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# Flow pattern transition driven by the combined Marangoni effect and rotation of crucible and crystal in a Czochralski configuration

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ABSTRACT

In order to understand the flow pattern transition driven by the combined Marangoni effect and rotation of crucible and crystal, a series of unsteady three-dimensional numerical simulations were conducted for this complex flow in a Czochralski configuration. Results show that the basic flow is axisymmetric and steady at small driving forces. The flow structures are represented as meridian circulations rotating in different directions, which are dependent on the differential rotation rates of the crystal and the crucible. When the thermocapillary Reynolds number exceeds a threshold value, the basic flow undergoes a transition to the three-dimensional oscillatory flow. Without rotation, the three-dimensional thermocapillary flow is characterized by standing waves or by spoke patterns with fluctuations growing and decaying periodically. When the crystal and/or crucible rotate, the oscillatory flow behaves as temperature and velocity fluctuation waves traveling in the azimuthal directions. The direction and velocity of wave propagation, fluctuation amplitude and wave number, which are dependent on the interaction of the thermocapillary, centrifugal and Coriolis forces, are discussed. Furthermore, the critical conditions for the onset of instabilities are determined and the stability diagrams are mapped. For the counter-rotation of the crystal and the crucible, two flow transitions occur with the increase of the thermocapillary Reynolds number, and three state regimes are zoned. The characteristics of the flow instabilities in each state regime are analyzed.



## 1. Introduction

Rotating flow and thermal convection are ubiquitous in the natural and industrial processes. In the past few decades, many researchers have been devoted to these phenomena that affect the fluid flow from the laboratory scales to the planetary scales, and from the fundamental perspectives to the industrial applications. In the material processing industry, an important example is the Czochralski (Cz) crystal growth technology, where both the crucible containing the melt and the crystal growing at the melt surface are rotated. Under the effects of temperature gradient and rotation, buoyancy, thermocapillary, centrifugal and Coriolis forces are coupled to drive the undesired flows and ensuing instabilities, which directly affect the crystal quality. Therefore, understanding this complex flow and the instabilities will help to improve the qualities of the crystal growth.

It is well known that the thermocapillary force is one of the major causes for the undesired convection. Smith and Davis [1,2] performed a linear stability analysis of the thermocapillary flow in a thin and infinitely extended fluid layer with the free surface subjected to a horizontal temperature gradient. Two types of three-dimensional (3-D) instabilities were reported. The first one behaves as a spanwise traveling wave for small Prandtl numbers ($Pr$). The second one moves in the steamwise direction and occurs for large Prandtl numbers. Afterward, many investigators were devoted to the research of thermocapillary and thermocapillary-buoyancy flows [3–7]. It was found that thermocapillary flow exhibits various types of 3-D flow instabilities. Subsequently, the effect of rotation on the thermocapillary flow was analyzed by Zebib [8]. Results showed that the system rotation has a great influence on the flow pattern transitions and the effect of Coriolis force must be taken into account. Shi et al. [9,10] performed a linear stability analysis of the effect of pool rotation on the basic thermocapillary flow and determined the critical conditions for the onset of hydrothermal waves in a rotating annular pool heated from the outer wall. The test fluids of both silicone oil ($Pr = 6.7$) and silicon melt

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**Nomenclature**

| | |
|---|---|
| $f$ | dimensionless frequency |
| $h$ | depth, m |
| $H$ | dimensionless depth |
| $m$ | wave number |
| $P$ | dimensionless pressure |
| $Pr$ | Prandtl number, $Pr = \nu/\alpha$ |
| $r$ | radius, m |
| $R$ | dimensionless radius |
| $Re$ | thermocapillary Reynolds number |
| $T$ | temperature, K |
| $U, V, W$ | dimensionless velocities |
| $\boldsymbol{V}$ | dimensionless velocity vector |
| $z$ | axial coordinate, m |
| $Z$ | dimensionless axial coordinate |

*Greek symbols*

| | |
|---|---|
| $\alpha$ | thermal diffusivity, $m^2\ s^{-1}$ |
| $\beta$ | growth rate constant |
| $\gamma_T$ | temperature coefficient of surface tension, $N\ m^{-1}\ K^{-1}$ |
| $\Theta$ | dimensionless temperature, $\Theta = (T - T_c)/(T_h - T_c)$ |
| $\mu$ | dynamic viscosity, $kg\ m^{-1}\ s^{-1}$ |
| $\nu$ | kinematic viscosity, $m^2\ s^{-1}$ |
| $\rho$ | density, $kg\ m^{-3}$ |
| $\tau$ | dimensionless time |
| $\psi$ | dimensionless stream function |
| $\Omega$ | rotation rate, rpm |

