

Thermal Modeling of Crystal Growth by the Czochralski Method Including Radius Control

Amit Kumar, Jyotirmay Banerjee and K Muralidhar*

Department of Mechanical Engineering, Indian Institute of Technology, Kanpur 208 016

Received: 17 December 2001; accepted: 02 May 2002

Analysis of thermal phenomena in the crystal grown by the Czochralski process has been addressed. The model has been employed for deriving conditions under which the crystal radius during growth can be kept a constant. Two parameters that influence the size of the crystal are the pull velocity and the base temperature of the crucible. The present work explores the sensitivity of the crystal radius to these parameters. The mathematical model is based on one dimensional unsteady heat conduction in the solid phase with radiation to the enclosure. The model can predict the time-wise variation of the pull velocity and the base temperature so that the radius of the crystal can be maintained constant to within a prescribed tolerance. Materials considered for analysis are silicon and Nd:YAG. The analysis can account for variation in transport properties with temperature and differences in properties between the liquid melt and the crystalline solid. Results derived in the present work show that the crystal radius exhibits greater sensitivity to the pull velocity as compared to the crucible base temperature.

1 Introduction

Crystals with a high degree of perfection are required in several sensitive applications. Examples are the semiconductor industry for making computer chips and optically transparent materials that are needed for making high power lasers. Manufacturing methods for high quality crystals, include chemical vapour deposition (CVD) and the Czochralski (Cz) technique. CVD involves growing crystals from the gaseous phase while the Cz process is a popular known method of growing a single crystal from its melt. In both approaches the crystal growing process is determined by principles of physico-chemical hydrodynamics and is extraordinarily complex. To control the process and ensure growth of large high quality crystals, it is important to understand the physical phenomena involved during crystal growth. These include all modes of heat transfer, phase change, interfacial transport, turbulence, and the influence of complex geometries.

The Czochralski technique is an important method for the bulk growth of semiconductor and oxide crystals. The technology is currently in use in major research institutions across the country. It

comprises a crucible containing the molten material, into which a seed is introduced. The crystalline material solidifies onto the seed; to maintain a steady rate of growth the seed is pulled away from the crucible with a certain velocity. Simultaneously the crucible carrying the charge is thermally controlled to account for heat losses to the environment. Details of this technology are available in literature^{1,2}. A schematic drawing of the Czochralski growth apparatus is shown in Figure 1.

The temperature gradients during crystal growth are large, and temperature distribution in the crystal is a major factor in determining the crystal quality and cross-sectional area. Adverse thermal gradients may result in a large variation in the crystal size and excessive thermal stresses. Alternatively the pull velocity mismatched with the rate of solidification of the crystal can result in bulging or thinning. These factors encourage the growth of dislocations and, in effect, degrade the crystal structure of the growing ingot³. In addition, variations in the crystal area during growth also represent a waste, since sections of uniform cross-section alone are of practical use. Thus, heat transfer, from and to the crystal, plays an important role during the crystal growth process⁴. A control of thermal parameters greatly influences the overall process performance.

* Author for correspondence

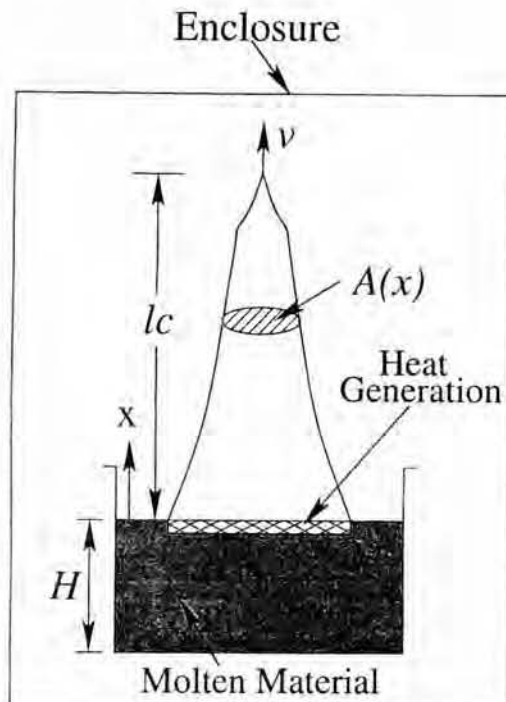


Figure 1 — Schematic drawing of the Czochralski crystal growth method; lc : length of crystal grown, $A(x)$: cross-sectional area of the crystal, v : pull velocity, H : melt height

The present work describes a mathematical model for the calculation of the temperature profile in the crystal during its growth from the molten phase. The model is in the form of an algorithm that includes the simultaneous evaluation and control of the incipient crystal radius at the solid-melt interface. The control action is provided by adjusting the pull velocity and the crucible base temperature. Additional details such as, heat transfer to a non-isothermal enclosure and changes in the melt level in the crucible are included in the model. Results in the form of temperature profiles in the crystal, and the variation in the pull velocity and the base temperature required to maintain a constant radius have been reported. Crystal materials analyzed include silicon and Nd:YAG. Billig⁵ has derived an approximate relationship between crystal radius and pull rate by solving the one-dimensional approximation for heat transfer in the crystal. Based on the analysis the author postulated that the radius of a steadily growing crystal should be inversely proportional to the square of the steady state growth rate of crystal. The present study can be viewed as a significantly improved thermal analysis of the crystal growth process with control.

