



3D-Numerical study of the effect of crystal rotation speed on interface shape in Czochralski growth for photovoltaic applications

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ARTICLE INFO

Article history:

Received September 02, 2025

Accepted October 20, 2025

Available online Oct 20, 2025

Published November 06, 2025

Keywords:

Silicon,
Czochralski,
Photovoltaic Application,
Melt-crystal interface,
Rotation speed,
Convection,
Heat Transfer,
Numerical simulation.

ABSTRACT

In this work, we conducted a 3D numerical simulation to investigate the shape of the melt-solid interface during the crystal growth of silicon using the Czochralski technique, which is widely employed in photovoltaic applications. Among the key parameters that influence the quality of the grown monocrystalline is the shape of the crystallization interface. This interface has a main role in determining the structural instability of the silicon ingot during the CZ pulling process. The primary aim of this study is to find the optimal rotation speed that results in a flat shape of the interface, which is conducive to forming a well-ordered atomic structure and thus ensuring superior crystal quality for photovoltaic use. Our findings indicate that, for a crucible with a diameter of 100 mm, an optimal rotation speed of 20 rpm gives a flat shape of the melt-solid interface. According to this study, we find that the Czochralski technique is the process that conserve the flow and the heat transfer of materials in the Cz crucible even for high rotation speed; Our results are in agreement with the experiment results. In our study for the Silicon, the heat transfer in the crucible is symmetrical even applying rotation crystal at high rates ($v_{rot} = 40 - 50 \text{ rpm}$).

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1. INTRODUCTION

The growth of Silicon single crystals using the Czochralski technique (Cz) remains essential for producing monocrystalline silicon used in photovoltaic applications, due to its ability to generate large, high-quality cylindrical ingots (Chen et al., 2023; Zhao et al., 2023). This Cz crystal growth technique is the predominant method for producing high-quality monocrystalline silicon, essential for the fabrication of high-efficiency solar cells. The monocrystalline silicon obtained through this method currently forms the cornerstone of high-efficiency solar cells (Deren Yang., 2019). The solid-liquid interface plays a key role in this process, as it governs the distribution of defects, mechanical stresses, the atomic structure of the pulled crystal, and the overall efficiency of the growth process (Sturm et al., 2023). Melt-crystal interfaces continue to pose major challenges in numerical modelling, particularly when it comes to determining the shape of the crystallization front (Ding et al., 2019). In this study, we aim to determine the optimal crystal rotation to obtain the flat shape of the melt-solid interface by varying the crystal's rotation speed. CFD analyses for silicon Czochralski growth systems were conducted using 3-D modelling in cylindrical coordinates where the radiative heat transfer, the melt forced convection and the Marangoni convection were conducted for Silicon melt in Cz crucible.

2. MODEL OF THE INDUCTIVELY HEATED CZOCHRALSKI SYSTEM

The Czochralski crystal growth furnace is illustrated in the below (fig. 1) (Azoui et al., 2018). In this technique; using the radiofrequency inductive technique, the silicon melt is heated beyond the melting temperature, the molten material (The raw silicon material) melted within a furnace in a cylindrical crucible. The crystal pulled has a cylindrical shape, it emerges due to phase change phenomena at the connection (interface) between the liquid and the solid (Tavakoli., 2018).

