William E. Langlois
Ki-Jun Lee

Digital Simulation of Magnetic Czochralski Flow Under Various Laboratory Conditions for Silicon Growth

Previous digital simulations have suggested that an axial magnetic field in the 0.1-T (1000-Gs) range can effectively suppress convection in Czochralski growth of silicon. The present paper treats the matter more quantitatively by investigating the convection in a variety of flow conditions corresponding to typical Czochralski growth of silicon on a laboratory scale.

Introduction

An external magnetic field dampens melt convection during Czochralski growth of silicon crystals, thereby hindering and controlling the erosion of the silicon dioxide crucible by the flowing melt. Usually the crucible and crystal are rotated coaxially but in opposite directions (counter-rotation) to smooth out thermal asymmetries, to control melt flow against the crucible, and to control the shear rate at the growth interface. A certain amount of dissolved oxygen in the melt is desirable, and this is regulated by controlled erosion from the silica crucible. Magnetic damping of flow is one important way of facilitating the growth of silicon crystals with controlled oxygen content. Various configurations have been tried, but one which has been simulated with existing digital codes [1] is the application of an axial magnetic field, as described by Kim, Schwuttke, and Smetana [2]. The present paper describes simulations of Czochralski flow using four different strengths for the applied axial field, viz., 0, 0.05, 0.1, and 0.2 tesla (T) [0, 500, 1000, and 2000 gauss (Gs)]. Flows with counter-rotation are examined, as well as those in which neither crystal nor crucible rotates. Also, two distinct values for the buoyancy parameter are used, since available density data for molten silicon are so scattered that the appropriate value of the volumetric expansion coefficient is rather in doubt. Other problem parameters are fixed at values appropriate to silicon growth on a laboratory scale, as suggested to us by K. M. Kim. These are listed in Table 1.

Table 1 Silicon growth parameters.

Melt density: 2.33 gm/cm^3
Specific heat: 975 J/kg-K (0.233 cal/gm-K)
Thermal diffusivity: 0.125 cm^2/s
Viscosity: 7 × 10^{-4} Pa-s (0.7 centipoise)
Thermocapillarity coefficient: 14.9 cm/s-K
Emissivity: 0.318
Crucible radius: 7.62 cm
Crystal radius: 4.125 cm
Melt depth: 5.0 cm
Crystal temperature: 1685 K
Crucible temperature: 1773 K at the wall, decreasing linearly with radius to 1723 K at the center of the bottom
Electrical conductivity: 1.25 × 10^4 (Ω-cm)$^{-1}$
Magnetic permeability: 1.0

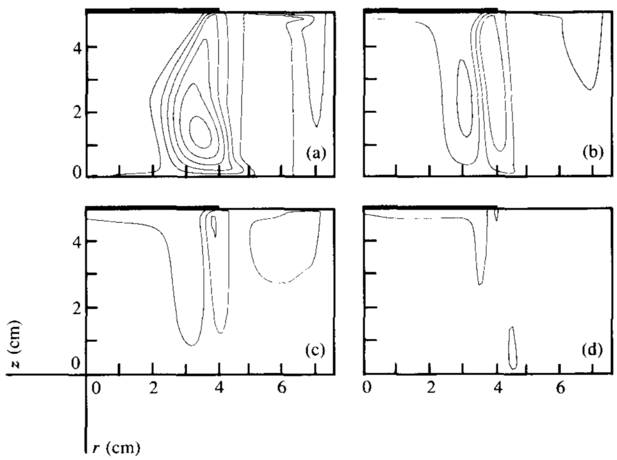

Figure 1 Meridional circulation patterns for the simulations of low-buoyancy flows with counter-rotation: a) $B = 0$; b) $B = 0.05$; c) $B = 0.1$; and d) $B = 0.2$ T. The contour spacing = 0.5 cm^3/s. The shaded bars above the figure represent the solid boundary formed by the growing interface.

