Proceedings of ALGORITMY 2005
pp. 64–72

BOUNDARY CONTROL OF SEMICONDUCTOR MELTS

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Abstract. In the present paper we investigate optimal boundary control of semiconductor melts. The flow is governed by the Boussinesq approximation of the Navier-Stokes system. The control goal consists in tracking of a prescribed flow field. As control action we consider Dirichlet boundary control. The first order optimality conditions of the underlying optimal control problems represent a coupled system consisting of the Boussinesq equations, an backward in time adjoint equation, and a boundary value problem for the boundary control temperature. Numerically we solve this system by damped Picard iteration and present results for a threedimensional model problem in a cylindrical configuration.

Key words. Free and forced convection, Boussinesq approximation, optimization of partial differential equations, crystal melt flow

AMS subject classifications. 65M60, 76D05, 76D55, 76R10

1. Introduction and motivation. During the growth of crystals in axisymmetric zone melting devices the transition from the twodimensional flow regime to an unsteady threedimensional behavior of the velocity and temperature field is observed in experiments under certain conditions of the growth device. This behavior leads to so called striations which from the crystal quality point of view should be avoided during the growth process. To avoid such crystal defects it is important to figure out those parameters, which guarantee a stable steady twodimensional melt flow during the growth process. There are several possibilities to determine these parameters. In the present work an optimization approach will be discussed.

From experiments and practical crystal production processes it is known that unsteady behavior of the melt and vorticies near the fluid-solid-interphase decrease the crystal quality. From the optimization point of view it therefore makes sense to gain

(i) flows, which are nearly steady, and/or
(ii) flows, which only have small vorticity in a certain region of the melt zone.

In a mathematical setting the goal in (i) may be achieved by minimizing tracking-type functionals of the form

$$J(\vec{u},\theta_c) = \frac{1}{2}\int_0^T \int_\Omega |\vec{u}-\overline{\vec{u}}|^2 \, d\Omega dt + \frac{\alpha}{2}\int_0^T \int_{\Gamma_c} (\theta_c^2 + \theta_{c_t}^2)\, d\Omega dt, \tag{1}$$

whereas goal (ii) may be related to minimal values of vorticity-type functionals of the form

$$J(\vec{u},\theta_c) = \frac{1}{2}\int_0^T \int_\Omega |curl\vec{u}|^2 \, d\Omega dt + \frac{\alpha}{2}\int_0^T \int_{\Gamma_c} (\theta_c^2 + \theta_{c_t}^2)\, d\Omega dt \; . \tag{2}$$

Above, $\vec{u}$ denotes the flow velocity vector field in the melt, and $\overline{\vec{u}}$ the desired state, which represents a physically favourable flow situation. The function θ_c denotes the

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temperature flux on the wall of the crucible and serves as control variable on the control boundary Γ_c. Both cost functionals contain two parts; the first part provides the mathematical formulation of the control gain, and the second part weighs the control cost.

2. Mathematical model. The flow in the crystal melt is gouverned by the Boussinesq approximation of the Navier-Stokes system for the velocity $\vec{u} = (u, v, w)$, the pressure p and the temperature θ;

$$\left\{\begin{array}{rl} \vec{u}_t + (\vec{u}\cdot\nabla)\vec{u} - \Delta\vec{u} + \nabla p - Gr\,\theta\,\vec{g} &= 0 \quad \text{on } \Omega_T, \\ -\text{div } \vec{u} &= 0 \quad \text{on } \Omega_T, \\ \theta_t + \vec{u}\cdot\nabla\theta - \frac{1}{Pr}\Delta\theta - f &= 0 \quad \text{on } \Omega_T. \end{array}\right. \tag{3}$$

Here $\vec{g} = (0, 0, 1)$ and $\Omega_T = \Omega \times (0, T)$ denotes the space-time cylinder with cylindrical melt zone of height H and radius R. Furthermore, Gr denotes the Grashof number, and Pr the Prandtl number. Since in the present work we are mainly interested in control via boundary temperatures the absence of external forces is assumed.

