

Modeling on Directional solidification of Silicon for Solar Cell Applications

M. Srinivasan¹, P. Ramasamy²

^{1,2} SSN Research centre, SSN College of Engineering, Chennai-603110, India.

Abstract: *The Directional Solidification is a very important technique for growing high quality multi-crystalline silicon at large scale for PV solar cells. The physics governing the growth of multi-crystalline silicon in the Directional Solidification System involves complex non-linear transport phenomena including but not limited to heat transfer, solidification, thermal stress development, and the formation of defects. Specifically, heat transfer and solidification process have significant impact on the quality and productivity of the crystals. This paper is aimed to achieve an advanced understanding of the heat transfer and solidification during the growth process and to identify important design and control parameters that can be modified to improve the processing conditions. To achieve this goal, a coupled heat transfer and fluid flow properties were analysed to investigate the heat transfer on the molten silicon in the crucible during solidification process. A 3D numerical approach is successfully used by finite element method. The temperature distribution, the primary and secondary vorticity generation in molten silicon are simulated and analysed for various Rayleigh numbers. The information obtained from this research will help to improve furnace design and process control for producing high quality multi-crystalline silicon ingots at high throughput.*

Keywords: Silicon; Simulation; Solar cell; Fluid flows, Heat transfer.

1. Introduction

The unsustainable nature of fossil fuels as an energy source, from the point of view of future availability and environmental impact, has spurred an interest in diversification of energy sources, with particular interest in renewable energy. The photovoltaic (PV) industry is a player in the renewable energy segment, and the electricity generation from photovoltaics (solar cells) is deemed to be one of the key technologies of the 21st century[1]. The multicrystalline Silicon (mc-Si) is the predominant material for solar cells, improvements are needed in order to increase the conversion efficiency. Since grain size significantly affects the conversion efficiency, grain growth is an important factor to consider in the mc-Si growth by directional solidification system. Basic studies of grain growth in mc-Si are essential to understand the crystal growth process[2]. Mainly mono-crystalline is grown by Czochralski (Cz), Floating zone (Fz) or Edge-defined film-fed growth (EFG) techniques and multi-crystalline Silicon (mc-Si) by directional solidification (DS) of large crystal ingots. The physical process in solidification of liquid is of great importance in natural and industry world. It can be described by mathematical model considering the transport of mass, momentum, and energy. To understand the physical phenomena inside furnace, theoretical analyses and numerical simulation with these models has been an attractive topic in the area of applied physics, materials science, and applied mathematics [3]

Crystal growth experiments are expensive and time-consuming, modeling becomes an effective tool for research and optimization of growth processes. Besides the crystal growth technology is more closely linked to fluid dynamics, thermodynamics, heat and mass transfer. The temperature distribution and velocity field are obtained by solving the heat transfer and Navier-Stokes equation simultaneously. The

finite element method (FEM) is employed to generate the grids (mesh) for simulation of melt flow. Melt convection is important for heat and mass transfer during the DS process, and can significantly affect the temperature distribution, impurity transport, and the melt-crystal (m-c) interface shape. Therefore, precise control of the melt flow pattern is crucial for optimizing the DS process and improving ingot quality[4]. In the conventional DS system, the melt flow is mainly driven by the buoyancy force resulting from the horizontal temperature gradient. The ability to control the buoyancy force for the melt flow pattern is limited. A careful control of the initial nucleation by low cooling rate and grain competition through the growth rate and the growth front shape are believed to be crucial.

In this study, we investigated the melt mechanism during mc-Si growth by directional solidification method. When a crystal is grown from a high-temperature melt, the temperature field often plays a significant role in determining the nature and the properties of the crystal. The temperature field in the melt gives rise to gradients of density, or surface tension, or both. Such gradients generate fluid motion which may substantially affect the growth process. The resultant fluid motion is often complex, but critical to crystal quality. The iterative process is tuned for a fast, efficient solution using nondimensional parameters and a Boussinesq term for the buoyant drive with the incompressible Navier-Stokes equation and the Convection and Conduction application modes. In the recent years, the finite element or finite volume based computer aided design packages have reached a new height and are being widely used in industries in designing, manufacturing and final testing of mechanical and thermal systems [5].