Low-buoyancy simulations with counter-rotation

With a volumetric expansion coefficient of 1.41×10^{-5} K^{-1}, a crucible rotation rate of 1.57 radians/s and a crystal rotation rate of −2.31 radians/s, we obtained the meridional circulation patterns shown in Fig. 1. In all four parts of this

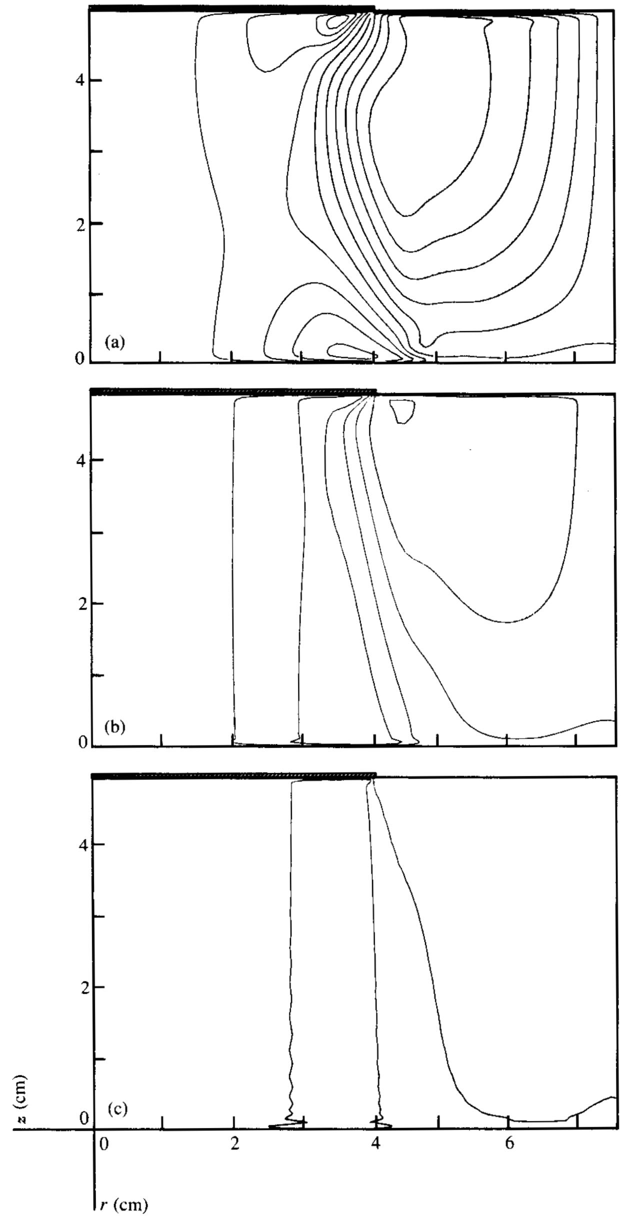

Figure 2 Current patterns for the simulation of low-buoyancy flows with counter-rotation: a) $B = 0.05$; b) $B = 0.1$; and c) $B = 0.2$ T. Contour spacing = 0.2 cm^3/s. Shaded bars as in Fig. 1.

figure, and in all our other streamline plots, the contour spacing is 0.5 cm^3/s. The shaded bars at the top of the figure represent the solid boundary formed by the growing interface. Figure 1 suggests that an applied field of 0.1 T (1000 Gs) substantially reduces the meridional circulation, and increasing the field to 0.2 T (2000 Gs) produces little added benefit.

The current patterns for the three simulations with magnetic fields are shown in Fig. 2. The meridional components

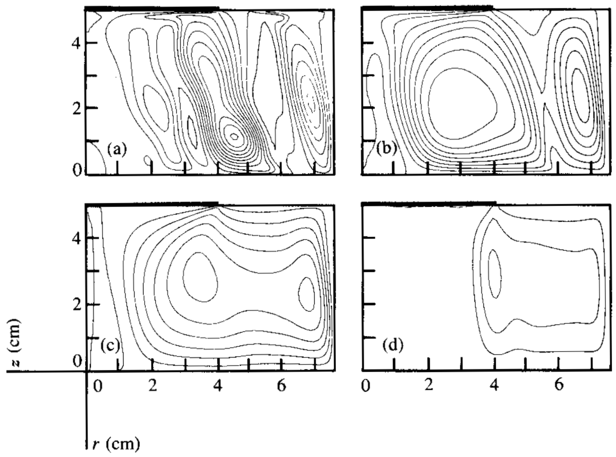

Figure 3 Meridional circulation patterns for the simulations of high-buoyancy flows with counter-rotation: a) $B = 0$; b) $B = 0.05$; c) $B = 0.1$; and d) $B = 0.2$ T. Contour spacing = 0.5 cm^3/s.