System (3) is supplied with temperature boundary conditions of third kind on the crucible walls (which form the control boundary Γ_c), and Dirichlet boundary conditions at the remaining parts Γ_d of the boundary. For the flow Dirichlet boundary conditions are prescribed on the whole boundary Γ. More precisely we set

$$\left\{\begin{array}{rl} u = u_d,\ v = v_d,\ w &= w_d \quad \text{on } \Gamma_T, \\ \lambda\frac{\partial\theta}{\partial\mathbf{n}} + \tilde{a}(\theta - \theta_0) &= \theta_c \quad \text{on the control boundary } \Gamma_{cT}, \\ \theta &= \theta_d \quad \text{on } \Gamma_{dT}, \end{array}\right. \tag{4}$$

with the boundary time cylinders $\Gamma_T = \Gamma \times [0, T]$, $\Gamma_{cT} = \Gamma_c \times [0, T]$ and $\Gamma_{dT} = \Gamma_d \times [0, T]$. θ_0 is some environmental temperature and $\lambda, \tilde{a}$ denote physical constants. It is convenient to rewrite the boundary condition on Γ_c in the form $a\frac{\partial\theta}{\partial\mathbf{n}} + b\theta = \theta_c$ on Γ_{cT}, with appropriate coefficients a, b which may not vanish simultaneously. We note that it is possible to include via u_d, v_d, w_d certain crystal and crucible rotations, as it is common in the case of Czochralski growth. In the case of zone melting techniques one would require $\vec{u} = \vec{0}$.

In the case of the Czochralski crystal growth technique with u_d, v_d, w_d we have the possibility to describe a certain crystal and crucible rotation. In the case of zone melting flow u_d equals zero. The initial state is assumed as the neutral position of the crystal melt

$$\vec{v} = \mathbf{0} \tag{5}$$

and an initial temperature field as a solution of the non convective heat conduction equation

$$-\frac{1}{Pr}\Delta\,\theta = 0 \text{ in } \Omega,\ \theta = \theta_0 \text{ on } \Gamma_c, \text{ and } \theta = \theta_d \text{ on } \Gamma_d. \tag{6}$$

The material properties and the dimensionless parameters for the investigated crystals close the initial boundary value problem for the description of the melt flow. We assume that prescribing Dirichlet boundary conditions on the walls of the crucible is possible, so that Dirichlet boundary controls may be utilized as control mechanism, i.e. $a = 0, b = 1$ in (4). The optimization goal then consists in finding an optimal boundary heating strategy by adjusting the boundary temperature distributions. Once this strategy is known, in a further step the methods developed in [1, 2] may be applied to provide optimal heater locations by solving an appropriate inverse problem.

3. Optimization. The optimization problem considered in the present work is given by

$$\text{(P)} \qquad \begin{cases} \min J(y, \theta_c) \\ \text{s.t.}(3) - (6). \end{cases} \tag{7}$$

To derive the first order necessary optimality conditions for this optimization problem we formally utilize the Lagrange technique. The related Lagrangian in the primitive setting is given by

$$\begin{aligned} L(\vec{u}, p, \theta, \theta_c, \vec{\mu}, \xi, \kappa, \chi) &= J(\vec{u}, \theta_c) + \langle \vec{\mu}, \vec{u}_t + (\vec{u} \cdot \nabla)\vec{u} - \Delta\vec{u} + \nabla p - Gr\,\theta\,\vec{g} \rangle_{\Omega_T} \\ &- \langle \xi, div\,\vec{u} \rangle_{\Omega_T} + \langle \kappa, \theta_t + \vec{u} \cdot \nabla\theta - \frac{1}{Pr}\Delta\theta - f \rangle_{\Omega_T} + \langle \chi, a\frac{\partial\theta}{\partial \mathbf{n}} + b\theta - \theta_c \rangle_{\Gamma_{cT}}, \end{aligned} \tag{8}$$

where $\langle \cdot, \cdot \rangle_{\Gamma_{cT}}$ and $\langle \cdot, \cdot \rangle_{\Omega_T}$ denote appropriate duality pairings, and $\vec{\mu}$, ξ, κ and χ are Lagrange parameters. For example for $\vec{u}, p$ and θ sufficiently regular one has

$$\begin{aligned} &< \vec{\mu}, \vec{u}_t + (\vec{u} \cdot \nabla)\vec{u} - \Delta\vec{u} + \nabla p - Gr\,\theta\,\vec{g} >_{\Omega_T} = \\ &\qquad \int_{\Omega_T} [\vec{u}_t + (\vec{u} \cdot \nabla)\vec{u} - \Delta\vec{u} + \nabla p - Gr\,\theta\,\vec{g}] \cdot \vec{\mu}\, d\Omega\, dt. \end{aligned}$$

A precise functional analytic setting, also containing the convergence analysis of the solution algorithms proposed in the subsequent sections will be given in a forthcoming paper, see also [3, 4, 5].

