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Thermal and solutal buoyancy convection in vertical zone melting configurations

During the growth of crystals crystal defects were observed 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 experimentally. This behavior leads to striations as undesirable crystal defects.
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 including the thermal and solutal bouyancy convection 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.

The superposition of thermal and solutal bouyancy convection effects sets up the possibility of avoiding undesirable behavior of the melt flow by a certain choice of the involved parameters.

1. Mathematical model and numerical solution method

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 and the diffusion equation. Heat conductivity and viscosity depend on the temperature. Thus we have the governing equations

$$u_t + (ruu)_r/r + (uv)_\varphi/r + (wu)_z - v^2/r = -p_r + \nabla\cdot(2\mu\vec{S_r}) - 2\mu S_{\varphi\varphi}/r\,, \tag{1}$$

$$v_t + (ruv)_r/r + (vv)_\varphi/r + (wv)_z + uv/r = -p_\varphi/r + \nabla\cdot(2\mu\vec{S_\varphi}) + 2\mu S_{r\varphi}/r\,, \tag{2}$$

$$w_t + (ruw)_r/r + (vw)_\varphi/r + (ww)_z = -p_z + \nabla\cdot(2\mu\vec{S_z}) + Gr_T\theta + Gr_c c\,, \tag{3}$$

$$(ru)_r/r + v_\varphi/r + w_z = 0\,, \tag{4}$$

$$\theta_t + (ru\theta)_r/r + (v\theta)_\varphi + (w\theta)_z = \frac{1}{Pr}(r\theta_r)_r/r + \frac{1}{Pr}(\theta_\varphi)_\varphi/r^2 + \frac{1}{Pr}(\theta_z)_z\,, \tag{5}$$

$$c_t + (ruc)_r/r + (vc)_\varphi + (wc)_z = \frac{1}{Sc}(rc_r)_r/r + \frac{1}{Sc}(c_\varphi)_\varphi/r^2 + \frac{1}{Sc}(c_z)_z\,. \tag{6}$$

in the cylindrical melt zone (height H, radius R). $\vec{S}$ denotes the stress tensor and u, v, w and p are the primitive variables of the velocity vector and the pressure, θ and c denote the dimensionless temperature and the Tellurit concentration.
For the velocity no slip boundary conditions are used. At the interfaces between the solid material and the fluid crystal melt we have for the temperature 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 physically correctly. At the bottom of the cylindrical melt zone we have a Tellurit deposit in form of a boundary layer. The boundary conditions are of the form

$$u = v = w = 0 \quad \text{on the whole boudary,} \tag{7}$$

$$-\frac{\partial\theta}{\partial r} = q \quad \text{for } r = 1, 0 \le z \le 2\alpha, \varphi \in (0, 2\pi), \tag{8}$$

$$\theta = 0, \quad \text{for } 0 \le r \le 1, z = 0,\ z = 2\alpha, \varphi \in (0, 2\pi), \tag{9}$$

$$\frac{\partial c}{\partial \mathbf{n}} = 0, \quad \text{for } 0 \le r \le 1, 0 < z \le 2\alpha, \varphi \in (0, 2\pi), \tag{10}$$

$$\frac{\partial c}{\partial z} + (1-k)\, v_0\, c = 0 \quad , \quad \text{for } 0 \le r \le 1, z = 0, \varphi \in (0, 2\pi). \tag{11}$$

The initial state was assumed as the neutral position of the crystal melt ($\vec{v} = 0$ and $c = 0$) and a temperature field, which solves the non convective heat conduction equation with the given temperature boundary conditions.
A threedimensional finite volume code is used for the numerical solution of the above described non linear initial boundary value problem.
The material properties and the dimensionless parameters for the investigated crystal $(Bi_{1-x}Sb_x)_2Te_3$ are given by

