPU-based approaches.

We will solicit participants from academia, industry and government institutions around the world. We anticipate three sessions for the presentation papers of the three topical areas discussed above, as well as one special session for Keynote lectures and invited papers, totaling four sessions.