The necessary optimality conditions for (P) are now given by

$$\nabla L = 0.$$

Assembling these conditions for the cost functions of (1) and (2) leads to the state equations (3)-(6), together with the so called adjoint system

$$\left\{ \begin{array}{rcll} -\vec{\mu}_t - \Delta\vec{\mu} + (\nabla\vec{u})^t\vec{\mu} - (\vec{u} \cdot \nabla)\vec{\mu} + \nabla\xi & = -\kappa\nabla\theta + \left\{ \begin{array}{l} -(\vec{u} - \overline{\vec{u}}) \\ \text{curl curl}\,\vec{u} \end{array} \right. & & \text{in } \Omega_T, \\ -\text{div}\ \vec{\mu} & = 0 & & \text{in } \Omega_T \\ \vec{\mu} & = \mathbf{0} & & \text{on } \Gamma_T, \\ \vec{\mu}(T) & = \mathbf{0} & & \text{in } \Omega, \\ & & & \\ -\kappa_t - \frac{1}{Pr}\Delta\kappa - \vec{u} \cdot \nabla\kappa & = Gr\,\vec{g} \cdot \vec{\mu} & & \text{in } \Omega_T, \\ \kappa & = 0 & & \text{on } \Gamma_{dT}, \\ a\frac{\partial\kappa}{\partial \mathbf{n}} + b\kappa & = 0 & & \text{on } \Gamma_{cT}, \\ \kappa(T) & = 0 & & \text{in } \Omega, \\ & & & \\ \chi & = \left\{ \begin{array}{ll} -\frac{1}{bPr}\frac{\partial\kappa}{\partial \mathbf{n}} & \text{if } b \neq 0 \\ \frac{1}{aPr}\kappa & \text{if } b = 0 \end{array} \right. & & \text{on } \Gamma_{cT}, \end{array} \right. \tag{9}$$

and the optimality conditions

$$\begin{array}{rcll} \alpha(-\theta_{c_{tt}} + \theta_c) & = \chi & \text{on } \Gamma_{cT} \\ \theta_c(0) & = \theta_0 & \text{on } \Gamma_c, \\ \theta_{c_t}(T) & = 0 & \text{on } \Gamma_c. \end{array} \tag{10}$$

Here θ_0 denotes a temperature distribution on Γ_c at the beginning of the melting process.

Alltogether, the necessary optimality conditions for problem (P) form a boundary value problem for $\vec{u}, p, \theta, \vec{\mu}, \xi$, and θ_c w.r.t. space and time in the space-time domain Ω_T, which inherits a very special structure.

From now onwards we assume that system (3) together with (4), (5) and (6) for given θ_c admits a unique solution (this is satisfied under appropriate assumptions at least in the two-dimensional case, see [6], [7]). Then the cost functionals in (1),(2) may be rewritten in the form

$$\hat{J}(\theta_c) = J(\vec{u}(\theta_c), \theta_c),$$

where the gradient of $\hat{J}$ is determined by the optimality condition (10). More precisley, there holds

$$\hat{J}'(\theta_c) = \alpha(\theta c_{tt} + \theta_c) - \chi. \tag{11}$$

To evaluate $\hat{J}'(\theta_c)$ for given θ_c amounts to solving (3)-(6) for $\vec{u}, \theta$, and then (9) for $\vec{\mu}, \theta$ and χ.

Let us close this section with noting that the approach to boundary control presented in the present work is designed to compute temperature distributions at every single point of the control boundary, since it follows from (11) that the gradient of the cost functional w.r.t. θ_c can be expressed in terms of adjoint variables, so that the directional derivatives in all directions are available once the adjoint variables are determined. This is different to the approach presented in e.g. [8], were control functions are sought which only depend on a few numbers of parameters and directional derivatives w.r.t these parameters are computed using finite difference techniques. We note that the latter approach requires the solution of an auxilliary linear problem for every directional derivative, so that its computationally complexity is proportional to the number of parameters.

