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ANALYTICAL STUDY OF MODIFIED CZOCHRALSKI CRYSTAL GROWTH PROBLEM

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An analytical study of Czochralski crystal growth problem is presented, therefore, we propose a model based on a three-dimensional axisymmetric approach using the Galerkin method for solving the system of equations of heat and momentum in a modified crystal growth process geometry as cylindrical-spherical. To facilitate the procedure of resolution related to the considered problem, we impose some approximation; the molten silicon is assumed to be a viscous, Newtonian and incompressible fluid satisfying the Boussinesq assumption. The thermophysical properties of the fluid are constant except for the density variation in the buoyancy force term. The flow is symmetric in the axial direction. Fixed temperatures are imposed at the walls of the melt crucible and the crystal melt interface. Thus we determine analytically the expressions of temperature and velocity field in the melt, and discuss the temperature properties for different values of the Grashof number.

1. Introduction. The silicon crystals used in the technology of semiconductors are produced primarily by the Czochralski technique. During the Czochralski process three modes of heat transfer are present, namely, conduction in melt and crystal, natural convection due to the temperature gradient between the crucible wall and the melt/crystal interface, forced convection induced by crystal and/or crucible rotation, thermocapillary convection known as the Marangoni convection due to the surface tension gradients on the free surface of the melt, also the heat transfer by radiation between various surfaces of the furnace. The effect of natural convection on the growth in the traditional system that is a cylindrical crucible was studied by several researchers; N. Kobayashi [1] and W.E. Langlois [2] were the first to do it. Turbulent natural convection in large melt volumes have been studied in recent works [3, 4]. V.Kumar *et al.* [5] showed that the Marangoni convection influences the thermal and dynamic field in the melt. K. Kakimoto and H. Ozoe [6] revealed in their three-dimensional numerical simulations that the surface tensions influenced the flow and the oxygen transport in the melt.

Our work consists in studying analytically the Czochralski crystal growth problem in the spherical crucible geometry. As a result, we propose a model based on a three-dimensional axisymmetrical approach using the Galerkin method for solving the system of equations of heat and momentum in a modified crystal growth process geometry as cylindrical-spherical.

2. Formulation of the problem. A.P. Anselmo *et al.* [7] and M.H. Tavakoli *et al.* [8] show that a cylindrical crucible with a curved bottom provides many advantages for crystallization. Therefore, it is proposed recently by F. Mokhtari *et al.* [9, 10] to modify the device as a cylindrical-spherical system. A schematic diagram of crystal growth in the hemispherical system is presented in Fig. 1.

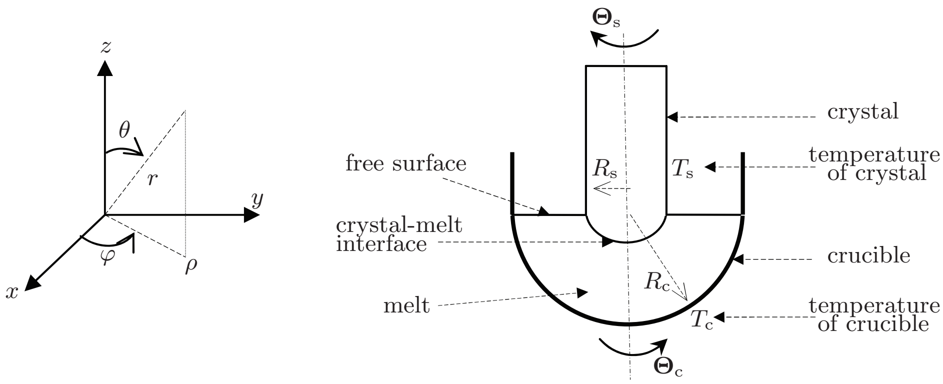

Fig. 1. Schematic diagram of crystal growth in the cylindric-spherical system.

In the framework of modeling related to the considered problem, we put some assumptions; the molten silicon is assumed to be a viscous, Newtonian and incompressible fluid satisfying the Boussinesq assumption. We assume the solid liquid interface to be spherical and the free surface to be flat. The thermophysical properties of the fluid are constant except for the density variation in the buoyancy force term. The flow is symmetric in the axial direction. Fixed temperatures are imposed on the walls of the melt crucible and the crystal melt interface.