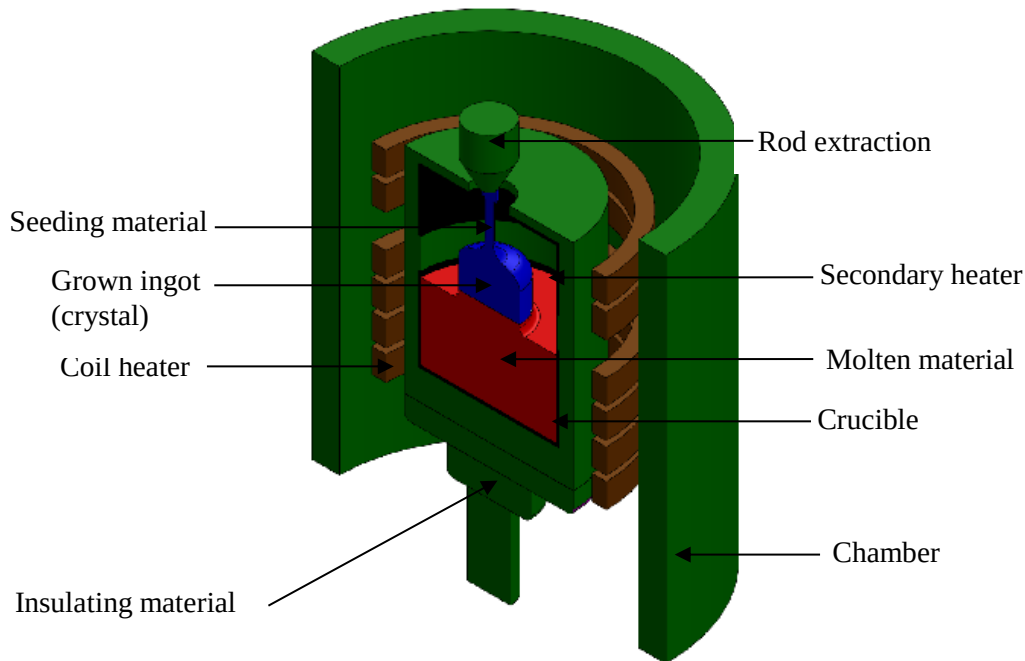


Fig 1. Schematization of the inductively heated Czochralski furnace (Azoui et al., 2018).

2.1. Mathematical model

The flow of a continuous, incompressible, viscous, Newtonian fluid is described by the unsteady Navier-Stokes equations. According to a reference (Azoui et al., 2018), three cylindrical-coordinate-based equations form the heart of the simulation model used are the following equations:

The equation for the radial component of momentum is given by:

$$\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial r} + \frac{v}{r} \frac{\partial u}{\partial \theta} - \frac{v^2}{r} + w \frac{\partial u}{\partial z} = -\frac{1}{\rho_m} \frac{\partial P}{\partial r} + \nu \left(\frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial u}{\partial r} \right) - \frac{u}{r^2} + \frac{1}{r^2} \frac{\partial^2 u}{\partial \theta^2} - \frac{2}{r^2} \frac{\partial v}{\partial \theta} + \frac{\partial^2 u}{\partial z^2} \right) + \frac{1}{\rho_m} (\rho g_r) \quad (1)$$

This equation represents the azimuthal component of momentum:

$$\frac{\partial v}{\partial t} + u \frac{\partial v}{\partial r} + \frac{v}{r} \frac{\partial v}{\partial \theta} - \frac{uv}{r} + w \frac{\partial v}{\partial z} = -\frac{1}{\rho_m} \frac{1}{r} \frac{\partial P}{\partial \theta} + \nu \left(\frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial v}{\partial r} \right) - \frac{v}{r^2} + \frac{1}{r^2} \frac{\partial^2 v}{\partial \theta^2} + \frac{2}{r^2} \frac{\partial u}{\partial \theta} + \frac{\partial^2 v}{\partial z^2} \right) + \frac{1}{\rho_m} (\rho g_\theta) \quad (2)$$

The axial component of momentum is described by this equation:

$$\frac{\partial w}{\partial t} + u \frac{\partial w}{\partial r} + \frac{v}{r} \frac{\partial w}{\partial \theta} - \frac{v^2}{r} + w \frac{\partial w}{\partial z} = -\frac{1}{\rho_m} \frac{\partial P}{\partial z} + \nu \left(\frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial w}{\partial r} \right) + \frac{1}{r^2} \frac{\partial^2 w}{\partial \theta^2} + \frac{\partial^2 w}{\partial z^2} \right) + \frac{1}{\rho_m} (\rho g_z) \quad (3)$$

The energy equation in this model is given by:

$$\frac{\partial T}{\partial t} + u \frac{\partial T}{\partial r} + \frac{v}{r} \frac{\partial T}{\partial \theta} + w \frac{\partial T}{\partial z} = \alpha \left[\frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial T}{\partial r} \right) + \frac{1}{r^2} \frac{\partial^2 T}{\partial \theta^2} + \frac{\partial^2 T}{\partial z^2} \right] \quad (4)$$

The continuity equation given by:

$$\frac{1}{r} \frac{\partial (ru)}{\partial r} + \frac{1}{r} \frac{\partial v}{\partial \theta} + \frac{\partial w}{\partial z} = 0 \quad (5)$$

Where: u, v, w expresses the radial, the azimuthal, and the axial velocity respectively.