4. The numerical approach. We solve problem (7) by applying a damped Picard iteration to the KKT system (3)-(6), (9),(10). The pseudo-algorithm reads

i) choose θ_c,
ii) solve the forward problem for $[\vec{u}, \theta](\theta_c)$
iii) solve the adjoint problem for $[\vec{\mu}, \kappa](\vec{u}, \theta)$
iv) update $\theta_c := \sigma_r \theta_c + (1 - \sigma_r)\mathcal{H}^{-1}(\chi)$, $\sigma_r \in]0, 1[$,
v) until convergence, go to ii),

where $\mathcal{H}^{-1}(\chi)$ for given χ denotes the solution of (10).

Next let us describe the numerical solution methods used in ii)-iv). For this purpose we denote by $t_i := i\tau$, $i = 0, \dots Z$ an equidistant time grid on $[0, T]$, where $\tau := \frac{T}{Z}$ for some $Z \in \mathrm{N}$. Moreover, unknown quantities are supplied with superscripts. In ii) we apply a semi-implicit time discretization scheme. Convective terms are treated explicitly, conductive terms implicitly. We obtain for $n = 0, \dots, Z - 1$

$$\frac{\vec{u}^{n+1}}{\tau} - \Delta \vec{u}^{n+1} + \nabla p^{n+1} - Gr\, \theta^{n+1} \vec{g} = \frac{\vec{u}}{\tau} - (\vec{u} \cdot \nabla)\vec{u}, \tag{12}$$

$$-div\ \vec{u}^{n+1} = 0, \tag{13}$$

$$\frac{\theta^{n+1}}{\tau} - \frac{1}{Pr}\Delta \theta^{n+1} = \frac{\theta}{\tau} - (\vec{u} \cdot \nabla)\theta, \tag{14}$$

supplied with the boundary conditions (4) at $t = t_{n+1}$. Here $\vec{u}$ and θ for $n = 0$ are taken from (5) and (6), respectively. Of course, given $\vec{u}$ equation (14) can be solved

for θ^{n+1}. To solve (12),(13) we apply a pressure-correction scheme which is explained next. Taking the divergence in (12) leads to

$$-\Delta p^{n+1} = -\frac{1}{\tau} div\ \vec{\hat{u}}, \tag{15}$$

where

$$\vec{\hat{u}} = \vec{u} + \tau[(\vec{u}\cdot\nabla)\vec{u} + Gr\,\theta^{n+1}\vec{g}]. \tag{16}$$

For the pressure we get Neumann boundary conditions. In the case of no slip walls the pressure boundary conditions are of the form $\frac{\partial p^{n+1}}{\partial \vec{n}} = 0$. Using the noted boundary conditions for p^{n+1} equation (15) can be solved for p^{n+1}, which in turn determines the velocity field $\vec{u}^{n+1}$ in terms of

$$\frac{1}{\tau}\vec{u}^{n+1} - \Delta\vec{u}^{n+1} = \frac{1}{\tau}\vec{u} - \nabla p^{n+1} \tag{17}$$

together with boundary conditions for $\vec{u}^{n+1}$ from (4) for $t = t_{n+1}$. In summary step ii) amounts to solving one poisson equation for p^{n+1}, three Helmholtz equations for $\vec{u}^{n+1}$, and one for θ^{n+1}. Spatially these subproblems are discretized by the finite volume method on a staggered grid in cylindrical coordinates developed in [9]. The resulting linear systems are solved by appropriately preconditioned cg methods.

For the time discretization of the adjoint system in iii) we for $n = Z, \ldots, 1$ apply the scheme

$$\begin{aligned}\frac{\vec{\mu}^{n-1} - \vec{\mu}}{\tau} - \Delta\vec{\mu}^{n-1} + (\nabla\vec{u}^{n-1})^t\vec{\mu} - (\vec{u}^{n-1}\cdot\nabla)\vec{\mu} + \nabla\xi^{n-1} \\ = -\kappa^{n-1}\nabla\theta + \begin{cases} -(\vec{u}^{n-1} - \overline{\vec{u}}) \\ \text{curl curl } \vec{u}^{n-1}, \end{cases} \end{aligned} \tag{18}$$

$$-div\ \vec{\mu}^{n-1} = 0, \tag{19}$$

$$\frac{\kappa^{n-1} - \kappa}{\tau} - \vec{u}^{n-1}\cdot\nabla\kappa - \frac{1}{Pr}\Delta\kappa^{n-1} = Gr\,\vec{g}\cdot\vec{\mu}, \tag{20}$$

where for $n = Z$ we have $\vec{\mu} = \mu(T) = 0$ and also $\kappa = \kappa(T) = 0$. The boundary conditions are taken from (9) for $t = t_{n-1}$. A motivation of this scheme together with a detailed discussion is given in [10]. Eq. (20) immediately can be solved for κ^{n-1}, the quantities $\vec{\mu}^{n-1}, \xi^{n-1}$ are obtained from (18),(19) by the pressure-correction method explained above. Spatially these subproblems are discretized again by the finite volume method of [9], and the resulting linear systems are also solved by appropriately preconditioned cg methods.