2 Mathematical Formulation

The present investigation aims to develop a mathematical model that correlates the crystal cross-sectional area with the pull velocity, thermal conditions in the melt and the temperature distribution in the solid material. For this purpose the crystal grown by the Czochralski process (Figure 1) is modeled as an unsteady, radiating, variable area fin of finite length, located within an enclosure. Utilization of this formulation may allow the prediction of the following:

- (i) Temperature distribution in the crystal grown as a function of time;
- (ii) Area distribution $A(x)$ at various instants of time;
- (iii) Crucible base temperature as a function of time needed to maintain the crystal area constant; and
- (iv) The time-dependent pull velocity needed to maintain the cross-sectional uniformity.

The following assumptions help in developing the mathematical model. The melt is considered to be incompressible. The physical properties of the melt can vary with the temperature. For definiteness, they have been evaluated in the numerical results at the melting point temperature. Heat transfer within the grown crystal is considered to be dominated by conduction, while radiation is the dominant mode at its surface. The pulling of the crystal from the melt is taken to be a continuous process. The crystal-to-enclosure thermal radiation is taken to occur between optically gray surfaces. Temperature variation in the growing crystal, as well as that over the enclosure length, have been included in the formulation. The geometric shape factors between any point on the crystal with respect to any other at the enclosure have been fully accounted for. The melt-crystal interface is assumed to be planar. The temperature at the interface is the freezing point for silicon, and the eutectic temperature for Nd : YAG. The latent heat per unit volume is thus generated entirely at the interface. The temperature gradient inside the crucible is prescribed to be linear, though time-dependent. This approximation neglects fluid motion in the melt, and is expected to be valid when the material thermal conductivities are quite large.

The differential equation governing the temperature distribution, $T(x,t)$ in the solid fin is

based on the conservation of energy principle and is given by⁶:

$$mC_p \frac{\partial T_s(x,t)}{\partial t} = \frac{\partial}{\partial x} \left[k_s(T_s) A(x) \frac{\partial T_s(x,t)}{\partial x} \right] - h_r P(x) (T_s - T_\infty), \quad \dots (1)$$

The notation used in Eq. (1) is explained in the nomenclature. Correspondingly the first term represents energy storage, the second term is the net energy transferred by diffusion and the third term is the radiative loss to the enclosure. Here, h_r is the radiative heat transfer coefficient between the crystal surface and the enclosure, at any given point on the crystal and is evaluated as⁷:

$$h_r = \sigma \epsilon F_{12} (T_s^2 + T_\infty^2) / (T_s + T_\infty).$$

Equation (1) can be solved by subjecting to suitable initial and boundary conditions of the form:

$$t=0, \quad T_s(x, 0) = \text{function of } x,$$

$$x=0, \quad T_s(0, t) = T_0,$$

$$x=lc,$$

$$\frac{\partial T_s}{\partial x} = 0.$$

In most calculations the initial temperature has been taken to be the freezing point temperature T_0 . With these conditions, Eq. (1) can be solved for the temperature distribution in the fin. The cross-sectional area $A(0)$ formed over an incremental time period at the base of the crystal can be obtained using the integrated form of Eq. (1), viz:

$$k_s(T_s) A_s(x) \frac{\partial T_s(x,t)}{\partial x} \Big|_{x=0} = \int_0^{lc} \sigma \epsilon P_s(x) (T_s^{n+1} - T_\infty^n) dx$$

$$- \int_0^{lc} m C_p \frac{T_s^{n+1} - T_s^n}{\Delta t} dx, \quad \dots (2)$$

where lc is the instantaneous length of the crystal at a time t . Equation (2) can be simplified by enforcing the condition of latent heat release⁶, viz.

$$-k_l(T_l) A_l(0) \frac{\partial T_l(x,t)}{\partial x} \Big|_{x=0} + k_s(T_s) A_s(x) \frac{\partial T_s(x,t)}{\partial x} \Big|_{x=0} = -\rho L v A_s(0), \quad \dots (3)$$

where suffixes l and s stand for the liquid and the solid phases, respectively.

When a chamber enclosing the crystal is included in the analysis, it is necessary to find the analytical expression for the diffuse view factor F_{12} between the crystal and the enclosure. In the absence of an enclosure the ambient is the equivalent enclosure at a fixed temperature T_∞ . The shape factor F_{12} is then unity.

