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Numerical investigation of the bifurcation behavior of a crystal melt flow

During the growth of crystals there were observed crystal defects under some conditions of the growth device. As a result of experiments a transition from the twodimensional flow regime of a crystal melt in axisymmetric zone melting devices to an unsteady threedimensional behavior of the velocity and temperature field was found. This behavior leads to striations as undesirable crystal defects [1].
To avoid such crystal defects it is importand to know the parameters, which guarantee a stable steady twodimensional melt flow during the growth process.
For the investigation of this symmetry break a mathematical model of the crystal melt was formulated for

i) the theoretical description of the experimental observed behavior and

ii) the identification of critical parameters of the growth device, i.e. the evaluation of bifurcation points.

1. Mathematical Model

The crystal melt is described by the Navier-Stokes equation for an incompressible fluid using the Boussinesq approximation coupled with the convective heat conduction equation. Heat conductivity and viscosity depend on the temperature.
For the velocity no slip boundary conditions are used. For the temperature we have at the interfaces between the solid material and the fluid crystal inhomogenous Dirichlet data, i.e. the melting point temperature. On the heated coat of the ampulla the experimentators gave us measured temperatures but we need Neumann conditions to describe the heating procedure physical correctly.
For the initial state we assume a neutral position of the crystal melt ($\vec{v} = 0$) and a temperature field, which solves the non convective heat conduction equation with the given temperature boundary conditions.

2. Numerical solution method and mathematical aspects

A threedimensional finite volume code based on a second order spatial discretization is used for the numerical solution of the above described non linear initial boundary value problem [2].
The validation of the finite volume code was done by the evaluation of the benchmark formulated in [3]. We got a vary good aggreement with the results of [4] and [5]. In the threedimensional computations we use a finite volume grid of 33 cells in the radial and axial direction and 20 cells in the azimutal direction. The time integration of the Navier-Stokes equation and the heat conduction equation is done with second order accurate Adams-Bashforth or leapfrog method.
Because of the information loss about the heat fluxes over the boundary we have to solve an identification problem for finding suitable heat flux densities q for the formulation of the Neumann boundary condition of the form $-\lambda\frac{\partial\theta}{\partial n} = q$.
q was identified in such a way, that the resulting temperature on the boundary is equal to a given measured value.
From mathematical point of view some bifurcation investigations are under consideration. But it's not possible to analyze the general nonlinear coupled problem described above. Simplifications with respect to the time dependency of the heat conductivity and the viscosity are necessary.
Quantitative bifurcation results of the general problem are only possible using numerical methods.

3. Results

A $(Bi_{1-x}Sb_x)_2Te_3$ crystal melt in an axisymmetric ampulla was investigated. We have the Prandtl number Pr, the Rayleigh number Ra and the aspect ratio α, i.e. height of the melt over the diameter of the ampulla, as parameters in the result of a dimension analysis.
During the computaions we found only stable twodimensional toroidal solutions using Dirichlet data as temperature boundary conditions. The more physical inhomogenous Neumann boundary for the temperature allows us to simul-

tate the transition from the twodimensional toroidal solution to a genuine non stationary threedimensional solution. With the numerical simulations critical parameters of the crystal growth configuration and bifurcation points of the time behavior of the velocity and temperatur could be identified and the experimetal phenomena could be verified with finding a critical value of $\alpha = \alpha_c = 1.45$.

Thus it was possible to define parameter intervals for a stable crystal growth configuration.

The following figure show the time history at two monitoring points of the melt and the frequency spectra for an over critical value of α, $\alpha = 3$, from the numerical simulation. Compared to the experiments we found a very good agreement of the base frequency of the experiment and the simulation [6].

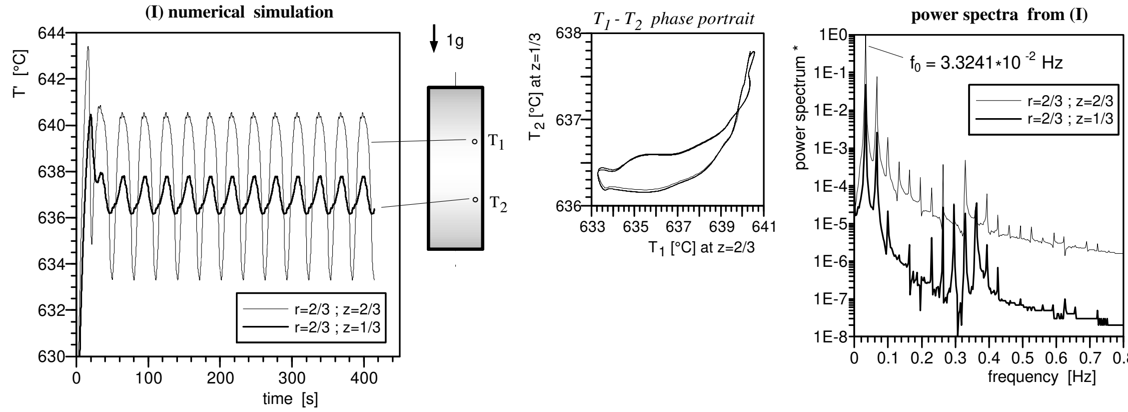

Figure 1: time history of the numerical simulation

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4. References

1 König, F., Bärwolff, G.: Crystal Growth of $(Bi_{0.25}Sb_{0.75})_2Te_3$ by zone melting technique under microgravity; AIAA-paper (**IAF-95-J.1.02**) IAF, Oslo, 1995.

2 Bärwolff, G.: Numerical Modelling of Two- and Three-Dimensional External and Internal Unsteady Incompressible Flow Problems; in Computational Fluid Dynamics (Ed. D. Leutloff and R.C. Srivastava), Springer-Verlag, Berlin Heidelberg New York 1995.

3 Wheeler, A.A.: Four test problems for the numerical simulation of flow in Czochralski crystal growth; J. Crystal Growth 102 (1990) 691.

4 Bückle, U., Schäfer, M.: Benchmark results for numerical simulation of flow in CZ growth; J. Crystal Growth 126 (1993) 682.

5 Baumgartl, J., Budweiser, W., Müller, G., Neumann, G.: Studies of buoyancy driven convection in a vertical cylinder with parabolic temperature profile; J. Crystal Growth 97 (1989) 9.

6 Bärwolff, G., König, F., Seifert, G.: Thermal buoyancy convection in vertical zone melting configurations; appears in ZAMM 1997.

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