The equations governing the dynamics of the flow result from the principles of conservation of mass, momentum, and the conservation equation of energy in the melt. We study the problem of crystal growth in an appropriate coordinates system, namely, the spherical coordinates, respectively, the radial position, r, the meridional angle θ and the azimuthal angle φ.

2.1. Flow control parameters. The dimensionless variables are given by $r = r'/R_c$, $V_r = V'_r R_c/\upsilon$, $V_\theta = V'_\theta R_c/\upsilon$, $V_\varphi = V'_\varphi R_c/\upsilon$, $P = P' R_c^2/\rho\upsilon^2$, $Q = Q' R_c^2/\rho\upsilon^2$, $T = (T' - T_f)/(T_c - T_f)$. V is the flow velocity, P and T are the associated pressure and temperature, g is the gravity field, and Q is a source term coming from the heating in the system.

2.2. Governing equations. We study the considered problem in the following dimensionless form.

Continuity equation:

$$\frac{1}{r^2}\frac{\partial}{\partial r}(r^2 V_r) + \frac{1}{r\sin\theta}\frac{\partial}{\partial\theta}(V_\theta \sin\theta) = 0. \tag{1}$$

Momentum equations:

$$V_r\frac{\partial V_r}{\partial r} + \frac{V_\theta}{r}\frac{\partial V_r}{\partial\theta} - \frac{{V_\theta}^2}{r} - \frac{V_\varphi^2}{r} = -\mathrm{Gr}\cdot T\cos\theta - \frac{\partial P}{\partial r} - \frac{2}{r^2}V_r$$
$$-\frac{2}{r^2\sin\theta}\frac{\partial}{\partial\theta}(\sin\theta\cdot V_\theta) + \frac{1}{r^2}\left[\frac{\partial}{\partial r}\left(r^2\frac{\partial V_r}{\partial r}\right) + \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial V_r}{\partial\theta}\right)\right] \tag{2}$$

$$V_r\frac{\partial V_\theta}{\partial r} + \frac{V_\theta V_r}{r} + \frac{V_\theta}{r}\frac{\partial V_\theta}{\partial\theta} - \frac{V_\varphi^2}{r}\cot\theta = \mathrm{Gr}\cdot T\sin\theta - \frac{1}{r}\frac{\partial P}{\partial\theta} + \frac{2}{r^2}\frac{\partial V_r}{\partial\theta}$$
$$-\frac{1}{r^2\sin^2\theta}V_\theta + \frac{1}{r^2}\left[\frac{\partial}{\partial r}\left(r^2\frac{\partial V_\theta}{\partial r}\right) + \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial V_\theta}{\partial\theta}\right)\right] \tag{3}$$

$$V_r\frac{\partial V_\varphi}{\partial r}+\frac{V_\theta}{r}\frac{\partial V_\varphi}{\partial \theta}+\frac{V_\theta V_\varphi}{r}\cot\theta+\frac{V_r V_\varphi}{r}=\frac{1}{r^2}\left[\frac{\partial}{\partial r}\left(r^2\frac{\partial V_\varphi}{\partial r}\right)\right.$$
$$\left.+\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial V_\varphi}{\partial\theta}\right)-\frac{1}{\sin^2\theta}V_\varphi\right]. \tag{4}$$

Energy equation:

$$V_r\frac{\partial T}{\partial r}+\frac{V_\theta}{r}\frac{\partial T}{\partial\theta}=\frac{1}{\mathrm{Pr}}\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial T}{\partial r}\right)+\frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial T}{\partial\theta}\right)\right]+Q, \tag{5}$$

where Gr and Pr are the dimensionless numbers defined as follows: the Grashof number $\mathrm{Gr}=g\beta R_\mathrm{c}^3(T_\mathrm{s}-T_\mathrm{f})\upsilon^{-2}$ characterizes the effect of natural convection; the Prandtl number $\mathrm{Pr}=\upsilon/\alpha$ characterizes the importance of thermal diffusivity compared to molecular diffusivity. $\mathrm{Re_c}$ and $\mathrm{Re_s}$ are the Reynolds numbers associated with the crucible and crystal defined as $\mathrm{Re_c}=R_\mathrm{c}^2\Omega_\mathrm{c}/\upsilon$ and $\mathrm{Re_s}=R_\mathrm{c}R_\mathrm{s}\Omega_\mathrm{s}/\upsilon$.