When the enclosure is present the view factor can be found by considering first a pair of annular rings of equal height δ and a spacing W , as shown schematically in Figure 2. Consider first the shell-to-tube view factor for the configuration in Figure 2. The derivation of the view factor starts with fundamental expression⁷:

$$F_{12} = \frac{1}{2\pi R_0 \delta} \int_0^{2\pi} \int_0^\delta \int_{-\pi}^\pi \int_0^\delta \frac{B}{[(W - x_1 + x_2)^2 + a]^2} dx_2 d\theta dx_1 d\phi, \quad \dots (4)$$

where

$$a = R_0^2 + R_i^2 - 2R_0 R_i \cos \theta,$$

$$B = \frac{R_0 R_i}{\pi(R_0 - R_i)^2}$$

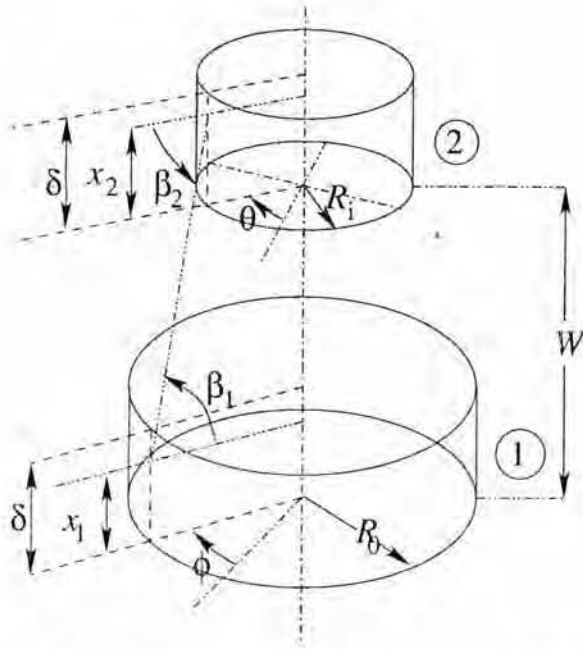


Figure 2—Coordinate system for the shell (1) to tube (2) view factor; δ : elemental ring thickness, W : separation distance between elemental rings, R_i : radius of tube (crystal), R_o : radius of shell (enclosure), φ and θ are azimuthal angles in 1 and 2, x_1 , x_2 , β_1 , and β_2 are local coordinates in the shell and tube elements

$$\left[R_o^2 + R_i^2 - R_o R_i (1 + \cos \theta) - 2R_i^2 \sin^2 \frac{\theta}{2} \right] \times$$

$$\left[R_o^2 + R_i^2 - R_o R_i (1 + \cos \theta) - 2R_o^2 \sin^2 \frac{\theta}{2} \right],$$

and

$$c = \cos^{-1} \left(\frac{R_i}{R_o} \right).$$

The quantities appearing in Eq. (4) are defined in Figure 2. Equation (4) assumes that the elements have equal thickness δ and the separation distance W is an integral multiple of δ . Equation (4) can be integrated three times analytically to yield⁸:

$$F_{12} = \frac{1}{R_o \delta} \int_0^c \frac{B}{a^{3/2}}$$

$$\begin{aligned} & (W - \delta) \tan^{-1} \frac{W - \delta}{a^{1/2}} + (W + \delta) \\ & \left[(W - \delta) \tan^{-1} \frac{W - \delta}{a^{1/2}} + (W + \delta) \tan^{-1} \frac{W + \delta}{a^{1/2}} - 2W \tan^{-1} \frac{W}{a^{1/2}} \right] d\theta. \end{aligned} \quad \dots (5)$$

The single integral can be numerically evaluated, e.g., by Simpson's rule to find the desired view factor. In order to find the view factor from the tube to the shell, one can use shape factor algebra to yield:

$$F_{12} A_1 = F_{21} A_2,$$

and therefore,

$$F_{21} = \frac{1}{R_i \delta} \int_0^c \frac{B}{a^{3/2}}$$

$$\begin{aligned} & \left[(W - \delta) \tan^{-1} \frac{W - \delta}{a^{1/2}} + (W + \delta) \tan^{-1} \frac{W + \delta}{a^{1/2}} - 2W \tan^{-1} \frac{W}{a^{1/2}} \right] d\theta. \end{aligned} \quad \dots (6)$$

The effective emissivity for a pair of two large gray concentric cylinders is given by⁷:

$$\frac{1}{\epsilon'(\text{effective})} = \frac{1}{\epsilon(\text{crystal})} + \frac{R_i}{R_o} \left[\frac{1}{\epsilon_{\text{encl}}} - 1 \right].$$

In the present study the enclosure surface has been taken to be black ($\epsilon_{\text{encl}} = 1$) and so the effective emissivity is that of the crystal surface itself.

3 Method of Solution

Equations (1-3) have been numerically solved by an implicit second order finite difference method⁹. Equation (1) is nonlinear, owing to the dependence of the material properties on the temperature distribution. This makes the computational algorithm iterative, wherein the properties are repeatedly improved using the temperature values of the previous iteration. A modular approach has been used for the calculations of the temperature profile in the crystal and crystal area at interface at any instant of time. After every time step the length of the crystal, increases by an amount equal to the nodal spacing of

the finite difference grid. Hence the number of grid points also increases with time. The crystal interface area calculated from Eq. (2 and 3) is supplied to the new grids formed and temperature distribution for the next time step is calculated from Eq. (1). The algorithm for the overall simulation proceeds as follows.

