

Model predictive temperature tracking in crystal growth processes



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ABSTRACT

The temperature gradients and distribution evolution within the crystal domain in Czochralski crystal growth process have important role in produced crystal's quality. Precise and tight regulation of temperature distribution and gradients is the most promising approach to ensure the crystal quality. In this work, the coupled crystal pulling dynamics and heat transfer models in Czochralski crystal growth with a time-varying boundary is considered. The moving boundary finite element method is used to obtain the optimal reference temperature trajectory associated with the reference crystal shape taking into account constraints on input and the temperature gradients. The obtained reference trajectory is used to implement a model predictive control strategy to track the reference temperature despite uncertainties in crystal domain geometry evolution and disturbances. Finally, the proposed method is implemented on a high fidelity finite element process model with non-planar interface and results are presented to validate the success of the proposed methodology.

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1. Introduction

Single crystals, due to unique mechanical, physical and electrical properties are common materials in microelectronics, optoelectronics and structurally robust and high temperature resistant applications (Sinno and Brown, 1999; Sinno et al., 2000). The Czochralski (Cz) crystal growth process is the most common mass production process to produce single crystal. In Cz process, the solid crystal is grown from molten material (Si, Ga, etc), starting from a small crystal seed and slowly growing by solidification of material at the melt-crystal interface. Due to the high-tech nature of single crystal applications, the quality of the grown crystal is of crucial importance. The crystal quality is defined by physical properties of the produced crystal such as defects density and developed residual stresses in the crystal. These defects and residual stresses are caused by significant temperature gradients in the crystal and can be regulated by introducing a controller to limit possibly large temperature gradient fluctuations (see (Gevlber and Stephanopoulos, 1987).

In order to realize process regulation in CZ crystal growth process one needs process model. The Czochralski crystal growth process modeling requires a sophisticated model of melt fluid flow, thermal and heat transfer phenomena, solid-liquid interface and pulling dynamics. There are recent studies focusing on modeling

and simulation of the coupled phenomena together (Cao et al., 2011; Demina and Kalaev, 2011). However for control purposes a simplified model of the phenomena of interest would suffice and usual assumptions are made to decouple specific processes to achieve a reduced order model as a basis for model based control synthesis. In the recent review on the automation of Czochralski crystal growth process (Winkler et al., 2013), both the classical and modern control realizations which are synthesized on the simplified process model description have been reported and critically accessed (Winkler et al., 2010a, 2010b). At present time, one can conclude that a successful controller synthesis relies on the interplay among feedback, feedforward control, the reference trajectory tracking and reconstruction of non directly measurable process states. Therefore, any controller realization is dependent on the quality of the model used in controller synthesis.

In particular, due to a specific feature of the Czochralski crystal growth process, the crystal shape undergoes time-varying changes which introduces moving boundaries to the parabolic partial differential equations (PDE) model of temperature evolution in the crystal growth process. Along this line, there are several works focusing on the model based controller design of parabolic PDE models with time-varying boundary domain, see Armaou and Christofides (2001a, 2001b), Rudolph et al. (2005). For example, Armaou and Christofides (2001a, 2001b) have reduced the 2-D heat transfer model on a rectangular domain of the crystal to a 1-D model and synthesized nonlinear controller for temperature regulation. Ng and Dubljevic (2012), Ng et al. (2013) studied optimal boundary control of the 2-D temperature model of the Cz crystal growth

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process with moving boundaries which is coupled with the crystal pulling dynamics. In these contributions, a simplified geometry (e.g. 1-D or 2-D rectangular domain) is used for control synthesis, however in realistic operation of Cz process, the crystal growth starts from a small three dimensional irregularly shaped seed and grows to a boule with relatively small fluctuations in desired radius.

One of the main obstacles in producing high quality large boules of a grown crystal is the presence of thermal stresses during the crystal cooling. The thermal stresses result in crystal cracking and fracture in the crystal during the cooling process. The critical stresses in the crystal depend on the crystal temperature and are usually caused by temperature difference in radial direction (Gevelber and Stephanopoulos, 1987; Gevelber et al., 1988; Fang et al., 2008). Controlling or limiting these stresses are crucial to avoid crystal cracking and to ensure the crystal quality. The conventional method to control these stresses are to adjust the heater temperature in order to maintain the temperature distribution around desired levels, however for larger crystals this method is not successful. In particular, the conventional methods are usually realized as off-line configuration accompanied with large scale simulation studies. The modern control strategies are helpful for on-line temperature distribution control, however limitations associated with distributed temperature measurement realization, the infinite-dimensional nature of the heat transfer process, time-varying crystal boundaries, stringent performance requirements reflected in grown crystal quality and coupled pulling and heat transfer dynamics make the control implementation a challenging task. One of the modern control realizations capable of accounting for the aforementioned performance and process characteristics in explicit way is the model predictive control.

