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Optimal control of convection–diffusion process with time-varying spatial domain: Czochralski crystal growth

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ABSTRACT

This paper considers the optimal control of convection–diffusion systems modeled by parabolic partial differential equations (PDEs) with time-dependent spatial domains for application to the crystal temperature regulation problem in the Czochralski (CZ) crystal growth process. The parabolic PDE model describing the temperature dynamics in the crystal region arising from the first principles continuum mechanics is defined on the time-varying spatial domain. The dynamics of the domain boundary evolution, which is determined by the mechanical subsystem pulling the crystal from the melt, are described by an ordinary differential equation for rigid body mechanics and unidirectionally coupled to the convection–diffusion process described by the PDE system. The representation of the PDE as an evolution system on an appropriate infinite-dimensional space is developed and the analytic expression and properties of the associated two-parameter semigroup generated by the nonautonomous operator are provided. The LQR control synthesis in terms of the two-parameter semigroup is considered. The optimal control problem setup for the PDE coupled with the finite-dimensional subsystem is presented and numerical results demonstrate the regulation of the two-dimensional crystal temperature distribution in the time-varying spatial domain.

1. Introduction

A large number of industrial systems exhibit time-varying features in which certain parameters of the system change over the course of the process. The methods employed in the formation and treatment of materials may result in, for example, chemical reactions, phase transitions, deformations or a combination of these behaviours, and therefore introduce complexities in model-based controller design. The Czochralski (CZ) crystal growth process, utilized for the production of semiconductor materials for the microelectronics industry, is a prime example in which a time-dependent feature of the system is the change in material domain and is the motivating example behind our study.

In the CZ crystal growth process, large boules of single crystals, typically Si, GaAs, InP, and CdTe, are formed in a thermal environment, whereby a crystal seed is slowly drawn from a pool of melt by a mechanical pulling arm. The material growth by solidification at the crystal–melt interface is affected by variations in the thermal fields of the ambient and melt temperatures, as well as the rate of pulling. These conditions are significant factors which contribute to the overall product quality where the objective of the batch processing strategy is to yield high-purity, defect and dislocation free crystals with constant diameter. The latter specification is vulnerable to fluctuations in heat transfer caused by turbulent convection in the melt environment, and also to longer term disturbances in the ambient temperature and changes in the melt level.

The complexity in modelling the dynamics of the CZ crystal growth process is reflected in the numerous works dedicated to the analyses of the multi-physics system which include studies of the transport phenomena associated with the crystal temperature, crystal–melt interface, melt dynamics, and crystal pull rate (see [6–9]). A more complete survey of the modelling and dynamical analyses of the process is contained in the review articles by Brown [6] and Lan [16], which also describe the usage and challenges in the design and implementation of active control methodologies for single crystal growth. For example, the maintenance of the crystal shape is a subject of considerable interest. Several controlled growth methods are based on models which incorporate the relationships between the crystal, ambient and melt temperatures, and have led to proposed strategies in which diameter control is achieved via combinations of crucible heater, bottom heater and crystal pull rate actuation (see [7–9]).

Another important control problem which has garnered less attention is the regulation of the crystal temperature distribution during the process which is important in counteracting the

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