of induced current density are defined in terms of the current function ψ_J according to

$$j_r = \frac{\sigma B}{r}\left(\frac{\partial \psi_J}{\partial z}\right), \qquad j_z = -\frac{\sigma B}{r}\left(\frac{\partial \psi_J}{\partial r}\right),$$

where B is the applied field and σ is the electrical conductivity. The induced current arises from the interaction of the applied magnetic field with the fluid motion. In the case of the meridional components, the source is the azimuthal flow. For purposes of the numerical simulation, this is best expressed in terms of the angular momentum per unit mass, usually called the swirl, since this is a physically conserved quantity. It is most often denoted by Ω and is defined by $\Omega = rv$, where v is the azimuthal velocity. Specifically, the current function is determined from

$$\frac{\partial}{\partial r}\left(\frac{1}{r}\frac{\partial \psi_J}{\partial r}\right) + \frac{1}{r}\left(\frac{\partial^2 \psi_J}{\partial z^2}\right) = \frac{1}{r}\left(\frac{\partial \Omega}{\partial z}\right),$$

subject to the boundary condition that ψ_J vanishes on the periphery of the computational domain. All current plots in this paper exhibit isolines of ψ_J, with a contour spacing of 0.2 cm^3/s.

High-buoyancy simulations with counter-rotation

Increasing the volumetric expansion coefficient by a factor of ten leads to the more intense circulation patterns shown in Fig. 3. Applying an 0.1-T (1000-Gs) axial field again yields a relatively quiescent flow, but now increasing the field to 0.2 T (2000 Gs) leads to additional improvement. Current patterns for these cases are shown in Fig. 4.

Low-buoyancy simulations without rotation

When neither the crystal nor crucible rotates, the flow is due entirely to thermal and thermocapillary convection. With the

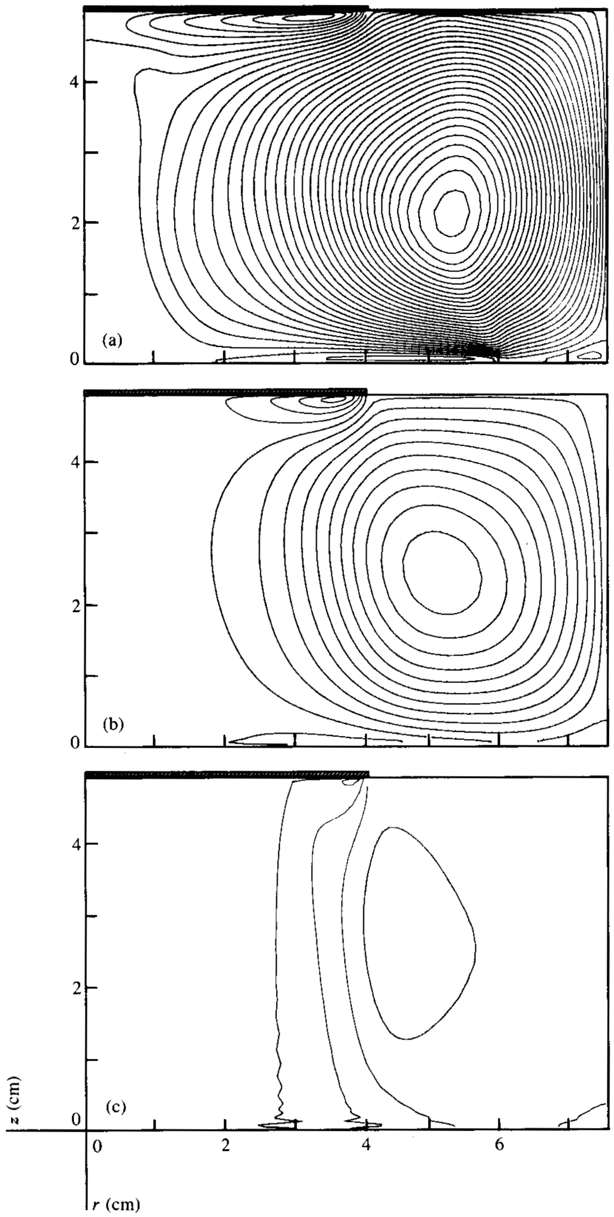

Figure 4 Current patterns for the simulations of high-buoyancy flows with counter-rotation: a) $B = 0.05$; b) $B = 0.1$; and c) $B = 0.2$ T. Contour spacing = 0.2 cm^3/s.