Model Predictive Control (MPC) strategies due to their practical and industrially appealing advantages attracted quite a few contributions in the area of Czochralski crystal growth and temperature control. For example, Lee et al. (2005) used the MPC to determine a feedforward trajectory for crystal growth control. Temperature distribution control in solid crystal and melt is also performed by Ng et al. (2013), Irizarry-Rivera and Seider (1997) where the main approach in these contributions is to use a reduced order model of the complex dynamical system to apply the MPC and ensure that desired performance objectives are satisfied. In Irizarry-Rivera and Seider (1997) work, the lumped models are considered for both the pulling dynamics and bulk heat transfer and then two different MPC are coupled to control the radius and pulling velocity. Although utilizing a more sophisticated model of the process would be more accurate and due to the improved performance recommended, the complexity and the computational efforts associated with more detailed models must be weighted against ability of these algorithms to be implemented on-line in real-time setting.

The control strategies have been previously developed to control the crystal radius (Gevelber and Stephanopoulos, 1987; Neubert and Winkler, 2012; Winkler et al., 2010a), pulling velocity (Winkler et al., 2010a; Lee et al., 2005), melt temperature (Irizarry-Rivera and Seider, 1997) and for stabilization of temperature distribution (Ng et al., 2013; Irizarry-Rivera and Seider, 1997; Armaou and Christofides, 2001a), however to the best of authors' knowledge, there are no control strategies developed for optimal temperature distribution tracking with the ultimate objective of reducing the dislocation concentration distribution in grown crystal. Motivated by this, the crystal growth practitioners would seek the control strategy which maximizes crystal cooling without inducing a significant dislocation generation.

In this work, a framework is provided for reference temperature profile tracking in the Czochralski crystal growth process in the presence of temperature distribution and gradient constraints which are directly linked to the quality of grown crystal. A predefined reference crystal shape evolution is used to calculate the opti-

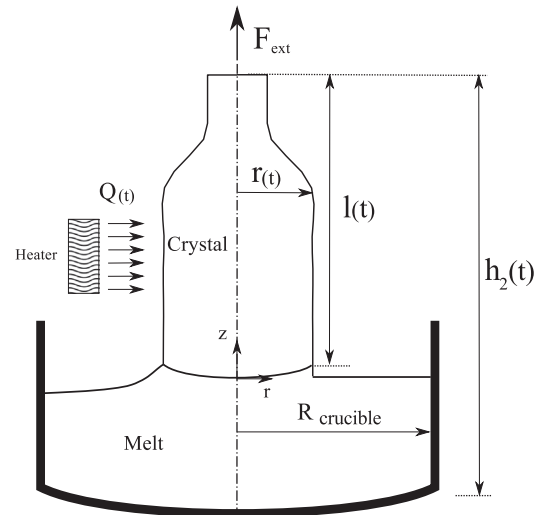


Fig. 1. Schematic of the Cz crystal growth process with the realistic geometry of the process given in the left figure side, and geometric simplifications and parameters given in the right figure side.

mal temperature trajectory. The reference trajectory is determined to achieve the maximum rate of crystal cooling and all constraints associated with temperature and gradient distributions are taken into account along with constraints on available actuator input. The moving boundary finite element model (FEM) of the conduction-convection thermal phenomena within the reference crystal shape is used to determine the optimal temperature distribution trajectory. Then the MPC is designed to track desired temperature distribution and satisfies stringent performance criteria.

The organization of the paper is given as following: after Section 1, a brief description of the pulling dynamics, heat transfer model and thermal stresses are provided in Section 2. In the following sections the optimization and the MPC controller realizations are presented and followed by numerical results and discussion.

2. Heat transfer model on moving boundary domain

The solid crystal growth process model, that we considered in this work, consists of coupled crystal boule growth and heat transfer dynamics. In general, the crystal growth model dynamics depicts crystal radius and length evolution which determines the domain boundaries of heat transfer model. On the other hand, the crystal shape evolution is influenced by temperature distribution and thermal phenomena (see Fig. 3). This two-way coupling is reduced to one-way coupling model realization using a robust controller such that the influence of the temperature distribution on the crystal growth dynamics is considered as a parametric uncertainty in the crystal growth rate.

2.1. Crystal pulling dynamics model

The schematic of the crystal pulling dynamics along with the notations are presented in Fig. 1. The pulling dynamics model is derived assuming horizontal melt–solid interface (see Abdollahi et al. (2014), Abdollahi and Dubljevic (2013)). The pulling dynamics model is given by:

$$\begin{aligned} \dot{x}_1(t) &= x_2(t) \\ \dot{x}_2(t) &= \frac{2}{\rho_c x_3(t)} \left[F_{ext}(t) - \rho_c \pi C_{growth} \left(\frac{x_2(t)}{2} - \frac{C_{growth}}{R_{cruc}^2} \right) \right] \\ \dot{x}_3(t) &= \pi C_{growth} \end{aligned} \quad (1)$$

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