- (i) Specify all parameters of the process, including the geometric dimensions, material properties, surface properties, and the initial and boundary temperatures.
- (ii) Find the shape factor F_{ij} using Eq. (6), where F_{ij} indicates the shape factor for the i th elemental ring on the crystal to the j th elemental ring on the enclosure.
- (iii) Calculate the radiative heat transfer coefficient for each ring on the crystal as per:

$$hr(i) = \frac{\sum_{j=1}^{n(m)} \sigma \epsilon F_{ij} (T_i^4 - T_{encl}^4) A_i}{A_i (T_i - T_{amb})},$$

where summation is to be carried out over all the j elemental rings of the enclosure, and

$$A_i = 2 \pi R_i \delta,$$

for each elemental ring i on the crystal.

- (iv) Compute the temperature profile along the crystal at the next time level, using the discretized form of Eq. (1).
- (v) Calculate the cross-sectional area of the crystal at the interface using Eq. (2 and 3).
- (v) If the calculated area is different from the desired area, adjust the velocity suitably and repeat the calculation. When the crystal area is controlled by varying the base temperature, Eq. (3) is used to calculate the temperature gradient in the melt for a given crystal area. The base temperature needed to produce the desired area is then calculated as:

$$T_{base} = T_0 - \frac{\partial T_i}{\partial x} H,$$

where H is the height of the crucible.

- (vii) Once the computed area at the interface is sufficiently close to the desired value, it is assigned to the newly formed grid.
- (viii) The temperature at the newly formed grid point is assigned the freezing point of the material. That of the previously formed grid is determined by using the condition that energy balance with respect to the latent heat release, energy storage, and that conducted into the crystal is maintained at every time instant.
- (ix) *Treatment of melt surface velocity* — In a batch process the melt level decreases as the solid crystal is formed. This can be accounted for by computing a melt velocity based on the conservation of mass principle. When the material in the crucible is continuously fed the melt level is a constant and the melt surface velocity is zero.
- (x) For the new time step the shape factor for the newly solidified crystal of thickness Δx ($=\delta$) is to be calculated with respect to all the elemental rings of the enclosure.
- (xi) The above steps are repeated till a crystal of a prescribed length is grown, or the melt in the crucible is fully exhausted.

3.1 Material Properties

A summary of the material properties employed in the present simulation is given in Table 1.

3.2 Parallel Computing

Calculations arising from the numerical algorithm, referred above, become computationally intensive, even when crystals of modest size are considered. To circumvent the difficulty the computer code was parallelized, to run on a system of 9 PCs. The PCs used were P-III, 600 MHz, 512 MB RAM. The ANULIB software¹⁰ was used to send and receive data between the processors. The parallelization steps employed were the following:

- (i) Send the required parameters for the calculation of the shape factor and the radiative heat transfer coefficient to all the slave processors.
- (ii) Partition the crystal into elemental rings and send the individual sets to all the slave

Table 1-Thermophysical properties of silicon and Nd:YAG.
Suffixes *s* and *l* refer to the solid and the liquid phases,
respectively

	Nd:YAG	Silicon
ρ_s , kg/m ³	4560.0	2300.0
ρ_l , kg/m ³	3620.0	2420.0
k_s , W/m-K	13.0	22.0
k_l , W/m-K	12.0	64.0
C_p , J/Kg-K	590.0	1000.0
Melting point, K	2243.0	1683.0
L , J/kg	9.18×10^5	18.0×10^5
ϵ	0.3	0.64

The geometric parameters used in the present simulation are listed below:

Initial seed length, m	= 0.03
	= 50
Crucible base area, cm ²	= 300
Crucible height, m	= 0.183
Enclosure area, cm ²	= 3000
Enclosure height, m	= 0.75
Emissivity of enclosure	= 1.0

processors. Partition the enclosure as well into elemental rings and distribute among the slave processors.

- (iii) Calculate the shape factor for each of the rings of a particular set on each slave processor.
- (iv) Communicate all the shape factors to the master processor.
- (v) Calculate the heat transfer coefficient at the ring locations in the master processor.
- (vi) Calculate the temperature distribution at the next time step in the master processor. This is followed by the calculation of the area of the newly grown crystal.
- (vii) The above procedure is to be repeated when the crystal area is controlled by the pull velocity; otherwise the integration is advanced to the next time level.

With these alterations, a practically linear speed up, namely a reduction in CPU time by a factor of 9

on 9 (1 master and 8 slave) processors, was evident. A typical simulation run took 15 min of CPU time on 9 PCs, while the time on a single PC was around 120 min.

4 Result and Discussion

Numerical results have been presented below for the temperature profiles in the crystal, and the crystal base radius as a function of time when the growth is uncontrolled. When the radius is controlled to a tolerance of 0.1 per cent, the control parameters namely, the pull velocity and the crucible base temperature, respectively, change with time. These results have also been reported in the present study. In addition the role of the presence of the enclosure, and the replenishment of the melt during the growth process have been discussed.