In the recent research and development of crystal growth processes it was clearly demonstrated that simulation of heat and mass transfer in bulk growth has become an indispensable tool for an efficient, time and cost saving optimization procedure. The melt flow in the crucible has

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Department of Physics, Government College (A), Rajahmundry, Andhra Pradesh, India

significant effects on the formation of micro - defects and segregation of impurity concentration in the grown crystals which are studied to control the flow pattern[6]. The temperature distribution and velocity field, Vorticity generation are obtained by solving the heat transfer and Navier-Stokes equation simultaneously. The finite element method is employed to generate the grids (mesh) for simulation of melt flow. A 3D numerical approach is also successfully used by finite element method to study the thermal characteristics and melt flow properties on molten silicon in directional solidification silicon. In this paper, we have presented only vorticity generation in molten silicon for various Raleigh numbers at constant Prandtl number. The aim is to increase average grain size in silicon multi-crystals and reduce the dislocation density by controlling the melt flow patterns during solidification process.

2. DS Model

The schematic diagram of industrial-scale DS system is shown in Figure 1. The DS system mainly consists of Silicon nitride (Si3N4)coated silica crucible, graphite susceptor, Gas tube, heat exchange block, graphite resistance heater, insulations, chamber wall. The simulation model is defined as follows: A directional solidification apparatus consists typically of a square shaped silica crucible in furnace which has Si melt with crystal seed. A model is assumed only for Si melt system with small temperature gradient. Known thermo-physical properties of silicon are given in the table.1[7].

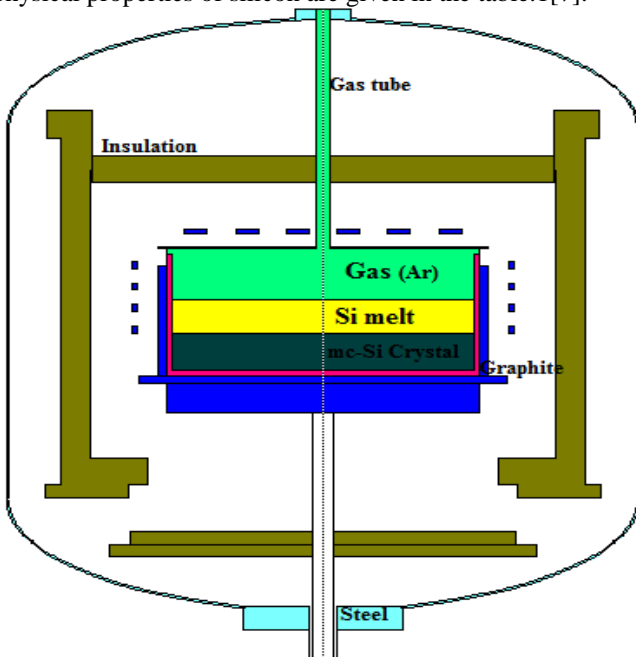


Figure 1: Schematic diagram of mc-Silicon growing directional solidification system

Table 1: Thermo- Physical properties of silicon (liquid)

Symbol and Description	Values (units)
β heat expansion coefficient	$5.5 \times 10^{-6} (K^{-1})$
γ surface tension	0.74 (N/m)
$d\gamma/dT$ rate of change of surface tension	$-2.8 \times 10^{-4} (N/m.K)$
ρ density	2530 (kg/m ³)

C_p specific heat capacity	1040 (J/kg.K)
T_{melt} melting point temperature	1685 K
η dynamical viscosity	$7 \times 10^{-4} (kg/ ms)$
λ heat conductivity	67 (W/m.K)
σ electrical conductivity	$1.2 \times 10^6 (S/m)$
L latent enthalpy	$1.8 \times 10^6 (J/kg)$
ΔT temperature difference	10K
Prandtl number	0.01
Rayleigh numbers	10,1000 and 100000