Since the pulling rate in the Czochralski process is upward, the gravity term is taken into account along the axial direction (oz). In this case, $\mathbf{g}_z = -9.81$. The radial and azimuthal terms of gravity are negligible in both the radial and azimuthal directions: $\mathbf{g}_r = \mathbf{g}_\theta = 0$.

2.2 Boundary conditions

The boundary conditions used in our simulation for both velocity and temperature parameters according to the reference (Azoui et al., 2018 and Soltani et al., 2017) are:

At the interface of crystallization: $0 \leq r \leq R_s, 0 \leq \theta \leq 2\pi, Z = H$

$$T = T_f \text{ and } u = 0, v = R_s \omega_{cri} = 0, w = 0 \quad (6)$$

ω_{cri} : Rotation speed of the crystal (rad/s).

At the interface with the air (free surface) [10]:

$$R_{cri} \leq r \leq R_{cru}, 0 \leq \theta \leq 2\pi, Z = H$$

Where the radius of the crystal is R_{cri} and the radius of the crucible is R_{cru} .

The convection and the Marangoni convection are the heat transfer phenomena take place at the free surface; they are expressed by:

$$\vec{n} \cdot \mathbf{k}_{\text{mel}} \vec{\nabla} T = -\text{Bio}(T - T_{\text{am}}) \quad (7)$$

According to the reference (Lan et al.,1998) : $\vec{n}$ is the unit vector directed outward normal to the surface of the molten material.

$\mathbf{k}_{\text{mel}}$: denotes the melt's thermal conductivity.

h : expresses the heat transfer coefficient.

T_{am} : the room temperature that is considered constant.

The Biot number for the molten material is defined:

$$\text{Bio} = hH/k_{\text{mel}}$$

On the side walls of the crucible:

$$R = R_{\text{cruc}}, 0 \leq Z \leq H$$

$$T = T_f + \Delta T = T_{\text{cruc}}$$

ΔT : The temperature difference between the melting temperature and the temperature of side walls of the crucible. T_f is the melting temperature of material.

For the side walls and the bottom of the crucible the conditions at the boundaries are:

$$u = 0, v = 0, w = R_{\text{cruc}}\omega_{\text{Cruc}} = 0 \quad (8)$$

At the bottom of the crucible:

$$-R_{\text{cruc}} \leq r \leq R_{\text{cruc}}; z = 0, 0 \leq \theta \leq 2\pi$$

$$u = 0, v = r\omega_{\text{cri}} = 0, w = 0$$

$$T = T_{\text{cruc}} \text{ (crucible temperature).} \quad (9)$$

3. RESULTS AND DISCUSSION

In this section, our intention is to identify the ideal rotation rate (the optimal rotation speed) of the crystal that leads to the formation of a flat solid–liquid interface. By varying the rotation speed of the solid (silicon crystal), we investigate the resulting interface shape in order to identify the conditions under which a planar interface is achieved.

3.1 Convective heat transfer

The figures below illustrate the convective heat transfer for different crystal silicon rotation speeds. These results are presented along the vertical mid-plane of the Czochralski crucible. The difference in the temperature between the crucible's walls and the silicon's melting temperature is kept constant.

According to these results, it can be observed that the convective heat transfer is influenced relatively by low rotation speeds, ranging from 4 rpm - 14 rpm.

Under these conditions, the solid silicon crystal primarily contributes to heat transfer through conduction and convection. This is evidenced by the clear diffusion of lower temperatures across the width of the

crucible (crystal-based cooling), as illustrated by the presence of blue, light blue, green, and yellow regions in the temperature contour plots.

For these low rotation rates the convective temperature distribution is symmetrical; this implies that the silicon flow is symmetric in the Cz crucible.