Temperature profiles in the crystal for controlled as well as uncontrolled conditions are shown in Figure 3 and 4, for silicon and Nd : YAG, respectively. Figure 5 and 6 are a companion plot for the variation of crystal radius at the base, as a function of time, when the process is uncontrolled. For a pull velocity of 1 m/d, the crystal bulges with time. When the pull velocity increases to 2 m/d, there is a better match with the solidification speed and the crystal size shows a smaller variation with time. In view of the differences in the thermal properties the growth of Nd : YAG is faster than silicon. The major parameters which affect the crystal radius are crucible size, volume of the melt, enclosure, base temperature of the crucible and the pull velocity. The decrease in level of melt has several interesting effects. Most importantly the relative pull velocity of the crystal with respect to the melt surface increases. Hence the crystal grown in batch production is of smaller radius as compared to that with continuous melt replenishment. There are secondary influences as well. As the melt level drops, radiative heat transfer from the crucible directly to the growing crystal affects growth. Secondly the amount of heat transfer to the melt from the crucible sides decreases because of the reduction in the contact area with the wall. Figure 5 and 6 also show that the presence of the enclosure near a crystal, increases the radiative heat loss from the crystal surface in comparison to one grown in an open ambient. Hence, for a given set of parameters, the crystal size with the enclosure will be smaller, as compared to one grown in the ambient. Simultaneously, the temperature levels along the crystal are smaller when compared to those without

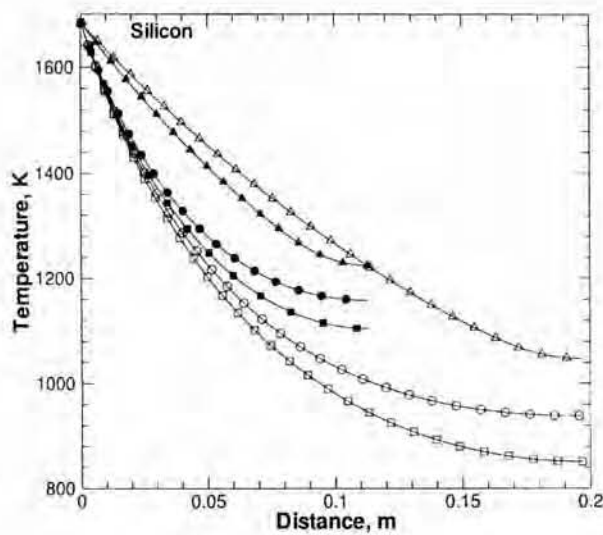


Figure 3 — Variation of temperature along the crystal length. Enclosure considered with continuous melt replenishment: Δ : No control, $\square$: Base temperature control, $\circ$: Pull velocity control. Shaded symbols show data after 2h, unshaded symbols after 4 h

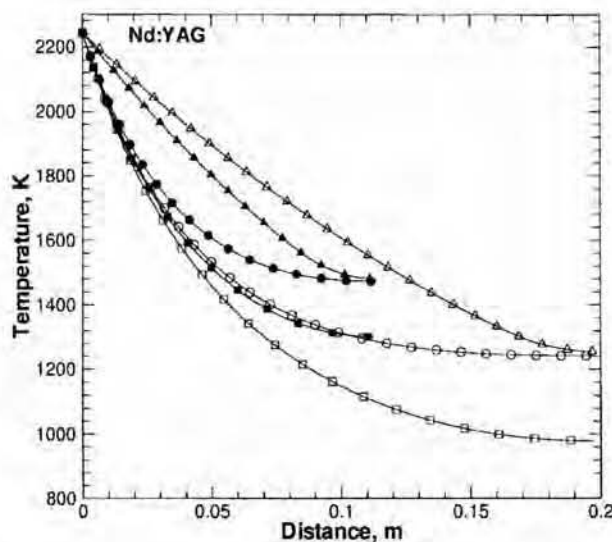


Figure 4 — Variation of temperature along the crystal length. Enclosure considered with continuous melt replenishment; Δ : No control, $\square$: Base temperature control, $\circ$: Pull velocity control. Shaded symbols show data after 2 h, unshaded symbols after 4 h

the enclosure. Lower temperatures are indicative of higher gradients at the crystal base, but lower gradients elsewhere in the crystal. This result shows that temperature uniformity will lower thermal stresses when the crystal is grown within an enclosure.

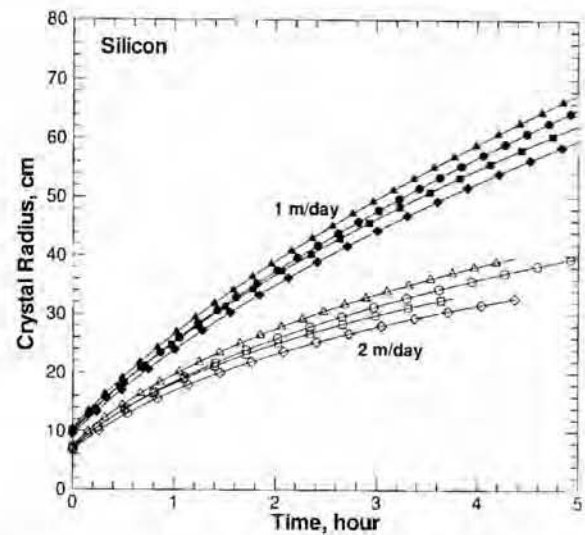


Figure 5 — Variation of crystal radius with time; $\square$: With enclosure and batch production, Δ : With enclosure and continuous melt replenishment, $\diamond$: Without enclosure and batch production, $\circ$: Without enclosure and continuous melt replenishment, shaded symbols: 1 m/d, unshaded symbols: 2 m/d