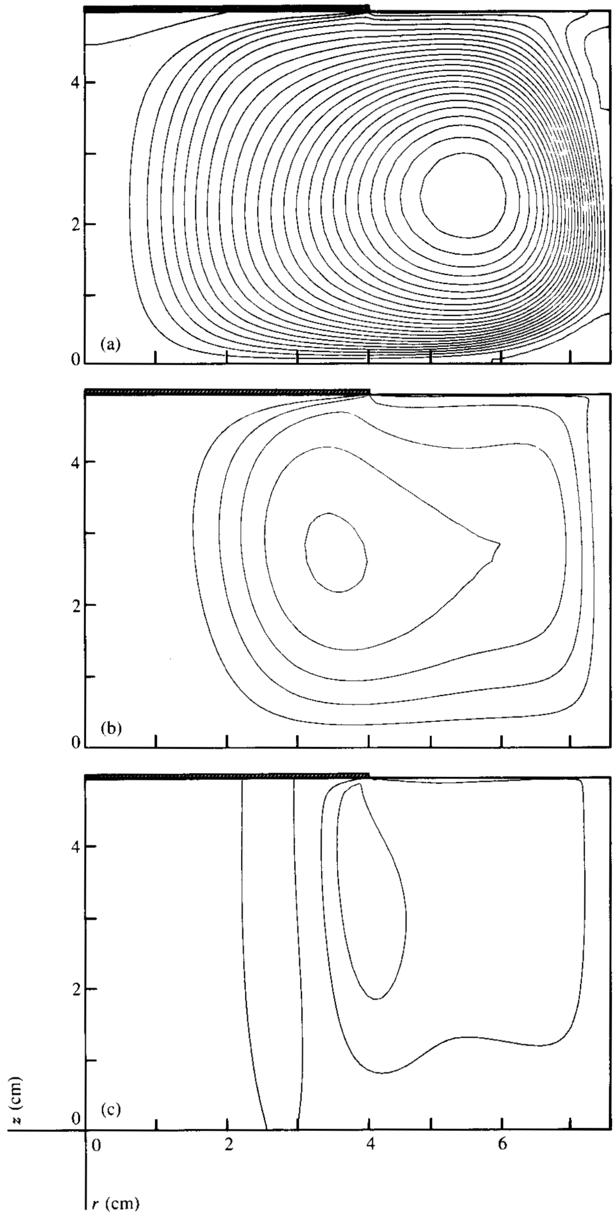

Figure 5 Meridional circulation patterns for the simulations of low-buoyancy flows without rotation: a) $B = 0$; b) $B = 0.05$; and c) $B = 0.1$ T. Contour spacing = 0.5 cm^3/s.

volumetric expansion coefficient set to 1.41×10^{-5} K^{-1}, the flow patterns of Fig. 5 were obtained. Since the 0.1-T (1000-Gs) field effectively shuts off convection except for a small, weak eddy near the edge of the crystal, the result for 0.2 T (2000 Gs) is not plotted.

Since there is no swirl, ψ_J vanishes everywhere; i.e., the induced current is purely azimuthal.

High-buoyancy simulations without rotation

With the volumetric expansion coefficient increased to 1.41 $\times$ 10^{-4} K^{-1}, intense flow fields again result. Figure 6 shows that, as in the case for high-buoyancy flows with counter-rotation, a 0.1-T (1000-Gs) field reduces the circulation considerably, but a 0.2-T (2000-Gs) field yields additional improvement.

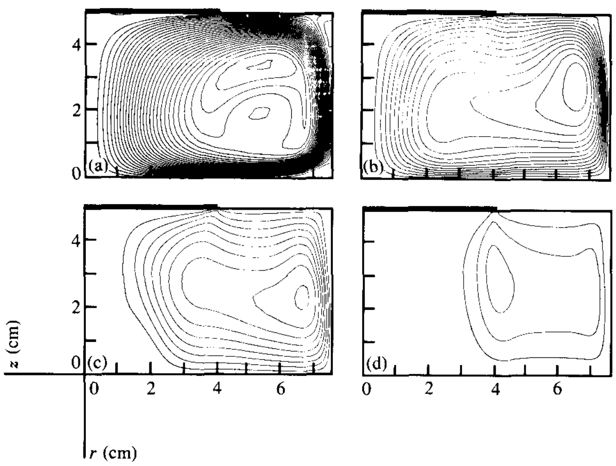

Figure 6 Meridional circulation patterns for the simulations of high-buoyancy flows without rotation: a) $B = 0$; b) $B = 0.05$; c) $B = 0.1$; and d) $B = 0.2$ T. Contour spacing = 0.5 cm^3/s.