2.3. Boundary conditions. The dimensionless boundary conditions are the following:

$$\begin{aligned} &r=1, \quad V_r=0, \quad V_\theta=0, \quad V_\varphi=\mathrm{Re_c}\sin\theta, \quad T=1;\\ &r=A, \quad V_r=0, \quad V_\theta=0, \quad V_\varphi=\mathrm{Re_s}\sin\theta, \quad T=0;\\ &\theta=\frac{\pi}{2}, \quad V_\theta=0, \quad \frac{\partial V_\varphi}{\partial\theta}=0, \end{aligned} \tag{6}$$

where A is the radius ratio: $A=R_\mathrm{s}/R_\mathrm{s}$. The system of differential equations (1)–(5) with partial derivatives with respect to (r,θ) associated with the boundary conditions (6) is the problem of crystal growth to be solved.

3. Method of resolution. To solve the system of equations, we use the Galerkin method to the second order as employed previously [9]. We eliminate the pressure from equations (2) and (3) by differentiating with respect to θ and to r, then we can establish the temperature distribution $T=(r-A)^3\Theta(\theta)/\mathrm{Gr}$. We replace by the velocity expressions V_r, V_θ and V_φ, and multiplying by $W=(1+\gamma/r)(a+b/r^2)$ we obtain the following equation

$$\frac{\partial}{\partial\theta}(\Theta\cos\theta)+p\cdot\Theta-\frac{G(\theta)}{\sin\theta}=0, \tag{7}$$

where $G(\theta)$ is a function of $\Phi(\theta)$ and its first, second and third derivatives; the solution of equation (7) is given by

$$\Theta=\cos\theta^p\left(\int^\theta\frac{G(\theta')}{\cos\theta'^{p+1}}\mathrm{d}\theta'+\Theta_0\right), \tag{8}$$

and Θ_0 denotes a constant to be determined from the boundary layer satisfying θ. In our previous work [9] we found

$$\Phi=\frac{M}{\sin\theta^{1+N}}\left(\int^\theta\sin\theta'^{1+N}\mathrm{d}\theta'-\int_0^{\frac{\pi}{2}}\sin\theta'^{1+N}\mathrm{d}\theta'\right), \tag{9}$$

where N and M are constants as integral expressions depending on the constants a, b, β_3, γ and A.

4. Results and discussion. Previously, we were interested in the law of distribution of the velocity field [9]. Here, we would like to focus on the study of the temperature field. From equation (5), the expression for the temperature