To provide $\mathcal{H}^{-1}(\chi)$ in iv) equation (10) is solved for the control θ_c by a finite volume method in space and time, where the boundary conditions $\theta_c(\gamma, 0) = \theta_{c0}$ and $\theta_{c_t}(\gamma, T) = 0$ for $\gamma \in \Gamma_c$ are taken. We note that $\mathcal{H} := -\partial_{tt} + id$.

Let us note that for the computation of $\vec{\mu}^{n-1}, \xi^{n-1}, \kappa^{n-1}$ the flow $\vec{u}^{n-1}$ is required for $n = Z, \ldots, 1$. This means that we have to store these flow velocities in order to compute the adjoint solution $\vec{\mu}^{n-1}, \kappa^{n-1}$, and θ_c.

5. Numerical results. To test our optimal control approach we consider a cylindrical threedimensional zone melting configuration with the crystal $(Bi_{0.25}Sb_{0.75})_2Te_2$ which forms a composition of bismuth point fifty antimony one point fifty telurium two, whose geometrical and material parameters are summarized in in Table 1 (see

parameter	symbol	value
radius	R	0.004 m
height	H	0.016 m
melting point	θ_s	613 K
diffusivity	a	0.44000e-05 $\frac{m^2}{s}$
viscosity	ν	0.36310e-06 $\frac{m^2}{s}$
expansion	β	0.96000e-04 K^{-1}

TABLE 1
Parameters of $(Bi_{0.25}Sb_{0.75})_2Te_2$-melt and of the melt geometry

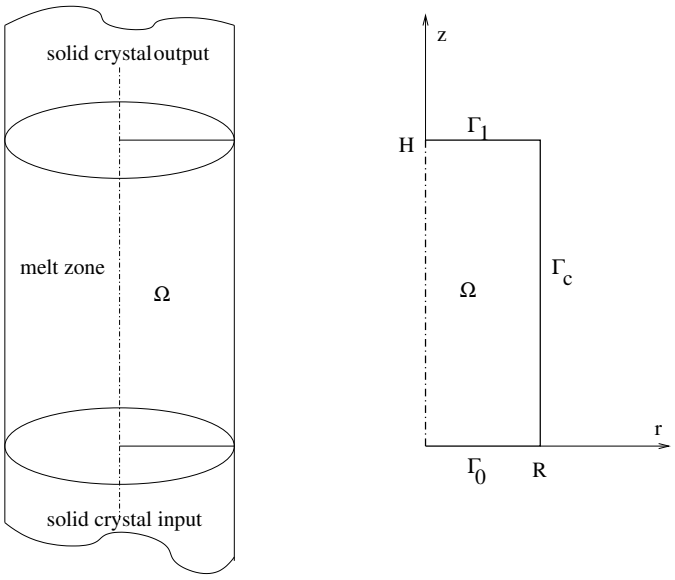

FIG. 1. *Physical domain for the zone melting growth*

also [9]).

$(Bi_{0.25}Sb_{0.75})_2Te_2$-crystals are used for small cooling devices. The Figure 1 shows the physical domain of the melt zone. We note that $\Gamma_d = \Gamma_1 \cup \Gamma_0$. For the velocity we use homogeneous dirichlet data on the whole boundary. For the temperature we use the boundary conditions

$$\theta = \theta_c, \text{ for } r = R, 0 \le z \le H, \varphi \in (0, 2\pi), \tag{21}$$

$$\theta = \theta_s, \text{ for } 0 \le r \le R, z = H, \tag{22}$$

$$\theta = \theta_s, \text{ for } 0 \le r \le R, z = 0, \tag{23}$$

i.e. we set $a = 0, b = 1$ in (4). For $t = 0$ we start with a given temperature profile $\theta_c = \theta_{c0}$ on Γ_c and with $\theta_s = 613\,K$, $\delta\theta = 25\,K$ for θ_{c0} we use

$$\theta_{c0}(z) = \theta_s + 4\frac{z}{H}(1 - \frac{z}{H})\delta\theta\ .$$

The control goal is tracking of a velocity field $\overline{\overline{u}}$, which either is given by

i) a typical twodimensional toroidal flow, or by a

ii) a non moving melt, i.e. $\overline{\vec{u}} = \mathbf{0}$.