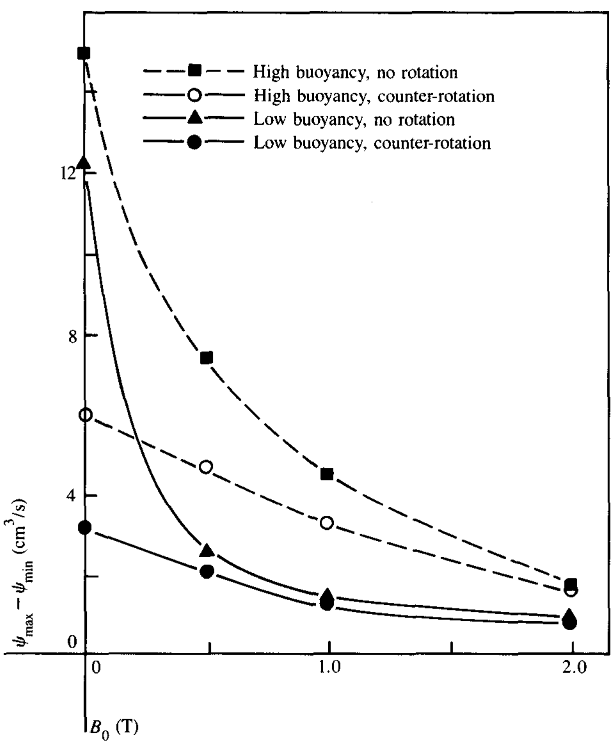

Figure 7 Effect of magnetic field intensity on the strength of the meridional circulation.

Summary

The volume of melt which circulates in the meridional flow is proportional to the difference between the maximum and the minimum of the Stokes stream function, which therefore provides a scalar measure of the convection strength. In Fig. 7, this quantity is plotted versus the magnetic field intensity for each of the sixteen simulations just discussed. It illustrates that, whether or not counter-rotation is used, there is little advantage in strengthening the field beyond 0.1 T (1000 Gs) if the low value of the buoyancy coefficient is correct. On the other hand, if the high value is more appropriate, increasing the field to 0.2 T (2000 Gs) gives a substantial further decrease in convection. The slopes of the two corresponding curves suggest that still more improvement could be obtained by passing to even higher field intensities.

References

1. W. E. Langlois and J. S. Walker, "Czochralski Crystal Growth in an Axial Magnetic Field," *Proceedings of the 2nd International Conference on Boundary and Interior Layers—Computational and Asymptotic Methods,* Trinity College, Dublin, June 16–18, 1982, Boole Press, Dublin, pp. 299–304.
2. K. M. Kim, G. H. Schwuttke, and P. Smetana, "Apparatus for Czochralski Silicon Crystal Growth through Axial Magnetic Field Fluid Flow Damping," *IBM Tech. Disclosure Bull.* **24,** 3376–3377 (1981).

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William E. Langlois *IBM Research Division, 5600 Cottle Road, San Jose, California 95193.* Dr. Langlois joined the San Jose research laboratory in 1959. His work has been in the area of computational fluid dynamics. Currently he is with the dynamic system modeling group and involved in the simulation of the fluid flow in the Czochralski crystal-pulling process. Dr. Langlois received an Sc.B. in physics from Notre Dame University, Indiana, in 1953 and a Ph.D. in applied mathematics from Brown University, Providence, Rhode Island, in 1957. Prior to joining IBM, he did research in non-Newtonian hydrodynamics for E. I. Du Pont de Nemours & Co. laboratories from 1956 to 1959.

Ki-Jun Lee *IBM Research Division, 5600 Cottle Road, San Jose, California 95193.* As a visiting scientist from Seoul National University, Dr. Lee has been involved in collaborative efforts with physical science at the research laboratory since early 1982. His research interests are in the area of theoretical studies on slow viscous flow systems, which he is pursuing with the dynamic system modeling group. In Korea, Dr. Lee is a Professor of Chemical Engineering. He received his B.S. in 1961 and his M.S. in 1964 from Seoul National University and his Ph.D. in 1972 from the University of Washington, all of these degrees in chemical engineering. Dr. Lee is a member of the American Institute of Chemical Engineers and the Korean Institute of Chemical Engineers.