It can be seen that according to the temperature contour corresponding to a rotation speed of 14 rpm, 16 rpm, 18rpm, we observe that the heat transfer moves downward toward the bottom of the crucible, forming a clear jet heat transfer. The contours illustrating convective heat transfer for rotation speeds between 14 rpm and 18 rpm show a symmetrical thermal distribution, where the melt jet expands down to the bottom of the crucible.

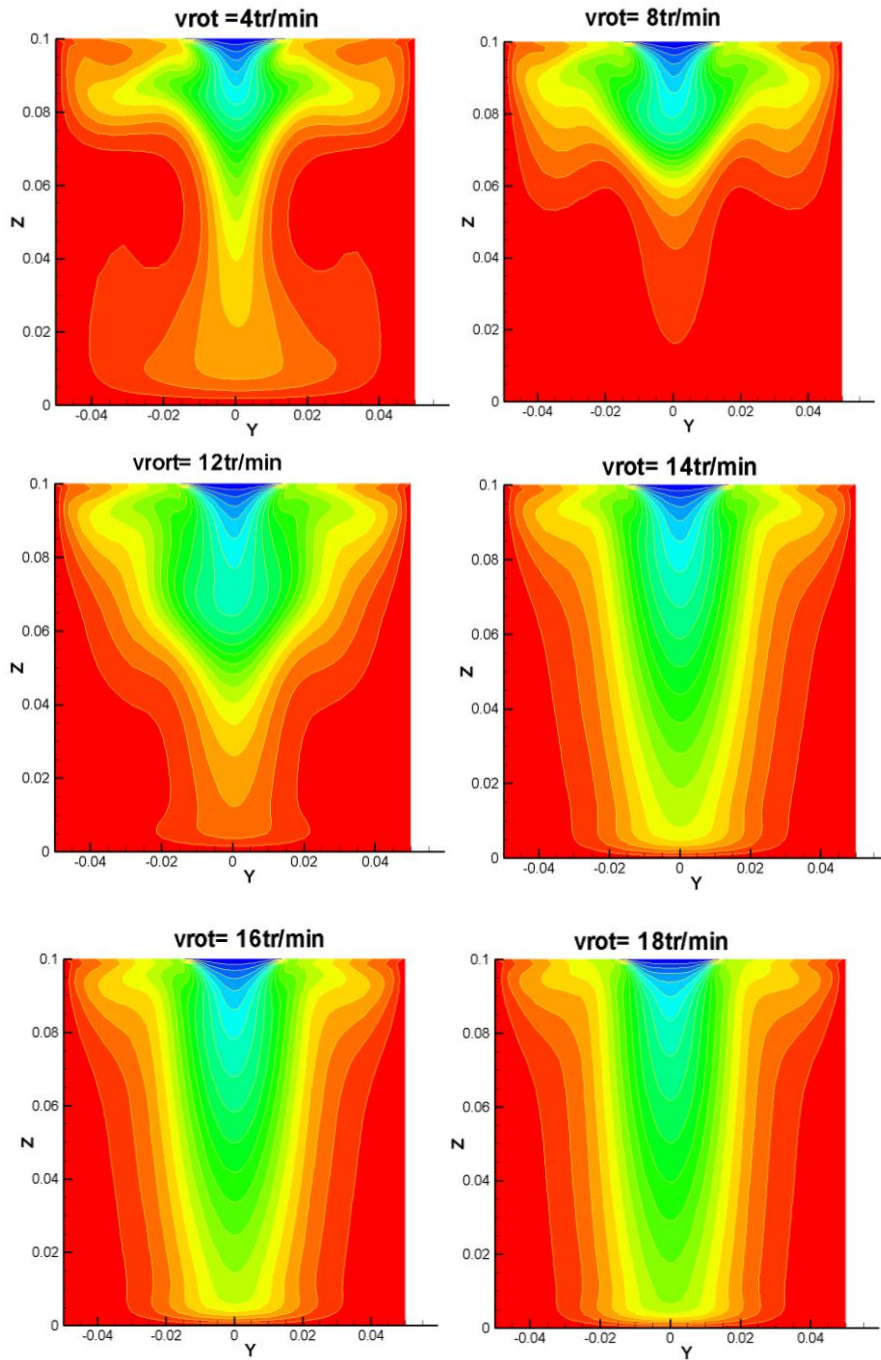


Fig 2. Convective heat transfers in the vertical median plane from 4rpm-14rpm rotation rates crystal.