The case ii) is artificial but serves as a good test case since $\theta_c = \theta_s = const.$ implies $\vec{u} = \mathbf{0}$, and this velocity field together with $\theta = \theta_s$ is a solution of the Boussinesq approximation. Artificial in this context means that $\theta = \theta_s$ on Ω is not a realistic assumption for a crystal melt and the input mixed crystal will never change to a single homogeneous output crystal. We consider the time interval $[0, T] = [0, 8\,\text{seconds}]$ and $Z = 60$ time steps of duration 0.1222 seconds each. For the spatial discretization we use a grid containing 20×30 finite volumes. As regularization and damping parameters we use $\alpha = 0.25$ and $\sigma_r = 0.1$.

The Figures 2 - 4 show the results of the optimization for the case i) and case ii), i. e. the resulting control temperature on the boundary-time cylinder and the development of the functional values, where the temperatures are dimensionless defined by $\bar{\theta} = \frac{\theta - \theta_s}{\delta\theta}$. As one can see a remarkable reduction of the value of the cost functional is obtained already within the first few iterations of our solution algorithm.

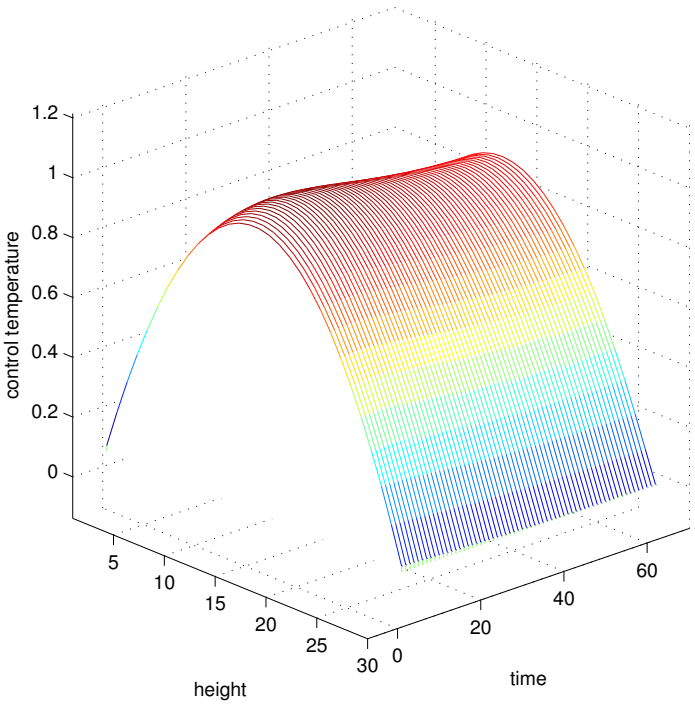

FIG. 2. *Control temperature (problem (i))*

6. Conclusion. Optimal boundary heating control strategies for fully time-dependent thermally coupled flow problems in spatially 3-dimensional cylindrical domains are developed. Optimal heating strategies are obtained as solutions of certain minimization problems and are computed from the related Karush-Kuhn-Tucker system by applying a damped Picard iteration.

Numerical results are presented for zone melting growth configurations in realistic 3-dimensional cylindrical domains. While boundary heating control for zone melting configurations seems to offer a practically relevant control mechanism numerical results for Czochralski growth in [10] indicate, that boundary heating for this

