ACCGE-17 ABSTRACT

Stability of Detached Solidification

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Abstract

Bridgman crystal growth can be conducted in the so-called "detached" solidification regime, where the growing crystal is detached from the crucible wall. A small gap between the growing crystal and the crucible wall, of the order of 100 micrometers or less, can be maintained during the process. A meniscus is formed at the bottom of the melt between the crystal and crucible wall. Under proper conditions, growth can proceed without collapsing the meniscus. The meniscus shape plays a key role in stabilizing the process. Thermal and other process parameters can also affect the geometrical steadystate stability conditions of solidification. The dynamic stability theory of the shaped crystal growth process has been developed by Tatarchenko [1]. It consists of finding a simplified autonomous set of differential equations for the radius, height, and possibly other process parameters. The problem then reduces to analyzing a system of first order linear differential equations for stability. Here we apply a modified version of this theory for a particular case of detached solidification. Approximate analytical formulas as well as accurate numerical values for the capillary stability coefficients are presented. They display an unexpected singularity as a function of pressure differential. A novel approach to study the thermal field effects on the crystal shape stability has been proposed. In essence, it rectifies the unphysical assumption of the model [1] that utilizes a perturbation of the crystal radius along the axis as being instantaneous. It consists of introducing time delay effects into the mathematical description and leads, in general, to stability over a broader parameter range. We believe that this novel treatment can be advantageously implemented in stability analyses of other crystal growth techniques such as Czochralski and float zone methods.

[1] V. A. Tatarchenko, *Shaped Crystal Growth*, Springer, 1993, pp. 19.

STABILITY OF DETACHED SOLIDIFICATION

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DETACHED BRIDGMAN GROWTH



SYSTEM RESPONSE TO PERTURBATIONS

Linear response of perturbed crystal radius and height

$$\delta \dot{R} = A_{RR} \delta R + A_{Rh} \delta h$$
$$\delta \dot{h} = A_{hR} \delta R + A_{hh} \delta h$$

Stable growth if

$$A_{RR} + A_{hh} < 0$$

 $A_{RR}A_{hh} - A_{Rh}A_{hR} > 0$



CAPILLARITY PROBLEM

Young-Laplace equation

$$\frac{z''}{\left(1+z'^2\right)^{3/2}} + \frac{z'}{r\left(1+z'^2\right)^{1/2}} = a - b z(r)$$
$$a = \frac{\Delta P_m r_c}{\gamma} \qquad b = \frac{\rho g_0 r_c^2}{\gamma} \qquad \Delta P_m = \left(P_{top} + \rho g\right) P_{tot}$$

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CAPILLARY COEFFICIENTS - THEORY

$$A_{RR} = -V \frac{\partial \beta}{\partial R}$$

$$A_{Rh} = -V \frac{\partial \beta}{\partial h}$$

$$\frac{\partial \beta}{\partial R} = \frac{\left(aR - \cos \alpha_{gr}\right) \sin \left(\alpha_{gr}\right)^2}{R \operatorname{s} \left(i\alpha_{gr}\right)^3 - 1b\left(5 - R\right)^2 \left(2 - 4 + R - 8\right)}$$

$$\frac{\partial \beta}{\partial h} = -\frac{r_c^2 \rho g}{2\gamma} \frac{\left(1 - R^2\right) \sin \alpha_{gr}^2}{R \, \mathrm{s} \, i \alpha_{gr}^3 - \hbar \left(-5 \, R\right)^2 \left(2 - 4 + R - 8\right)}$$



CAPILLARY COEFFICIENTS - NUMERICS





THERMAL RESPONSE - BASICS

Boundary condition at the interface

$$V_{C}L = k_{S} \frac{\partial T_{S}}{\partial z} - k_{L} \frac{\partial T_{L}}{\partial z}$$