*Subscripts*

| | |
|---|---|
| c | crucible or critical or cold |
| h | hot |
| s | crystal |
| $R, Z, \theta$ | coordinate directions |

($Pr = 0.011$) were used. The results showed that pool rotation destabilizes the basic steady axisymmetric thermocapillary flow. Gelfgat [11] studied the destabilization of buoyancy flow by a weak rotation. For this case, thermocapillarity was excluded. It was found that for low Prandtl numbers, the weak rotation splits the main convective circulation into several vortices with an unstable boundary between them that generates the instability; for larger Prandtl numbers, rotation steepens the unstable thermal stratification, which causes the Rayleigh–Bénard instability. Recently, Kahouadji et al. [12] investigated the effect of rotation on the thermocapillary flow in a laterally heated liquid bridge. The buoyancy effect was neglected. Results showed that when the feed rod co-rotates with the crystal, the weak rotation effect is destabilizing and the strong rotation effect is stabilizing. However, the counter-rotation always destabilizes the thermocapillary flow. Meanwhile, Shvarts [13] analytically studied the stability of thermocapillary flow in a slowly rotating liquid layer. He also concluded that within a certain range of Taylor numbers, the rotation destabilizes the flow, but after a critical value of Taylor number, the rotation has a stabilizing effect.

On the other hand, experimental investigations on the instabilities of melt flow in the Cz configuration have been performed either by measuring temperature or velocity oscillation, or by the visualization of the flow on the free surface or inside the melt [14–16]. Fein and Pfeffer [17] conducted an experiment in a rotating annulus and found that the baroclinic waves counter-rotate with the annulus in the slow-rotation regime, but they co-rotate with the annulus in the high-rotation regime. Contrarily, Seidl et al. [18] observed in both experiments and numerical simulations that the azimuthal $m$-folded ($m = 2, 3, 4,\ldots$) waves propagate in a direction that was opposite to the crucible at higher crucible rotation rates. For the crystal rotation, Hintz and Schwabe [19] found that the critical value of the crystal rotation rate for the incipience of oscillatory convection monotonically increases with the temperature difference between the crystal and the crucible. For the combined rotation of the crystal and crucible with a horizontal temperature gradient, Son et al. [20,21] reported that the counter-rotation of the crystal and crucible can decrease the traveling velocity of the oscillation wave. Two different modes of temperature transition were observed.

Numerical simulations facilitated the understanding of the characteristic of the flow instability and the flow pattern transition by providing detailed data such as the 3-D time-dependent flow fields [16,22–24]. Numerical simulations of the combined action of the temperature gradient and rotation date back to the work of Rojo and Derby [25]. They performed high-resolution calculations by using a parallel finite element method to simulate the flow of molten bismuth silicon oxide driven by the combined rotational and buoyant forces during Cz crystal growth. For the first time, the spoke patterns were predicted along the surface at high crystal rotation rates. Subsequently, many 3-D numerical simulations have been performed for the hydrodynamic model of the Cz crystal growth [14,15,26]. The results showed that the asymmetrical phenomena of the fluid flow and the critical temperature difference for the flow pattern transition are dependent on both the crystal and crucible rotation. However, Gunzburger et al. [27] reported that the crucible and crystal rotation are ineffective in reducing the velocity perturbation and the temperature gradient. With these divergences, Shi et al. [10] and Li et al. [28] reported the results of 3-D numerical simulations of the thermocapillary flow for silicone oil and silicon melt in a rotating shallow annular pool, respectively. They concluded that the rotation of the annular pool has an important effect on the critical temperature difference and the propagating direction of the traveling waves.

In the investigations above, the flow driven by the Coriolis and the centrifugal forces combined with the thermocapillary and/or buoyancy forces are very complicated. However, it is known that the rotation can lead to fluid-dynamic instabilities even in isothermal liquids. The 3-D rotating flow produces beautiful patterns and has attracted the interest of physicists as examples of pattern formation in flow [29]. Most interest about rotating flow is related to the rotor-stator cavity or the closed/open cylindrical enclosure, but only several works have been reported to take relevance to the Cz configuration, which has a partly free surface. Kanda [30] performed an experiment on the instability behaviors of isothermal fluid in a differential rotation system that was derived from the Cz crystal growth process. He observed various flow patterns as the increasing rotation rate difference between the crystal and the crucible. At a relatively small rotation rate difference, the well-known barotropic instability forms multiple vertically coherent vortices along the Stewartson layer. To extract the effect of rotation during the Cz process, Li and his colleagues [31,32] numerically investigated the detailed characteristics of the forced flow driven by iso- and counter-rotation of the crystal and crucible regardless of the temperature gradient. It was indicated that the rotation-driven flow undergoes a transition from the axisymmetric and steady state to the 3-D oscillatory flow when the rotation Reynolds number exceeds a critical value. The stability diagram was