MATHEMATICAL AND COMPUTATIONAL ASPECTS OF THE CONTROL OF SOLIDIFICATION AND CRYSTAL GROWTH PROCESSES

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Solidification and crystal growth processes involve the interaction of a variety of physical phenomena at different length scales. Due to the required large scale, high resolution simulations for solidification modeling, solidification control provides a number of mathematical and computational challenges.

We will review our recent work on the control of solidification processes of various materials (particularly semiconductors) using an externally imposed magnetic field. The ability to achieve a homogeneous distribution of the solute and a flat freezing interface are usually the main objectives in the control of such solidification processes. The control of the fluid flow in the melt has been shown to have a direct impact on the above two objectives. We focus on the design of a tailored magnetic field (both spatially and temporally varying) that controls the fluid flow in the melt. The design problem is posed as an infinite-dimensional optimization problem. The solution to this problem is achieved through the solution of direct, sensitivity and adjoint partial differential equations. The computational parallel framework needed to address such problems will be discussed.

In addition, we will address a number of mathematical challenges required for: (i) multi-scale solidification control e.g. control of dendritic morphology using macro design variables (e.g. combination of optimal furnace conditions and optimal external magnetic field), (ii) real time control of solidification processes (model reduction for multi-physics multi-scale processes, role of uncertainty, etc.) and (iii) control of protein crystallization processes.