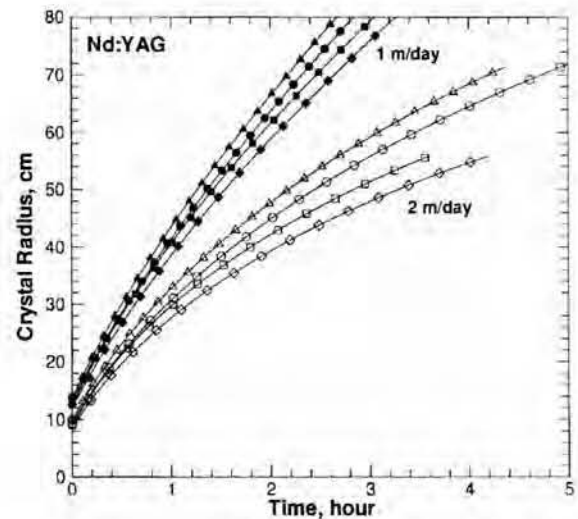


Figure 6 — Variation of crystal radius with time; $\square$: With enclosure and batch production, Δ : With enclosure and continuous melt replenishment, $\diamond$: Without enclosure and batch production, $\circ$: Without enclosure and continuous melt replenishment, shaded symbols: 1 m/d, unshaded symbols: 2 m/d

Crystal growth in the presence of size control is discussed subsequently. The time-variation of the crucible base temperature, required to maintain constant crystal radius at pull velocities of 1 and 2 m/d are depicted in Figure 7 and 8. Initially the base temperature needs to be raised to compensate for a

large heat transfer from the crystal surface, which is initially at the freezing point of the material. After the passage of time, thermal gradients stabilize within the crystal and the losses increase only in response to the additional increment in the crystal length. Thus the temperature distribution does not depend on the crystal length. For germanium, this length has been estimated from preliminary analysis to be $6\sqrt{a}$, m , where a in meters is the crystal radius¹⁰. Therefore, after the passage of the initial transients the temperature profile is quasi-steady. In response the temperature gradient in the crucible, and hence the crucible base temperature also becomes a constant. With batch production, an increase in heat transfer from the crystal surface, and the lowering of the melt level play important roles. Initially heat losses predominate, and the base temperature has to be raised. Afterwards the heat loss stabilizes, but the drop in the melt level plays an important role. Initially the base temperature is required to be raised, but later it has to be reduced because of the reduced melt height. The crystal radius for batch production (without melt replenishment) is smaller, and the heat loss from the surface is consequently smaller. This factor, along with a higher relative pull velocity, decreases the numerical value of the crucible base temperature needed to maintain the constancy of the crystal size. The present discussion reveals that base

temperature control with a constant melt height is best suited for controlling the crystal size. The limiting factor here is the speed of thermal response of the molten material in the crucible.

When the crystal is grown in an enclosure maintained at the ambient temperature, the heat loss is higher and leads to a higher base temperature requirement. This trend suggests that crystal size can also be controlled by the enclosure temperature when the base temperature and the pull velocity are held constant.

For crystal growth controlled by the pull velocity, an appropriate amount of latent heat is generated at the interface to compensate for changes in the radius that occurs in an uncontrolled system. As presented in Figure 5 and 6 the crystal radius is inversely related to the pull velocity. Therefore, to attain a fixed crystal radius the pull velocity should have a specific value that ensures energy balance among the latent heat release, diffusion into the crystal and the radiation loss at all time instants. The pull velocity as a function of time, determined from the mathematical model, is summarized in Figure 9 and 10 for silicon and Nd:YAG. With an enclosure around the crystal the axial temperature gradient along the crystal is low away from the base. It leads to a higher crystal radius at a fixed pull velocity.

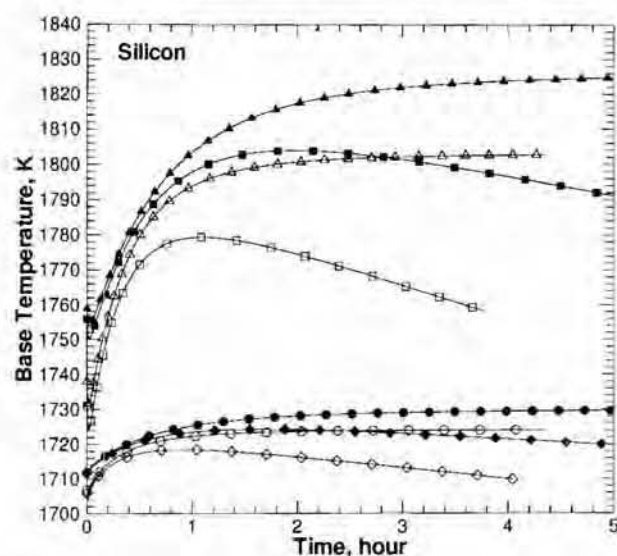


Figure 7 — Variation of crucible base temperature with time to control the crystal radius; $\square$: With enclosure and batch production, Δ : With enclosure and continuous melt replenishment, $\diamond$: Without enclosure and batch production, $\circ$: Without enclosure and continuous melt replenishment, shaded symbols: 1 m/d, unshaded symbols: 2 m/d

