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Abstract. We present an optimal control approach for the crystallization of a GaAs melt in a VGF configuration. The solidification process is described by a two phase Stefan problem including flow driven by convection and Lorentz forces. The interface between the liquid and the solid phase is modelled as a graph.

The control goal consists in tracking a prescribed shape and evolution of the free boundary (phase interface) using the crucible temperature and/or Lorentz forces. In particular we intend to achieve a flat free boundary in order to keep the density of dislocations small, compare e.g. [8].

We achieve this goal by minimizing an appropriate cost functional. The resulting optimization problem is solved numerically using an adjoint approach.

In the present work we apply the concept developed in [2, 3, 13] to growth from a melt to a practically relevant configuration [6]. Among other things we show that both, the control with Lorentz forces as well as the control with crucible wall temperature may be applied to achieve the control goal.

1 Introduction

Gallium Arsenide (GaAs) is a semiconductor material with increasing importance. The high electron mobility recommend GaAs in high frequency applications such as transmitting and receiving circuits in mobile phones. GaAs is also very important in optoelectronic, especially for the production of Lasers, LED's, and highly specialised solar panels (e.g. for satellites). GaAs mono crystals are grown using the LEC (Liquid Encapsulated Czochralski) method or the VGF (Vertical Gradient Freeze) method, see [4] for a comparison.

The structural quality of the crystals is strongly influenced by the amount and the distribution of dislocations of the crystal structure which are mainly caused by thermomechanical stress at the phase interface, These tensions can be reduced by a small radial temperature gradient, [6, 8]. Because the temperature gradients occurring with the VGF method are usually small, crystals grown with this technique show a very small dislocation density in comparison to LEC grown crystals, [8].

Assuming that the temperature at the free boundary is constant (equal to melting temperature), the free boundary must become flat in order to eliminate the radial temperature gradient at the free boundary. Thus, our control goal consists in achieving a flat free boundary. In addition to that, we also consider the direct reduction of the radial temperature gradient.

We emphasize that the control approach developed in the present work also allows to increase the crystallization speed of the VGF method while keeping the quality of the crystal.

The mathematical model used in this work governs heat conduction in the solid phase and heat conduction, heat transport and flow in the liquid phase. The two phases are coupled through the Stefan condition and the melting temperature condition at the free boundary. A third order boundary condition models heat transfer between the phases and the crucible wall.

The mathematical approach used in the presented work is described in [2, 3, 13], where solidification of Aluminium is considered as test configuration, and where also a detailed discussion about the related literature [5, 12, 11] can be found.

The results of the numerical experiments are presented in Section 3. There we consider a cylindrical crucible with a GaAs melt and a diameter of $D = 5\,\mathrm{cm}$ and a height of 10 cm. This configuration is relevant at least for experiments considered [6]. Our control goal is to obtain a flat free boundary with a velocity of $5\,\frac{\mathrm{cm}}{\mathrm{h}}$. The results presented in Section 3 strongly differ from the results presented in [3]. This is due to the fact that the physical properties of GaAs strongly differ from that of aluminium.

2 Problem definition

2.1 Mathematical model

Let $\Omega = G \times H$ be a cylindrical domain containing the substance, where G denotes the bottom domain and $H \subset \mathbb{R}$ the height, see Figure 1. The crucible wall, i.e. the boundary of Ω, is denoted by $\partial\Omega$. The time dependent domains $\Omega_s(t)$ and $\Omega_l(t)$ denote the solid and the liquid phase and satisfy $\Omega_s(t) \cup \Omega_l(t) = \Omega$ The free boundary Γ (the phase interface) is described as a graph

$$\Gamma(t) = \left\{ \begin{pmatrix} y \\ f(t,y) \end{pmatrix} : y \in G \right\}$$

with $f : G \to H$. Figure 1 depicts such a configuration.

As mathematical model for the temperatures $u_{s/l}$ in the solid and liquid phase respectively, the velocity $\boldsymbol{v}$ and the pressure p we take

$$\partial_t u_s = \frac{k_s}{c_s \rho} \Delta u_s \qquad \text{in } (0,T] \times \Omega_s, \quad (1)$$

$$\partial_t u_l + \boldsymbol{v} \cdot \nabla u_l = \frac{k_l}{c_l \rho} \Delta u_l \qquad \text{in } (0,T] \times \Omega_l, \quad (2)$$

$$\nabla \cdot \boldsymbol{v} = 0 \qquad \text{in } (0,T] \times \Omega_l, \quad (3)$$

$$\partial_t \boldsymbol{v} + (\nabla \boldsymbol{v})\boldsymbol{v} - \frac{\varepsilon}{\rho} \Delta \boldsymbol{v} + \frac{1}{\rho} \nabla p = -\boldsymbol{g}\gamma(u_l - u_M) + \boldsymbol{A} \qquad \text{in } (0,T] \times \Omega_l, \quad (4)$$