Fig. 3 represents the heat transfer under forced convection at a crystal rotation speed of 20 rpm. According to the isotherms in the upper part of the crucible, shown in blue region, the first isotherm revealed a flat shape of the solid-liquid interface. So this is the optimal rotation rate. We will confirm this result using the radial temperature profile 2mm just below the melt free surface.

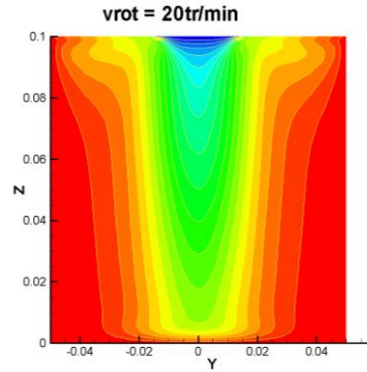


Fig 3. Convective heat transfer in the vertical median plane of 20 rpm rotation rate crystal.

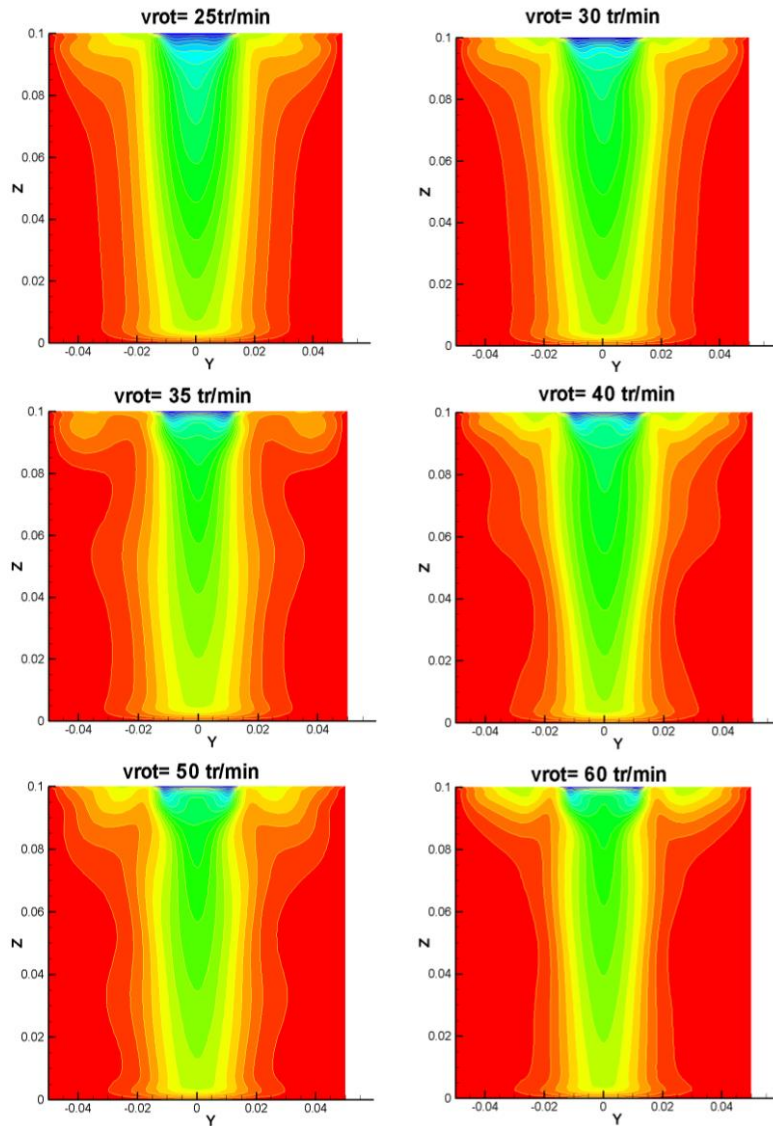


Fig 4. Convective heat transfers for high crystal rotation rates 25 rpm- 60 rpm.