Growth rate $V_C = V + \partial h / \partial t$

Height perturbation – Tatarchenko's model

$$\frac{\partial \delta h}{\partial t} = L^{-1} \left(k_{S} \frac{\partial G_{S}}{\partial h} - k_{L} \frac{\partial G_{L}}{\partial h} \right) \delta h + L^{-1} \left(k_{S} \frac{\partial G_{S}}{\partial R} - k_{L} \frac{\partial G_{L}}{\partial R} \right) \delta R$$
$$\delta G_{S} \neq \frac{\partial G_{S}}{\partial R} \delta R$$
questionable

ONE-DIMENSIONAL LUMP HEAT MODEL

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For melt

 $\frac{\partial^2 T_L}{\partial z^2} + \frac{V}{\kappa_L} \frac{\partial T_L}{\partial z} - \frac{\mu_L}{k_L} \frac{2}{r_C} \left(T_L - T_e\right) = 0$

For crystal

$$\frac{\partial^2 T_s}{\partial z^2} + \frac{V}{\kappa_s} \frac{\partial T_s}{\partial z} - \frac{\mu_s}{k_s} \frac{2}{R + \delta(z)} (T_s - T_e) = 0$$

$$A_{hh} = -L^{-1}k_L \frac{T_{hot} - T_0}{H^2} - L^{-1}k_S \frac{T_0 - T_{cold}}{l^2}$$

Perturbation of thermal gradient at the interface due to crystal radius variation (convolution): $\sqrt{2}$

$$\delta G_{S} = -\frac{2\mu_{S}\left(T_{0} - T_{cold}\right)V}{R^{2}k_{S}}\int_{0}^{t}\delta R(t')e^{-V(t-t')\sqrt{\left(\frac{V}{\kappa_{S}}\right) + \frac{8\mu_{S}}{k_{S}R}}}dt'$$



GENERALIZED RESPONSE

$$\delta \dot{h} = \int_{0}^{t} \delta R(t') G(t-t') d' + A_{hh} \delta h$$
$$\delta \dot{R} = A_{RR} \delta R + A_{Rh} \delta h$$

Laplace transform solution

$$h(s) = \frac{G(s)\delta R(0) + s(\delta h(0) - A_{RR})}{s^2 - s(A_{RR} + A_{hh}) + A_{RR}A_{hh} - A_{Rh}G(s)}$$
$$R(s) = \frac{\delta R(0)(s - A_{hh}) + A_{RR}\delta h(0)}{s^2 - s(A_{RR} + A_{hh}) + A_{RR}A_h} - \beta (s_R)A_h$$



GENERALIZED RESPONSE CONT.

Tatarchenko model gives

$$A_{hR} = -\frac{2V\mu_S\left(T_0 - T_e\right)}{LR^2s_0}$$

Our model

$$G(s) = \frac{A_{hR}s_0}{s+s_0} \qquad s_0 = V \sqrt{\left(\frac{V}{\kappa_s}\right)^2 + \frac{8\mu_s}{k_s H}}$$

Response for the induced perturbation can be studied by analyzing the roots of the following polynomial

$$s^{2}(s+s_{0}) - s(s+s_{0})(A_{RR} + A_{hh}) + A_{RR}A_{hh}(s+s_{0}) - A_{Rh}A_{hR}s_{0} = 0$$

MODIFIED STABILITY CRITERION

Conditions for stable growth

Our model

$$A_{RR}A_{hh} - A_{Rh}A_{hR} > 0$$

 $A_{RR} + A_{hh} < S_0$

 $A_{RR}A_{hh} - S_0(A_{RR} + A_{hh}) > 0$

Tatarchenko model

$$A_{RR}A_{hh} - A_{Rh}A_{hR} > 0$$

$$A_{RR} + A_{hh} < 0$$



MODEL APPROXIMATIONS

- Environmental temperature is constant
- One-dimensional lump type approximation
- Capillarity zero order model no meniscus motion effects, no triple point effects



CONCLUSION

- × Capillarity coefficients display singularity
- * Thermal response for the radius perturbation is of the convolution type – this modified model is applicable for other types of shaped crystal growth: Czochralski, Float Zone, etc.

