Optimal control of the phase interface during the solidification of a GaAs melt

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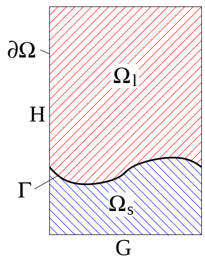
1 Introduction

The solidification process of a GaAs melt in a cylindrical crucible with a diameter of $5\,\mathrm{cm}$ is considered. The goal consists in controlling the shape and evolution of the free boundary (phase interface) using the crucible wall temperature and/or near-wall Lorentz forces. In particular we intend to achieve a flat free boundary in order to keep the density of dislocations small, compare e.g. [3].

2 Problem definition

We consider the depicted crucible $\Omega = G \times H$, with th solid phase Ω_s, the liquid phase Ω_l und the free boundary Γ.



The solidification process is modelled using the heat equation (1) in the solid phase Ω_s and in the liquid phase Ω_l. In the liquid phase additionally flow driven by convection and near-wall Lorentz forces (3), (4) are considered, where the convection term is modelled using the Boussinesq approximation. The phase transition is constituted by the Stefan condition (5) and the melting temperature condition (7) at the free boundary Γ. The Robin-type boundary condition (6) models the heat transfer at the crucible wall $\partial\Omega$. Altogether one obtains the nonlinear system

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

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

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

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

$$V_\Gamma L = \frac{k_s}{\rho}\partial_{\boldsymbol{\mu}} u|_{\Omega_s} - \frac{k_l}{\rho}\partial_{\boldsymbol{\mu}} u|_{\Omega_l} =: -\Big[\frac{k_{s/l}}{\rho}\partial_{\boldsymbol{\mu}} u\Big]_\Gamma \qquad \text{in } (0,T] \times \Gamma, \tag{5}$$

$$\tfrac{k_{s/l}}{\alpha_{s/l}}\partial_{\boldsymbol{\nu}} u = u_b - u \qquad \text{in } (0,T] \times \partial\Omega, \tag{6}$$

$$u = u_M \qquad \text{in } (0,T] \times \Gamma. \tag{7}$$

Here, u denotes the temperature, u_M the melting temperature, $\boldsymbol{v}$ the velocity and p the pressure. The near-wall Lorentz forces $\boldsymbol{A}(A_c)$ depend on the control values A_c and are modelled using the Riga plate configuration presented in [2] and [4]. The function A_c and the crucible wall temperature u_b serve as control variables.

The free boundary is modelled as a graph $\Gamma(t) = \big\{(x,\ f(t,x))^T\big\}$. By $\overline{f}$ the desired evolution of the free boundary is denoted. The control goal mathematically is formulated as a pde-constrained optimization problem;

$$\begin{aligned} &J(f,u_b,A_c) := \frac{1}{2T}\int_0^T \int_G \big(f(t,y) - \overline{f}(t,y)\big)^2 dy dt = \min_{f,u_b,A_c}! \\ &\text{s.t. } (1) - (7)\,. \end{aligned} \tag{P}$$

The functional J models the objective in our minimization problem, namely the reduction of the error between the free boundary and the desired free boundary in the mean square sense.

The optimization problem (P) is solved using a adjoint approach, which allows to compute the gradient of the reduced functional $K(u_b, A_c) = J\big(f(u_b, A_c), u_b, A_c\big)$ in a efficient way. The computational costs for one gradient computation consist in solving the forward system (1) – (7) with given A_c, u_b and one backward-in-time adjoint system, which contains the state of the forward system as input data. Utilizing this an efficient gradient method is developed.

For a detailed derivation of the gradient of K and description of the algorithm we refer to [1, 4].

3 Results

We consider a GaAs melt in in a rotational symmetric crucible. The desired free boundary is a moving plane with a velocity of $5\,\frac{\text{cm}}{\text{h}}$.

The figures show the free boundary (black line), the temperature (colored stripes) and the velocity (arrows) at different time instances, for the uncontrolled problem (right side), with crucible wall temperature control (bottom left), and with near-wall Lorentz forces control (bottom right).

One clearly sees that tracking of the desired flat free boundary works very well using crucible wall temperature as control variable. In contrast to the aluminum test problem considered in [2] the control of the free boundary using near wall Lorentz forces also works well for the GaAs test problem considered here. This is due to the significant lower crystallization speed of GaAs in comparison to aluminium and is described in detail in [4].

