

STABILITY OF A ROTATING WEIGHTLESS LIQUID PHASE IN
ZONE MELTING

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Numerical analysis is used to determine the parameters of the critical equilibrium states of a weightless uniformly rotating melt in a model of single-crystal growth by the floating zone technique. The treatment focuses on nonzero angles of growth.

Consider a liquid of density ρ , occupying the region bounded by the ends of two coaxial cylindrical rods of equal radius ξ_0 and by a free surface Γ . No external force fields are acting; the system rotates with constant angular velocity ω about the axis ζ of the rods, and is in equilibrium under the effect of centrifugal and surface-tension forces. We assume that Γ is axisymmetric and that the tangent to its axial cross section (profile) at the point of contact with the edge of either rod makes an angle β_0 with the horizontal, i.e., the endface of the rod (see Fig. 1). Our object is to analyze the stability of this state.

The above problem models the stability of a rotating weightless melt in single-crystal growth by zone melting. We define the angle $\beta_0 = \pi/2 - \gamma$ (where γ is the angle of growth [1]) at the endface which is the front of solidification. The angle γ is close to zero; for actual semiconductor materials (e.g., silicon or germanium), it is 10-15°.

Let us introduce a cylindrical coordinate system (ξ, θ, ζ) , with its origin at the center of the endface and its ζ axis pointing towards the liquid. The arc length τ along the profile is measured from the point at which $\zeta = 0$. Using the linear scale $p^{-1/3}$ ($p = \rho\omega^2/2\sigma$, where σ is the coefficient of surface tension), we convert to the dimensionless quantities $r = \xi p^{1/3}$, $r_0 = \xi_0 p^{1/3}$, $z = \zeta p^{1/3}$, $s = \tau p^{1/3}$. The shape of the profile is then given by the solution $r(s)$, $z(s)$ of the problem [2]

$$\begin{aligned} r'' &= -z'(r^2 + c - z'/r), \quad z'' = r'(r^2 + c - z'/r), \\ r(0) &= r_0, \quad r'(0) = \cos \beta_0, \quad z(0) = 0, \quad z'(0) = \sin \beta_0. \end{aligned} \quad (1)$$

According to [2, 3], for any given parameter c a critical point in the solution of (1) is the first point $s = s^*$ at which either $d_0(s)$ or $\varphi_1(s)$ changes sign. Here

$$d_0(s) = \varphi_{01}(s) \int_0^s r(\varphi_{02} - \varphi_{03}) ds + [\varphi_{03}(s) - \varphi_{02}(s)] \int_0^s r\varphi_{01} ds,$$

and the functions $\varphi_{01}(s)$, $\varphi_{02}(s)$, $\varphi_{03}(s)$ and $\varphi_1(s)$ are the solutions of the following problems:

$$\begin{aligned} L\varphi_{01} &= 0, \quad \varphi_{01}(0) = 0, \quad \varphi'_{01}(0) = 1, \quad L\varphi_{02} = 0, \quad \varphi_{02}(0) = 1, \quad \varphi'_{02}(0) = 0, \\ L\varphi_{03} &= 1, \quad \varphi_{03}(0) = 1, \quad \varphi'_{03}(0) = 0, \quad L\varphi_1 - \varphi_1/r^2 = 0, \quad \varphi_1(0) = 0, \quad \varphi'_1(0) = 1. \\ L\varphi &\equiv \varphi'' + r'\varphi'/r + [2rz' + (r^2 + c - z'/r)^2 + (z'/r)^2]\varphi. \end{aligned}$$

Since $r(s_1) = r_0$ at the endpoint $s = s_1$ of the profile, in order to find the critical profile for given r_0 and β_0 it is necessary to choose c so that $r(s^*) = n_0$. A change in the sign of $d_0(s)$ or $\varphi_1(s)$ denotes a loss of stability with respect to axisymmetric or non-axisymmetric perturbations, respectively.