3. Mathematical Model

The square silica crucible with molten silicon is considered to the computational domain which is used for the local 3D-simulations. To formulate the directional solidification problem, the following assumptions are made: (a) melt flow is axisymmetric; (b) the melt is Newtonian fluid; (c) the Boussinesq approximation is applicable. The Si melt flow is described by conservation equations. The conservation equations for transport mechanism is written as momentum (Navier-Stokes equation) and continuity in differential form as below [7]

Momentum (Navier-Stokes) equation

$$-\nabla \cdot \eta [\nabla \vec{u} + (\nabla \vec{u})^T] + \rho \vec{u} \cdot \nabla \vec{u} = -\nabla P + F \quad (1)$$

Continuity equation

$$\nabla \cdot \vec{u} = 0 \quad (2)$$

Navier-Stokes equation with Boussinesq approximation

$$-\nabla \cdot \eta [\nabla \vec{u} + (\nabla \vec{u})^T] + \rho \vec{u} \cdot \nabla \vec{u} = -\nabla P + \rho g \beta (T - T_{ref}) \quad (3)$$

where $\eta, \rho, u, p, g, \beta, T$ are dynamic viscosity, density, velocity vector, pressure, acceleration due to gravity, thermal expansion and reference temperature respectively. Conduction-convection equation

$$\nabla \cdot (-k \nabla T + \rho C_p T \vec{u}) = 0 \quad (4)$$

The parameters k, T, C_p are thermal conductivity, temperature and heat capacity respectively. The boundaries for the Navier-Stokes equations are impermeable, no-slip conditions. The no-slip condition results in zero velocity at the wall, with pressure within the domain remaining undefined. The boundary conditions for convection and conduction application mode are the fixed high and low temperatures on the vertical walls, and others at insulation conditions. The model addresses a square crucible filled with silicon melt, fluid properties, and temperature drops using material (liquid Silicon) properties set up with dimensionless numbers like Raleigh and Prandtl numbers [8]. On the melt free surface, we consider slip/2D and axial symmetry condition [9],

$$\vec{u} \cdot \vec{n} = 0, \vec{u} \cdot \vec{t} = U$$

$$\vec{t} \cdot [-pI + \eta (\nabla \vec{u} + (\nabla \vec{u})^T)] \vec{n} = 0 \quad (5)$$

where, $p = 2\eta (\partial \vec{u} / \partial \vec{n})$, U is scalar velocity, \vec{t} and \vec{n} represent the boundaries of tangential and normal vectors, respectively. Since the boundary conditions involve \vec{u} alone,

the pressure can be eliminated. In this condition, vorticity is formed in fluid. So momentum equations can be written in curl form

$$\nabla^2 (\nabla \times \vec{u}) = \nabla^2 \omega = 0 \quad (6)$$

where $\omega = \nabla \times \vec{u}$ is the vorticity [10]. In the present case of two-dimensional motion with negligible inertia forces, it is convenient to introduce a stream function Ψ so that the conservation of mass equation is satisfied identically and the single non-zero component of vorticity becomes $\omega = -\nabla^2 \Psi$

$$\text{then } \nabla^2 (\nabla \times \vec{u}) = 0 \text{ becomes } \nabla^2 (\nabla^2 \psi) = 0 \quad (7)$$

The Raleigh number(Ra) denotes the ratio of buoyant to viscous forces.

$$Ra = (g\beta TL^3)/(\eta\rho^{-1}K CL^{-1}) \quad (8)$$

Here, η is dynamical viscosity L is the length of the system.

4. Mesh Generation

The quality of the grid plays a direct role on the quality of the analysis, regardless of the flow solver used. Additionally, the solver is more robust and efficient when using a well constructed mesh. Triangular grids(T-grids) were generated for in this numerical analysis for considered molten system. Figure 2 shows the mesh generated of molten silicon domain in DS furnace. Boundary conditions used in heat transfer computations are specified at the boundaries of the computational domain. A numerical method based on an adaptive mesh refinement discretization exhibits a computationally efficient technique to solve the transport process of conservation equations like mass, momentum, energy etc, describing the evolution and dynamics of thermal boundaries.