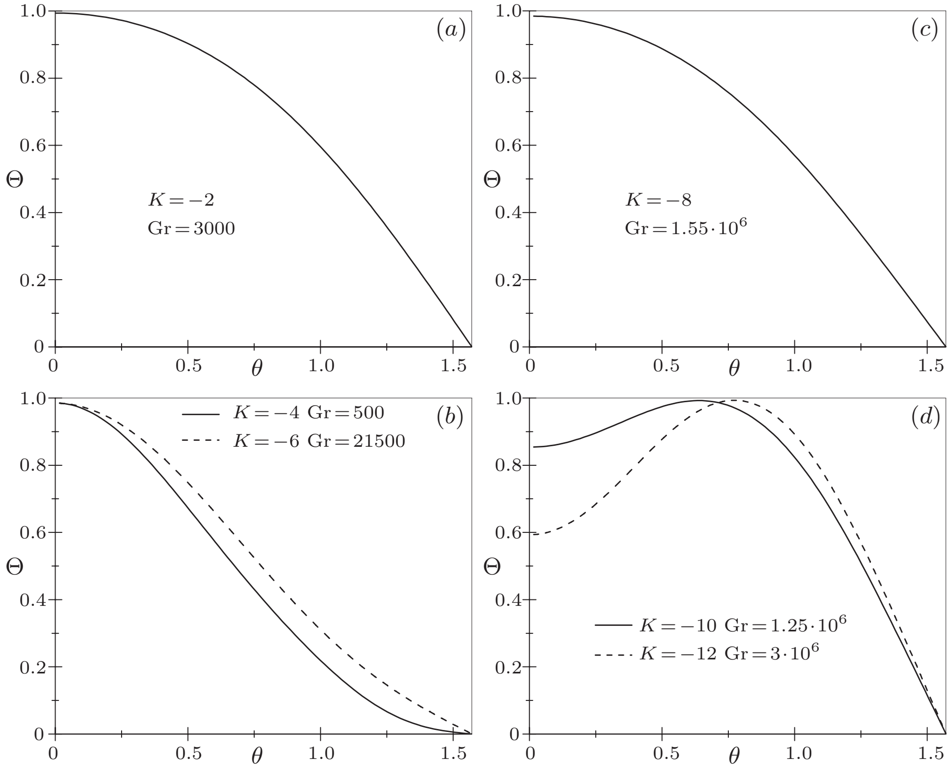

Fig. 2. The angular part of temperature Θ for different values of K and Gr.

$T(r,\theta) = F(r)$. $\Theta(\theta)$ is determined by cubic form for the radial part $\rho^3 = (r-A)^3$, but it depends in a very complex way on θ.

As it is done in our previous work [9], we introduce a control parameter $K = N + 1$, which is related to cinematic and geometrical characteristics of the device and connects all constants, which appear in the velocity components. In addition, we remind that by choosing positive values of K, the condition on the axis of symmetry, namely, the zero stream function is not satisfied. The odd values of K lead to a problem of indetermination, but for even negative integer numbers the preceding condition is satisfied.

Figs 2 and 3 display the evolution of the angular part of temperature Θ for different Grashof number and control parameter K values. We choose a value of 0.25 for the radius ratio A and $\gamma = 1$ and different values for the constant a. The choice of the parameter a is based on the sign of the temperature expression, which must be positive. The value of the Grashof number varies from one case to another, it depends strongly on the value of the control parameter K. The Grashof number is fixed from the maximum value of the angular part of temperature $\Theta(\theta)$; this is justified by the fact that the dimensionless temperature T must be less than 1, so the maximum value of $\Theta(\theta)$ represents the Grashof value.

In particular, one notes the existence of an inflection point (Fig. 2*b*), which confirms when the Grashof number tends to decrease. From the physical point of view the occurrence of a point of inflection involves the appearance of an unstable phenomenon for $r = A$ as a necessary condition. This value coincides with the melt-crystal interface indicating as well that the interface of solidification is a source of potential instability. On the other hand, the law of behaviour of $\Theta(\theta)$ changes considerably when the control parameter K grows in absolute value and Gr increases until reaching the value $Gr = 10^6$, which is the beginning of a strong natural convection (Fig. 2*c*). Indeed, one notes even the existence of a maximum $\Theta_{\max} = 1$ related to the existence of a critical angle for the value $\theta_c = 0.62$ (Fig. 2*d*). The angular axis $\theta \simeq \pi/4$ corresponds to the bisector passing by the center of the vortex of natural convection thus justifying the result already found previously [10]. It would seem through the streamlines that it is a privileged angular position to diffuse the temperature field within the melt so as to possibly homogenize the solution of the melt.

Beyond $K = -12$ and for $\mathrm{Gr} = 3\times10^6$, which is of the same order of magnitude as previously, the law of behaviour is appreciably similar (Fig. 2*d*) with a maximum more affirmed, and one notes a displacement of x corresponding to $\theta = 0.77$.

The preceding curves evolution led us systematically to exploit those being based on a new representation using the variable $x = \cos\theta$ for an interpretation based on a significant physical property. Therefore, we plotted the bisector $\Theta = x$ in order to evaluate the deviation of the angular effects compared to this symmetry of reference. The analysis of the curves thus obtained reveals a certain number of interesting properties.