According to the temperature contours shown in the previous figures, it is clear that heat transfer within the melt remains symmetric throughout the CZ crystal growth process across the different rotation speeds. This symmetry indicates that the molten silicon flow inside the crucible is likewise symmetric. Notably, a thermal plume can be observed descending toward the bottom of the crucible. Furthermore, the presence of two counter-rotating convection cells is clearly identified, which can be attributed to natural convection effects within the melt.

3.2 Radial temperature profile

In figure 5 we illustrated the temperature radiale profile for different rotation speeds just 2mm below the free surface of the melt.

According to these curves, it is confirmed that for the rotation velocity $v_{rot} < 20$ rpm, the melt-solid interface takes a concave shape. The curves shown the profiles of temperature for the rotation crystal velocity $v_{rot} > 20$ rpm indicate that the shape of the melt-crystal interface is convex.

It is clear that the flat shape of the crystallization interface corresponding to the flat curve in maroon color with value of 20 rpm. These curves shapes confirm the results illustrated in the contours of convective heat transfer of 20 rpm.

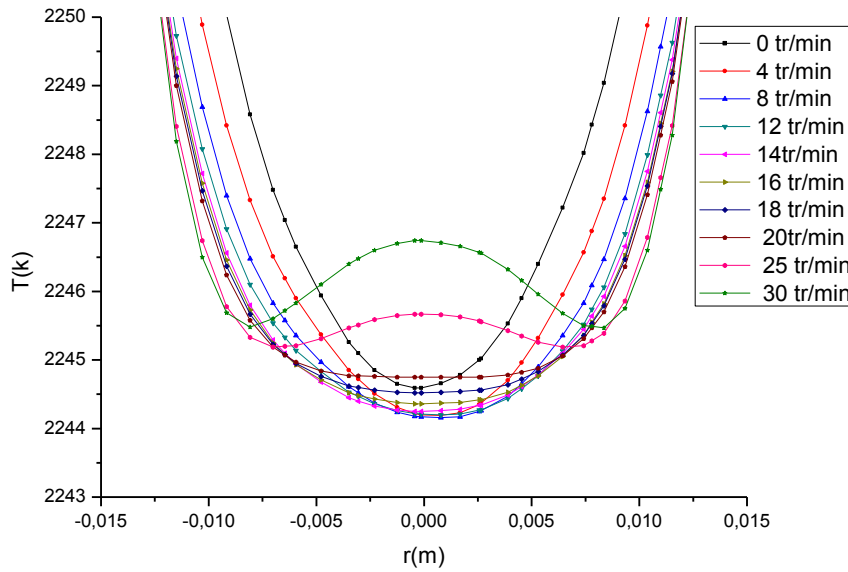


Fig 5. Profile of radial temperature 2mm just below the melt free surface.

4. CONCLUSION

CFD analyses for Cz growth systems were carried using three-dimensional modelling to examine the influence of the crystal rotation rate on the melt-crystal interface shape, the convective heat transfer and flow during Czochralski Silicon growth process and the behaviour in the crucible. This study shows that:

- We have been able to determine the flat shape of the melt-solid interface that gives the good atomic structure and high quality of the pulled crystal for photovoltaic applications.
- For crystal rotation rate $v_{rot} < 20$ rpm, the form of the solid-melt interface is concave.

- For rotation velocity $v_{rot} > 20$ rpm, the interface crystallization shape becomes convex.
- We identified the optimal rotation speed that minimizes the growth time while preserving the symmetry of the flow within the crucible. Our results show that the rotation crystal by 20 rpm the value of the optimal rotation speed for 100 mm diameter Cz silicon crucible.
- The Czochralski method is a process that maintains controlled heat transfer and material flow within the system in the crucible even applying crystal rotation at high rates; our results are in agreement with the experiment results (Stelian et al., 2018). In our study for the Silicon Cz growth, the flow in the crucible is symmetrical even for high rotation speed ($v_{rot} = 40 - 50$ rpm).

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