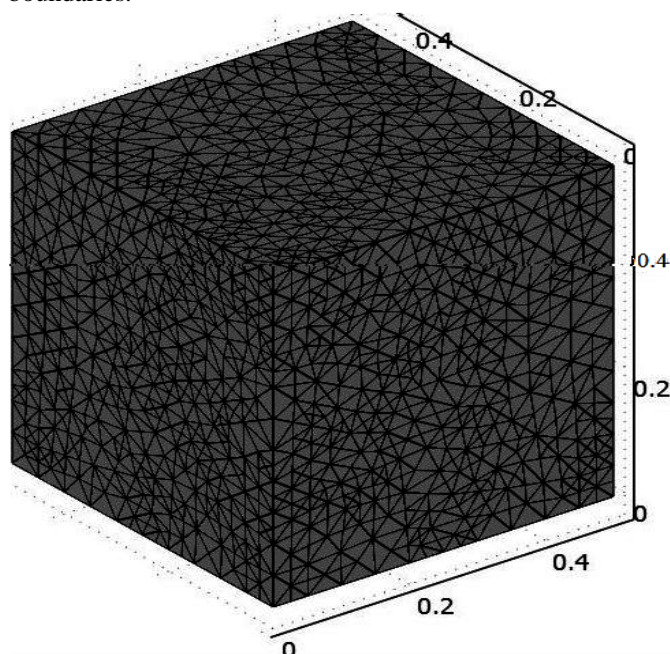


Figure 2: Mesh Generation for melt domain in DS system using finite element method

The governing equations and the boundary conditions for the melt flow and heat transfer characteristics in the molten Si system are solved numerically using finite element method in

which the calculation domain is discretized as triangular element into a finite number of elements. The mesh nodes are between 87954 and 119087 for considered system. The computations are performed using the three-dimensional(3D) axis-symmetry hypothesis for molten silicon of rectangular-shaped silica crucible. The time-independent, Newtonian, incompressible Navier-Stokes model for fluid flow, heat and mass transfer, along with weak form of the boundary is solved using the finite-element numerical technique. By default, the conditions of zero velocities (Wall boundary conditions) are used at the solid-gas boundaries.

5. Simulation Results and Discussion

The numerical simulations of molten Si flow properties such as stream line flow, Peclet numbers Reynolds numbers, convective and conductive heat flux, vorticity generations were carried out using finite element method for the various Rayleigh numbers. In this paper, we have focused only on the vorticity generation of molten silicon for the three Rayleigh numbers (10,1000 and100000) with constant temperature difference 10K at constant Prandtl number $Pr = 0.01$. Vorticity[11] is main physical phenomenon during directional solidification of mc-Si growth. Apart from the velocity field and temperature distribution, the vorticity generation is possible during melt crystal growth process. It could be controlled by rotating crucible or applying the magnetic field on the melt flow. Vorticity is related with the linear integrals of the velocity. From the obtained simulation results, there are two types of vorticities generated. One is primary vorticity at central melt regime, other one is secondary vorticity at periphery melt region which are shown in figure 3.

Figure 3(a) shows that the primary vorticity occupied most of the melt region with very low vorticity values, below 30(1/s), for low Raleigh number $Ra= 10$. At the same time, the secondary vorticities are formed only in very small region. So, the melt flow fluctuation may not be much for this Rayleigh number. Figure 3(b) displays that the primary vorticity is dominated at central region compared to the secondary vorticities of periphery region of melt domain at Rayleigh number $Ra =1000$. It may lead to heavy melt fluctuation and inhomogeneous dopant and impurities distributions in growing crystal. Figure 3(c) shows that secondary vorticities are heavily dominated to compare the primary vorticity with high vorticity values of more than 100(1/s). This has created more perturbation of melt flow during directional solidification growth process. So, we suddenly need to control using appropriate external force on the melt flow. Otherwise, the growing crystal becomes bad in quality. The Positive value of vorticity corresponds to the melt surface moving upwards and the negative value of vorticity corresponds to the melt surface moving downwards. We conclude from the obtained results that the low Rayleigh number is preferable.