At the beginning of the appearance of natural convection one notes the passage of Θ from area (1) towards area (2) when the control parameter of the flow K increases in absolute value from 2 to 4 (Figs. 3*a*,*b*) that indicates a process of transition from one state to another, which remains to be explained. Thus Fig. 3*a* can be considered as a starting point of a characteristic evolution of a first state

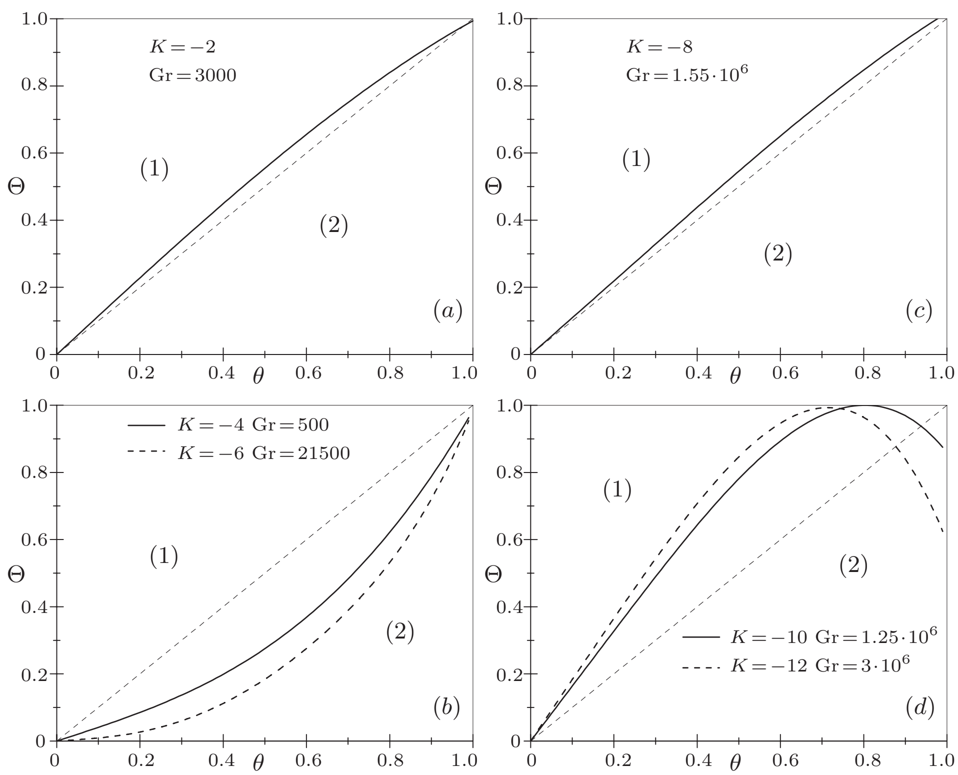

Fig. 3. The angular part of temperature Θ with respect to $x = \cos\theta$.

of crystal growth. Consequently, it is noted that there is not a notable qualitative change when the Grashof number increases from Gr = 500 up to Gr = 21500, corresponding, respectively, to $K = -4$ and $K = -6$ (Fig. 3*b*). Thus one can state that the corresponding evolution of these two cases appears stable.

However, near $\mathrm{Gr} = 1.5 \times 10^6$ for $K = -8$ (Fig. 3*c*) one finds a similar behaviour at the initial state characterized by a weak natural convection. In fact, this new state is very different from Fig. 3*a* because the convection here is reinforced through the intensification of the momentum transfer. For the Grashof number close to $\mathrm{Gr} = 1.25 \times 10^6$ (Fig. 3*d*), one observes a remarkable change of the evolution of Θ according to x, which highlights a maximum value in the interval $0 \le x \le 1$. This state becomes more sensitive to the increase in K as one passes from $K = -8$ to $K = -10$.

Concerning the property of extremality of the curve, one checks that this one is located in the vicinity of $\theta = \pi/4$. The evolution related to $K = -12$ and $\mathrm{Gr} = 3 \times 10^6$ is confirmed once again in Fig. 3*d*.

The Nusselt number Nu is assumed to give important information according to the evaluation of heat transfer Q between the crystal and the free surface and the crucible, on the other hand. We then define the Nusselt number for heat transfer as

$$\mathrm{Nu}(r,\theta) = \frac{Q(\theta) D_1}{k(T_c - T_s)},$$

where $Q = k\partial T/\partial r$ denotes the corresponding heat quantity, so that we can obtain $Q = 3kR_{\mathrm{c}}^{-1}\Theta(\theta)(r-A)^2(T_{\mathrm{c}} - T_{\mathrm{s}})$. Therefore we get $\mathrm{Nu}(r,\theta) = 6A(r-A)^2\Theta(\theta)$.