References

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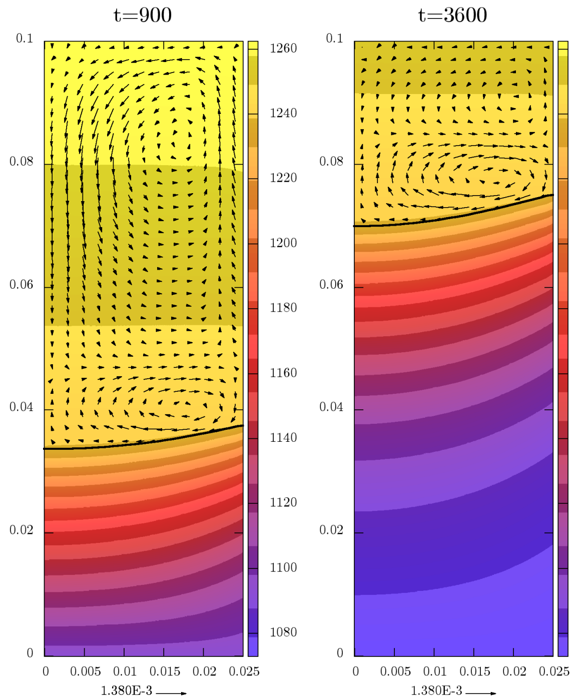
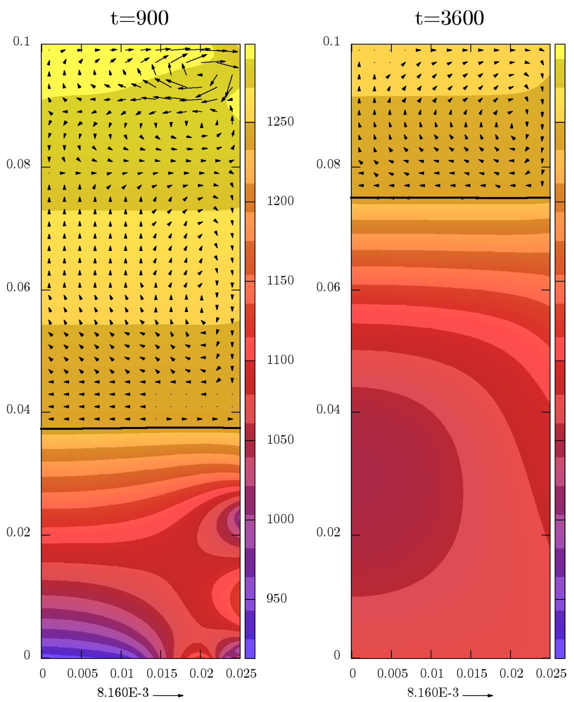
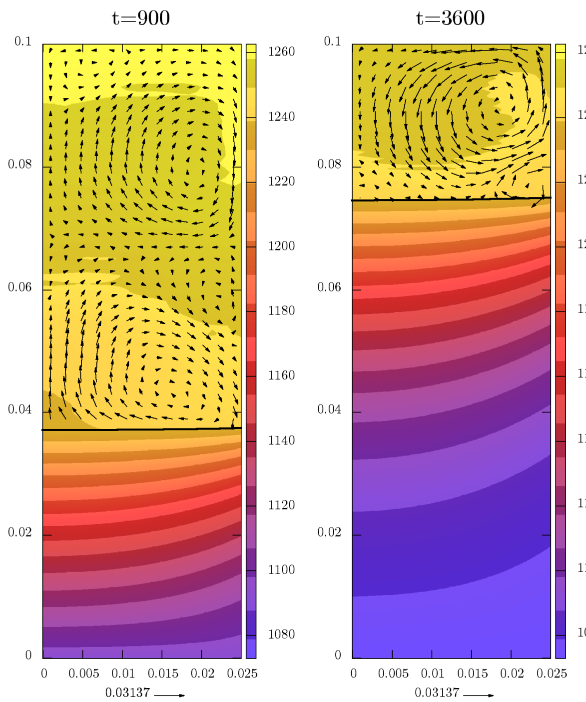


without control



with crucible wall temperature control



with near-wall Lorentz force control