$$\nu_0 = \nu(T_0) \quad , T_0 = 613^oC\,,$$
$$\mu = \nu(\theta)/\nu_0\,,$$
$$\nu = (c - d\,T) * 10^{-7}\, m^2/s\,,$$
$$c = 11.6,\ d = 1.3 * 10^{-2}/1^oC\,,$$
$$\kappa = 4.4 * 10^{-6} m^2/s\,,$$
$$\hat{\beta_T} = 9.6 * 10^{-5} K^{-1}\,,$$
$$\delta T = (5 + H/1mm)\,K$$
$$\hat{\beta_c} = 0.09,$$
$$\delta_c = 0.5\, mm$$
$$D = 5 \cdot 10^{-9}\, m^2/s\,,$$
$$L_0 = R \ \text{(radius)},$$
$$U_0 = \nu_0/L_0\,,$$
$$\theta = \frac{T - T_0}{\delta T}\,,$$
$$Q = 1.5 * 10^4 W/m^2\,,$$
$$Gr_T = g\hat{\beta_T}\delta T R^3/\nu_0^2 \ \text{(Grashof number)},$$
$$Gr_c = g\hat{\beta_c}\delta c R^3/\nu_0^2\,,$$
$$Pr = \nu/\kappa \ \text{(Prandtl number)},$$
$$Sc = \nu/D \ \text{(Schmidt number)},$$
$$\alpha = H/(2R) \ \text{(aspect ratio)},$$
$$V_0 = 1.0 * 10^{-6} m/s \ \text{(growth rate)},$$
$$k = 0.1\,.$$

The considered crystal material is of interest during the production of cooling devices.

2. Results

The experimental results of the oscillatory behavior for certain ascpect ratios could be confirmed by the thermal bouyancy convection model. With the generalization of the mathematical model by solutal bouyancy convection effects we figured out a damping/decreasing of the fluid motion in the melt zone when the Grashof number is increasing. These investigations have just begun and because of the computational amount (time and memory) we consider an axisymmetrical simplification.

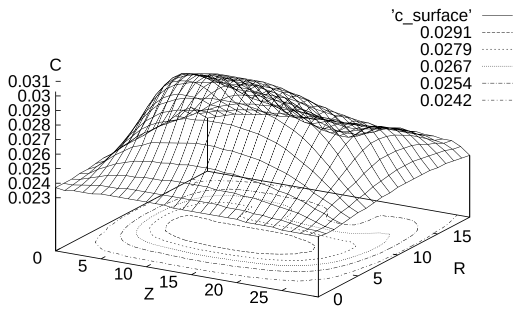

Figure 1: c-surface plot, $\alpha = 1.25$, $Gr_c = 47621$

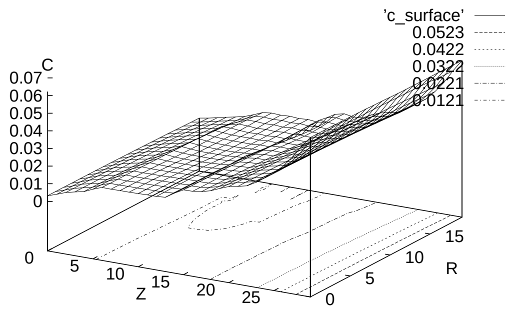

Figure 2: c-surface plot, $\alpha = 2.5$, $Gr_c = 428590$

The figures 1 and 2 show the surface plots of the Tellurit concentration for $\hat{\beta_c} = 0.01/Gr_c = 47621$ and $\hat{\beta_c} = 0.09/Gr_c = 428590$ respectively. The investigations show the principal possibility of stabilization of the melt flow for certain thermal and solutal parameter configurations. In consequence of the presented results the necessity of the investigation of the genuine unsteady threedimensional mathematical model of the coupled thermal and solutal convection is obvious.

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3. References

1 Bärwolff, G., König, F. and G. Seifert: Thermal buoyancy convection in vertical zone melting configurations, ZAMM 77 (1997) 10

2 König, F. and G. Bärwolff: Crystal growth of $(Bi_{0.25}Sb_{0.75})_2Te_2$ by zone melting technique under microgravity (IAF-Paper - 95 -J.1.02), 46th International Astronautical Congress, Oct. 2 - 6, Oslo, 1995

3 Müller, G, Neumann, G. and H. Matz: A two-Rayleigh-number model of buoyancy-driven convection in vertical melt growth configurations, J.Crystal Growth 84, (1987)

4 Bärwolff, G.: Numerical Modelling of Two- and Three-Dimensional External and Internal Unsteady Incompressible Flow Problems, in: Computational Fluid Dynamics - Selected Topics, D. Leutloff and R.C. Srivastava (Eds.), Springer-Verlag Berlin Heidelberg New York, 1994

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