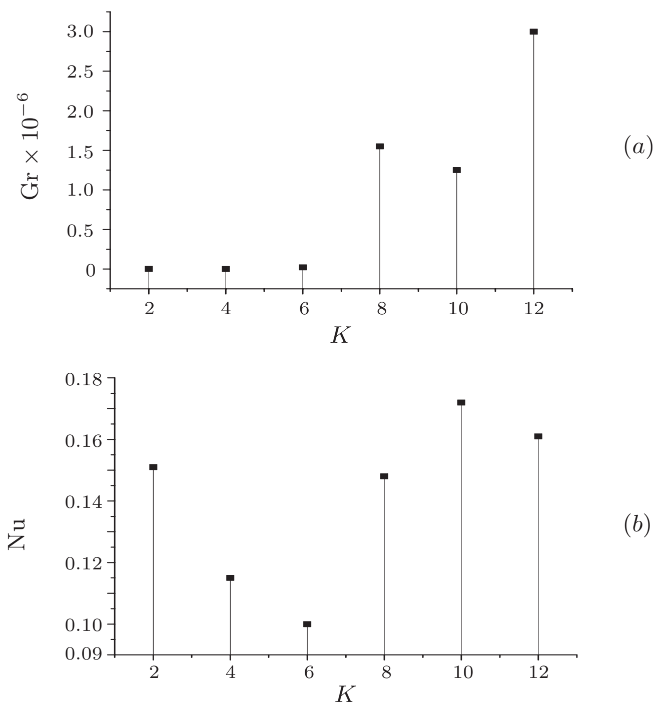

Fig. 4. Evolution of the Grashof and Nusselt numbers versus the control parameter K (an even integer number).

It is convenient to use the mean Nusselt number as

$$\mathrm{Nu} = \frac{1}{1-A}\int_A^1 \left(\frac{1}{\pi/2}\int_0^{\pi/2} \mathrm{Nu}(r,\theta)\mathrm{d}\theta\right) r\mathrm{d}r.$$

The result is simply the following

$$\overline{Nu} = 0.145 \int_0^{\pi/2} \Theta(\theta)\mathrm{d}\theta.$$

Clearly, $\overline{\mathrm{Nu}}$ is closely related to the angular properties due to the function Θ depending on θ. In Figs. 4*a*,*b* we present the evolution of the Nusselt number in order to evaluate the quality of the heat transfer. According to the evolution of the Nussel number Nu, the heat transfer process decreases as the control parameter $|K|$ increases, meanwhile the Gr number does not vary considerably in the same range of K.

However, for $|K| \geq 6$ the Nusselt Number Nu increases considerably until reaches its maximum $\mathrm{Nu}_{\max} = 0.175$ at $|K| = 10$ and decreases slightly then after at $|K| = 12$. Globally, the Grashof number Gr is the same range of $|K|$, except for $|K| = 10$. Indeed, it seems that the optimum conditions to make an efficient heat transfer process is located at $\mathrm{Nu} = 0.175$ corresponding to the values $|K| = 10$ and $\mathrm{Gr} = 1.25 \times 10^6$.

5. Conclusion. By means of the Galerkin method we solved analytically the system of equations of heat and momentum conservations corresponding to the crystal growth in a modified geometry, we evaluated the velocity and temperature fields in a spherical Czochralski crystal growth crucible and we gave the evolutions of temperature for different parameters of the system. Our main result shows that the parameter K controls the flow and the temperature for different crucible dimensions and rotation rates. We have found that the control parameter K is strongly related to the Grashof number Gr through the maximum value of the angular part of temperature Θ.

In future work, the most extensive information is to know the parameters; the Grashof number Gr and the mean Nusselt number $\overline{\mathrm{Nu}}$ play different roles, while the integer number $|K|$ determines the condition for growth or decay of the process.

In addition, one plans to examine the effect of the free surface or thermocapillarity effect on the flow when the height of the melt decreases compared to the radius of the hemispherical crucible.

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