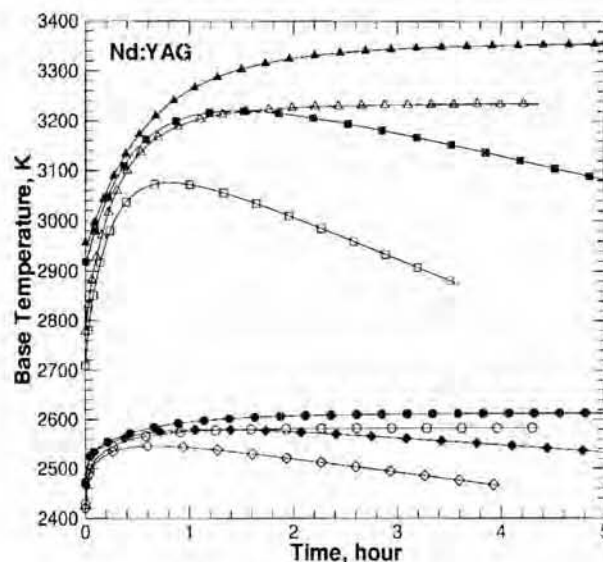


Figure 8 — Variation of crucible base temperature with time to control the crystal radius; $\square$: With enclosure and batch production, Δ : With enclosure and continuous melt replenishment, $\diamond$: Without enclosure and batch production, $\circ$: Without enclosure and continuous melt replenishment, shaded symbols: 1 m/d, unshaded symbols: 2 m/d

Hence the numerical value of the pull velocity needs to be higher for a crystal grown in an enclosure. A crystal of higher radius needs a smaller pull velocity so that sufficient time is available for solidification. On the other hand, an increase in crystal surface area with radius incurs a larger radiation loss. Hence, a stronger control action is expected when the pull velocity is utilized.

When the batch size is to be increased, larger crucibles can be employed, but the heat losses would then dramatically increase. It is preferable to increase the crucible capacity by increasing its depth rather than the diameter. There is a penalty to be paid with deeper crucibles in terms of the variable pull rate at steady state or a higher base temperature.

To compare the graphs of silicon and Nd:YAG the following difference in the material properties should be noted. Silicon has a higher density in the liquid phase, as compared to the solid phase, while Nd:YAG has just reverse of it. There is a large difference between the conductivities in the solid and liquid phases of Si, while they are practically equal for Nd:YAG. Owing to a lower value of density in the liquid phase of Nd:YAG the melt level decreases at a higher rate, in turn leading to a high relative pull velocity. Further, for Nd:YAG the specific heat, emissivity, heat conductivity, and latent heat are half

of that of silicon, while density is twice that of silicon. The high melting point of Nd:YAG also leads to a large temperature difference at the crystal surface with respect to the surroundings. The heat losses from the surface of the Nd:YAG crystal are greater (despite a lower emissivity) since radiative heat transfer is proportional to the fourth power of the absolute temperature. These differences together lead to a higher crystal radius for Nd:YAG, when compared to silicon, for similar simulation parameters. The large difference in the material properties is also responsible for a high crucible base temperature needed to maintain the crystal area of Nd:YAG, a constant. Similarly the optimal pull velocity is also higher for Nd:YAG, as against silicon.

Conclusions

A mathematical model for the temperature distribution in a growing crystal in a Czochralski process has been presented. Simulations for silicon and Nd:YAG crystals have been carried out. The model can predict the shape of the growing crystal for a given set of external conditions. More importantly the control functions in terms of the crucible base temperature and the pull velocity that can maintain the crystal radius, a constant, can be predicted. The model accommodates the presence of an enclosure,

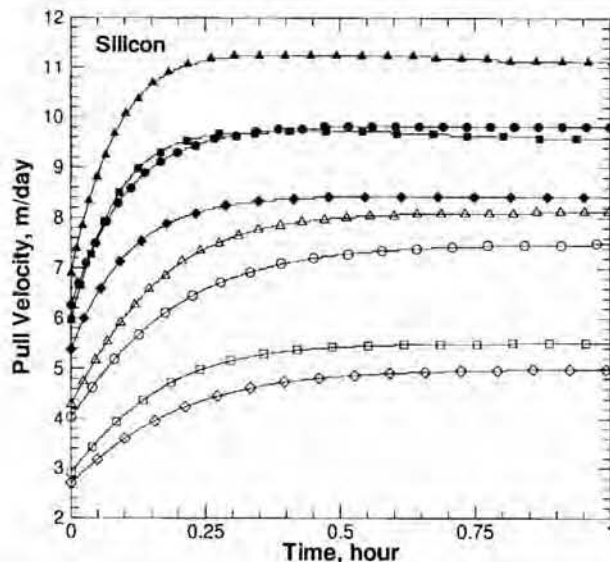


Figure 9 — Variation of pull velocity with time to control the crystal radius; temperature gradient in crucible neglected; $\square$: With enclosure and batch production, Δ : With enclosure and continuous melt replenishment, $\diamond$: Without enclosure and batch production, $\circ$: Without enclosure and continuous melt replenishment, shaded symbols: Crystal area = 50cm^2 , Unshaded symbols: Crystal area = 150cm^2

