

3D MODELING OF CZOCHRALSKI MELT FLOW AND EXPERIMENTAL VALIDATION

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Proposed session topic: convection

In Czochralski (CZ) semi-conductor growth, crystal quality strongly depends on the melt flow pattern under the interface. However, melt convection involves a complex combination of flow instabilities associated with buoyancy, surface tension and rotational forces. Therefore, except under the effect of a strong magnetic field, the flow becomes time-dependent (TD), three-dimensional (3D) and, more or less weakly, turbulent. It also exhibits azimuthal and temporal structured oscillations [1, 2].

In order to better understand the complex mechanisms occurring in the bulk flow, real and numerical experiments are complementary approaches. In addition to be a valuable tool to identify the melt flow dynamics, the experimental procedure provides relevant data which can be used to validate the numerical models.

Our experimental apparatus corresponds to a simplified isothermal CZ configuration and resembles the one used in [3]. It consists in a rotating cylinder filled with water and a faster rotating flat disk located on the free surface. Two dimensionless numbers characterize the flow regime, viz. the Rossby number Ro (ratio between Coriolis and inertial forces) and the Ekman number Ek (ratio between viscous dissipation and inertia). If the disk and cylinder angular velocities are close together, the flow is stationary and axisymmetric, and the flow domain can be separated in two bulk regions, viz. the region located under the disk ($r < R_s$) and an external liquid annulus ($R_s < r < R_c$). In both regions, the basic bulk flow is that of a rotating solid, but with slightly different angular velocities. However, since the disk rotates faster than the cylinder, the underneath fluid is pumped upwards, hence joining the Ekman layer that forms beneath the disk where it is radially ejected by centrifugal force (Fig. 1). As this inertial effect is not strong enough for the fluid to penetrate into the external annulus, the ejected fluid moves downwards inside the internal shear layer which separates the two bulk flows and then reaches a second Ekman layer on the cylinder bottom (Fig. 2). Now, if the difference between the two bulk angular velocities exceeds a critical value, the flow will leave the steady axisymmetric regime. Since inertial effects are strong enough for the fluid to penetrate into the external flow, thereby destabilizing the internal shear layer (Fig. 3). This instability generates a set of rotating waves whose wavenumber depends on the values of Ro and Ek (Fig. 4).

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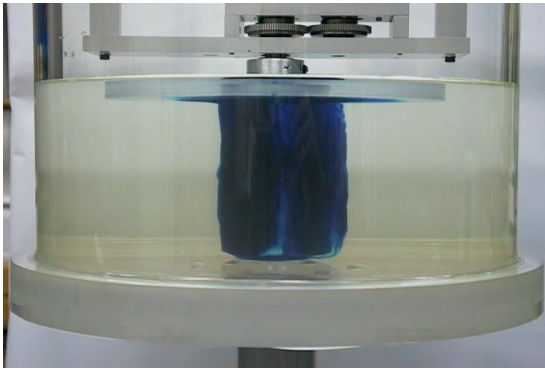


Fig. 1: Upwards pumping of core fluid.

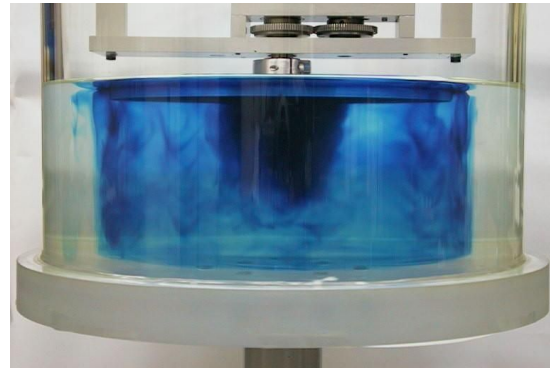


Fig. 2: Downwards motion of ejected fluid.

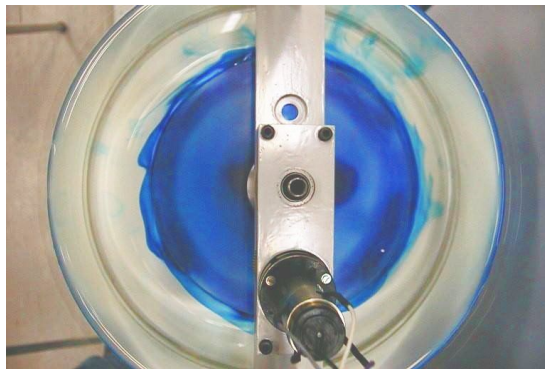


Fig. 3: Development of instabilities.

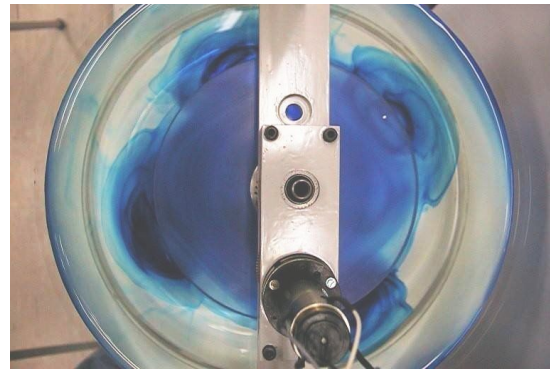


Fig. 4: Generated rotating waves.

As a second tool for investigating the CZ melt flow, we have developed a parallel 3D Finite Element (FE) solver. Simulating 3D TD melt convection is difficult, since the flow dynamics is complex due to the interaction of thin boundary and internal layers as confirmed by our model experiments. Hence fine graded meshes are needed to resolve these layers, and the discrete system has a number of unknowns that may amount to several millions, requiring parallel computing to assemble and solve the FE discrete problem. Here, besides the management of distributed data, the spatio-temporal discretization and the development of an iterative solver are critical issues. For the sake of robustness, we have implemented an effective preconditioner [4] that allows the scheme to converge to a given tolerance with a number of iterations which is essentially independent of the system size. Our 3D solver has been validated by comparison with the above model experiments and further used to simulate CZ melt flow.

References

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