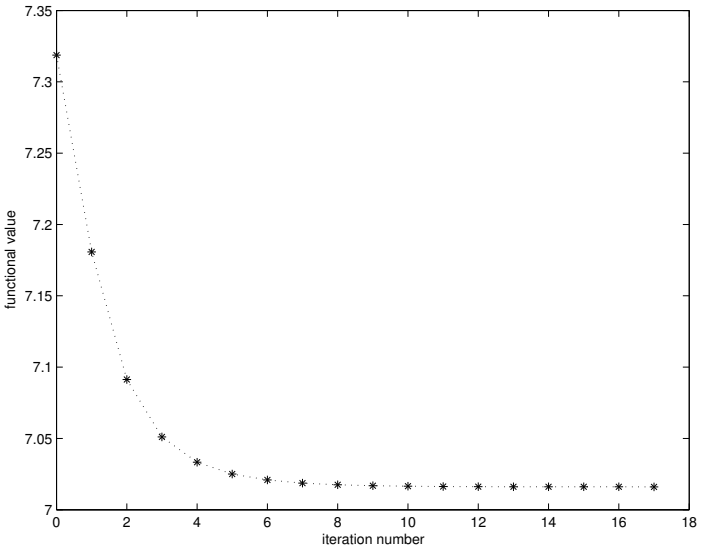

FIG. 3. *Functional vs. iteration (problem (i))*

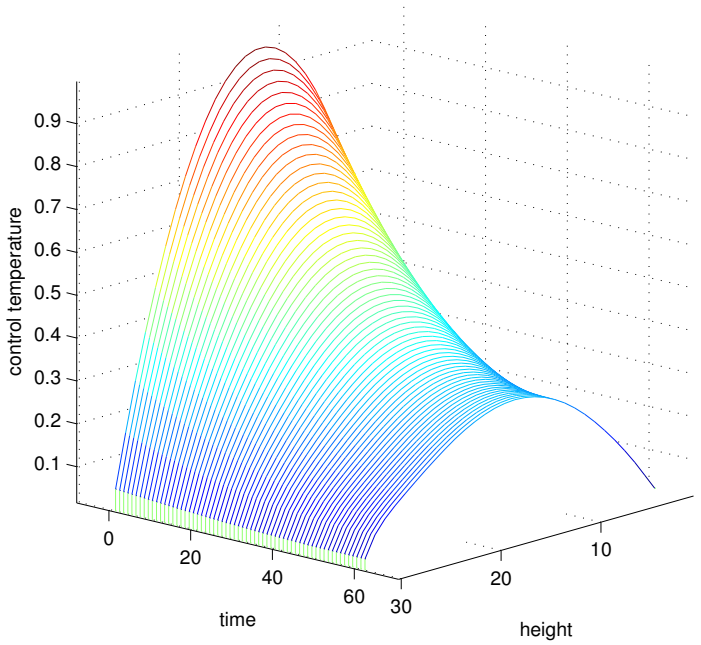

FIG. 4. *Control temperature (problem (ii))*

configuration seems to have only limited impact on the flow behaviour in the melt. As a result for Czochralski growth other control mechanisms should be considered, like control by magnetic fields and/or crucible/crystal rotation.

Acknowledgments. The authors thank their colleagues from the Institut für Kristallzüchtung in Berlin for many fruitfull discussions. The second author acknowl-

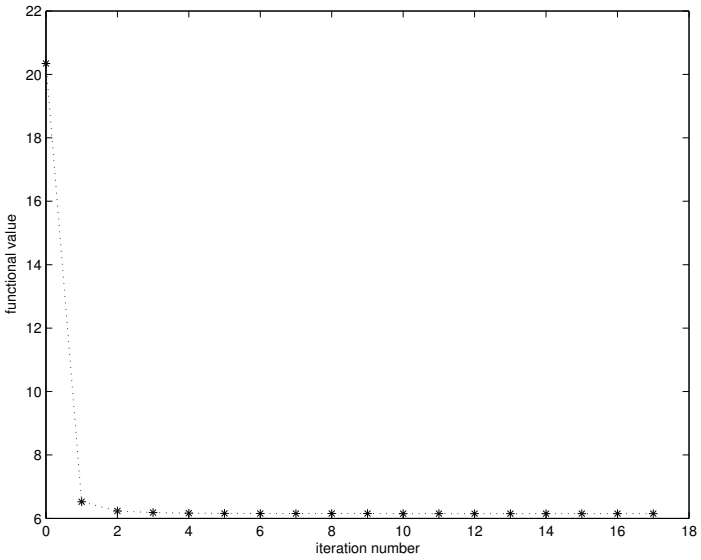

FIG. 5. *Functional vs. iteration (problem (ii))*

edges support of the collaborative research center SFB 609 located at the Technische Universität Dresden.

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