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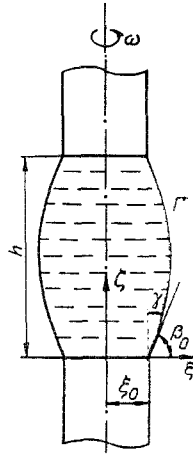


Fig. 1

TABLE 1

r_0	$\beta_0=75^\circ$			$\beta_0=80^\circ$		
	c_*	η_*	V_*	c_*	η_*	V_*
0,050	3,728	24,983	50,936	3,699	25,419	51,039
0,100	3,015	15,747	16,252	3,018	16,051	15,833
0,150	2,599	12,021	8,570	2,617	12,308	8,180
0,215	2,258	9,310	4,848	2,277	9,628	4,580
0,300	1,925	7,231	3,027	1,952	7,570	2,815
0,464	1,402	4,897	1,865	1,471	5,292	1,636
0,600	1,018	3,765	1,537	1,056	4,009	1,392
0,800	0,481	2,691	1,319	0,494	2,798	1,229
1,000	-0,069	1,991	1,228	-0,063	2,062	1,159
1,200	-0,644	1,548	1,174	-0,642	1,607	1,118
1,400	-1,264	1,247	1,138	-1,267	1,295	1,093
1,600	-1,941	1,031	1,113	-1,948	1,068	1,076
1,800	-2,683	0,871	1,095	-2,692	0,901	1,064
2,154	-4,167	0,672	1,073	-4,179	0,692	1,050
2,300	-4,842	0,611	1,067	-4,855	0,628	1,045
2,600	-6,359	0,511	1,056	-6,373	0,524	1,038
2,900	-8,046	0,435	1,048	-8,061	0,446	1,032
3,500	-11,942	0,329	1,037	-11,958	0,337	1,025
4,642	-21,302	0,216	1,025	-21,322	0,221	1,017
7,000	-48,827	0,118	1,015	-48,847	0,119	1,010

The mathematical formulation and a preliminary analysis of the problem are provided in [3], where a zero angle of growth is specifically considered. In that case, the only stable surfaces are circular cylinders $r(s) \equiv r_0$. It is shown in [4] that the cylindrical surface is stable as long as

$$\eta < 2\pi/(1 + 2r_0^3)^{1/2} \text{ for } r_0^3 \leq 1/6,$$

$$\eta < \pi/(2r_0^3)^{1/2} \text{ for } r_0^3 \geq 1/6$$

($\eta = h/\xi_0$, where h is the dimensional height of the zone). When these inequalities are violated stability is lost, with respect to axisymmetric perturbations in the first instance, and with respect to nonaxisymmetric ones in the second.

Let us now examine nonzero angles of growth. The boundary of the stability region of nonrotating ($r_0 = 0$) weightless axisymmetric equilibrium states is plotted and analyzed in [5]. It is shown there that convex (barrel-shaped) states with $0 < \beta_0 < \pi/2$ are stable, i.e., the line corresponding to these states with a given β_0 never intersects the boundary of the stability region. When $\eta \rightarrow \infty$, the relative volume $V \equiv v/(\pi\xi_0^2h)$ (where v is the dimensional volume of the liquid) also tends to infinity along such a line. The stability region plotted in the variables (η, V) is therefore unbounded. The deformation of the boundary of the stability region with rotation ($r_0 > 0$) is examined in [6]. Calculation of this boundary

for $r_0 = \sqrt[3]{0,1}$ and $r_0 = \sqrt[3]{0,5}$ shows that in this case the stability region is bounded and becomes smaller as r_0 increases. It is impossible, however, to determine from [6] the parameters of the critical states of a zone with a given $\beta_0 \neq \pi/2$ or for a particular $r_0 > 0$.

We solved this problem numerically by the foregoing method for $\beta_0 = 75$ and 80° and different values of r_0 . (The Weber number $We \equiv \rho\omega^2\xi_0^3/2\sigma$ often encountered in the literature is equal to r_0^3 .) We found that when $r_0 \geq 0.05$ the critical states are always barrel-shaped (and symmetric about the equatorial plane $\zeta = h/2$), and that stability is lost with respect to nonaxisymmetric perturbations whose component normal to the equilibrium surface is proportional to $\varphi_1(s)\cos\theta$.

The parameters $c = c_*$, $\eta = \eta_*$, $V = V_*$ which correspond to critical states are listed in Table 1 for $\beta_0 = 75, 80^\circ$ and different r_0 values. When $r_0 \rightarrow 0$, we have $\eta_* \rightarrow \infty$ and $V_* \rightarrow \infty$, in good agreement with [5]. The stable states are barrel-shaped, and in that case $c > c_*$, $\eta < \eta_*$, $V < V_*$.

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