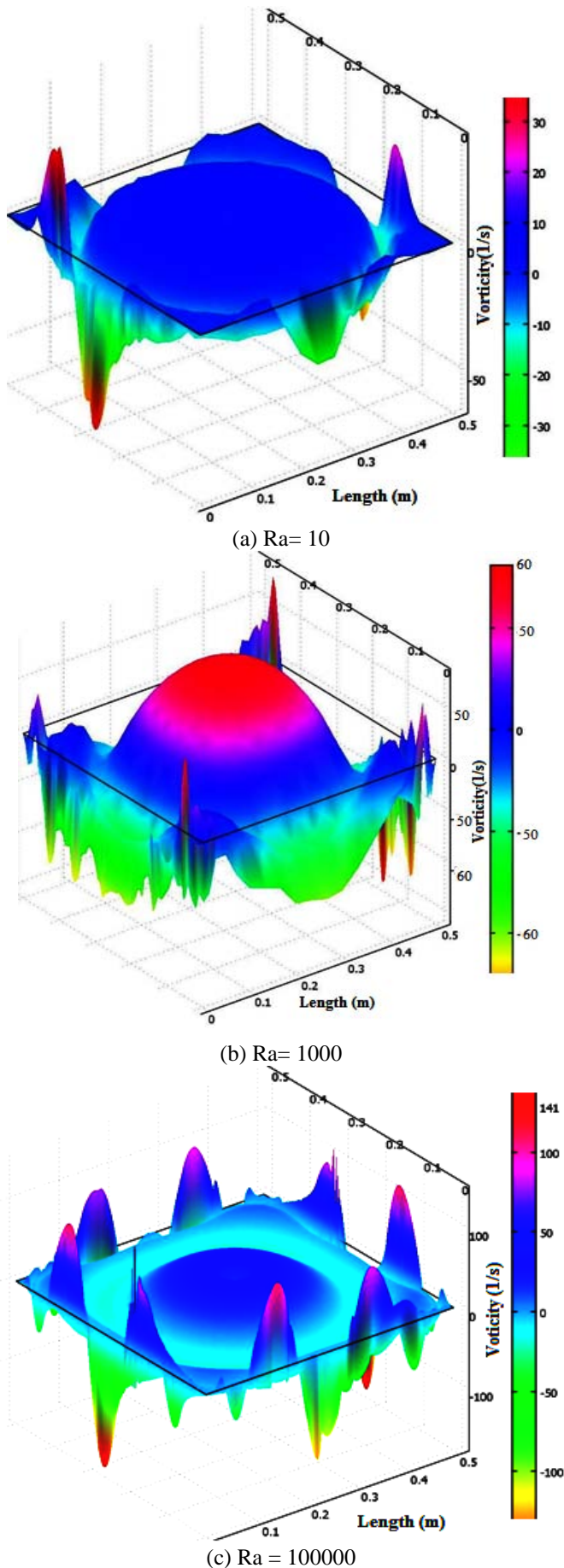


Figure 3: Vorticity generation in molten silicon at various Rayleigh numbers

6. Conclusions

We carried out numerical simulations of heat transfer and fluid flow characteristic of mc-Si melt in a directional solidification system for mc-Si ingot growth using finite element technique. A stationary model of the framework has been made using incompressible Newtonian fluid flow of Navier-Stokes equation in the Boussinesq approximation and the convection-conduction equation. Our objective in the present work was to study the convective flows induced by a temperature gradient and understanding the fluid mechanism for various Rayleigh numbers during multi-crystalline silicon crystal growth process for PV application. Vorticity generation study is essential to control the melt flow fluctuations. We have studied the vorticity generation of the melt flow due to buoyancy effect in silicon fluids. The present study is focused on the influence of Rayleigh numbers. The Rayleigh numbers ranging between $10 < Ra < 10000000$, are simulated at constant Prandtl number (0.01) and the results are given in the present paper only for $Ra=10$, $Ra=1000$ and $Ra=1000000$. The computed results reveal that dimensionless numbers should be incorporated with silicon melt growth of directional solidification process.

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Department of Physics, Government College (A), Rajahmundry, Andhra Pradesh, India