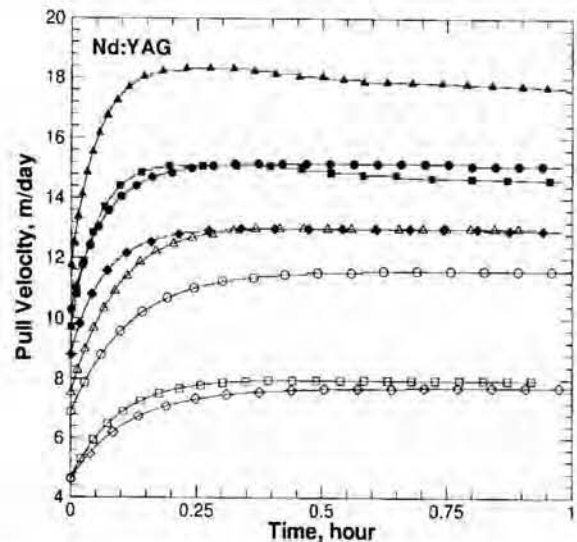


Figure 10 — Variation of pull velocity with time to control the crystal radius; temperature gradient in crucible neglected; $\square$: With enclosure and batch production, Δ : With enclosure and continuous melt replenishment, $\diamond$: Without enclosure and batch production, $\circ$: Without enclosure and continuous melt replenishment, shaded symbols: Crystal area = 50cm^2 , Unshaded symbols: crystal area = 150cm^2

batch vs continuous processes, and temperature-dependent material properties. It can be extended to include higher order effects during crystal growth. The temperature field in the crystal is an essential input for determining the thermal stresses in the crystal.

Results show that the magnitude of the pull velocity, crucible base temperature, and the size of the crystal that can be conveniently grown, depend on the choice of the material, and hence its material properties. Between the two methods of control the one involving the base temperature (with melt replenishment) is seen to be most robust, since a fixed crystal area results in a steady value of the base temperature. Under dynamic conditions, when the crystal area is required to be changed rapidly the pull velocity is expected to be more effective, since it does not experience the difficulties with thermal transients.

References

- 1 Shimura F, *Semiconductor silicon crystal technology* (Academic Press, New York) 1989.
- 2 Hurle D T J & Cockayne B, Czochralski growth, In *Handbook of crystal growth* (edited by D T J Hurle), 2a (North-Holland, New York) 1994, 99-211.
- 3 Derby J J & Brown R A, *J Cryst Growth*, **74** (1986) 605-624.
- 4 Rea S N, *J Cryst Growth*, **54** (1981) 267-274.
- 5 Billig E, *Proc R Soc*, (London), **A235** (1956) 37-54.
- 6 Ozisik M N, *Heat conduction* (John Wiley and Sons, New York) 1980.
- 7 Siegel R & Howell J R, *Thermal radiation heat transfer*, (McGraw-Hill Book Company, New York) 1984.
- 8 Reid R L & Tennant J S, *AIAA J*, **11**(10) (1973) 1446-1448.
- 9 Anderson D A, Tannehill J C & Pletcher R H, *Computational fluid mechanics and heat transfer* (McGraw-Hill, New York) 1984.
- 10 ANULIB, *Library of parallel computing interfaces developed by BARC*, Mumbai. 1998.
- 11 Vanderhart A & Uelhoff W, *J Cryst Growth*, **51** (1981) 251-256.

Nomenclature

$A(x)$	= Cross-sectional area of the crystal, m^2
F_{12}	= Shape factor between surfaces 1 and 2
h_r	= $\sigma \epsilon (T^2 + T_\infty^2) (T + T_\infty)$, radiative heat transfer coefficient, W/m^2-K
H	= Height of the melt in the crucible, m
$k(T)$	= Thermal conductivity, $W/m-K$
l_c	= Length of crystal grown, m
L	= Latent heat of fusion, J/kg
m	= Mass per unit length, $\rho A(x)$, kg/m
$P(x)$	= Perimeter of the crystal, m
t	= Time, s
T_0	= Temperature at the crystal-melt interface, K
T_{base}	= Temperature at the base of the crucible, K
T_∞	= Ambient temperature (no enclosure), or the average enclosure temperature, K
v	= Pull velocity, m/s
W	= Distance between rings in shape factor algebra, m
σ	= Stefan-Boltzman constant, W/m^2K^4
ϵ	= Emissivity of the crystal surface

Subscripts

Crystal	= Crystal surface
Encl	= Enclosure
l	= Liquid phase
s	= Solid phase
∞	= Reference condition