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Modelling of Multi-Crystalline Silicon Growth Process for PV Applications

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Abstract : Multi-crystalline silicon is an important material with advantages of low-production cost and high conversion efficiency of PV solar cells. Directional solidification method has become the preeminent technique for producing multi-crystalline silicon for solar cells because of its better feedstock tolerance, higher throughput and easier operation. Solar cell efficiency is decreased by impurities, precipitates, and structural defects in the mc-Si ingots, and the generation and distribution of these are mainly determined in the DS process. Numerical simulation is a comprehensive tool in modern process development which is extensively used for promotion of crystal growth processes. The melt flow in the crucible has 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**.** The control of grains as well as the grain boundaries is particularly important to the crystal quality and thus the solar cell efficiency. The computations are carried out in two dimensional (2D) axisymmetric model by the finite-element numerical technique. The melt flows and its thermodynamic properties like temprature distribution, stream line flow, X-velocity field, convective heat flux , vorticity are accurately simulated to analyze at constant prandtl number for two various Rayleigh numbers. In the present paper, stationary parametric dimensionless model of molten silicon on multi-crystalline silicon crystal growth by the directional soldifictaion method has been developed.
Key words: solar cell; heat transfer; simulation; directional soldification.

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 soldification 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 [3,4].

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 physics governing the growth of mc-silicon in the directional solidification system involves complex non-linear transport phenomena of heat and mass transfer processes. Crystal growth experiments are expensive and time-consuming, modelling 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[5]. 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[6]. 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 soldification 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[7]. 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 [8]. The effects of buoyancy on the melt flow and heat transfer like X-velocity field, Y- velocity field, pressure, convective and conductive heat flux were investigated for molten silicon by directional solidification system using the finite element technique.

DS System Model:

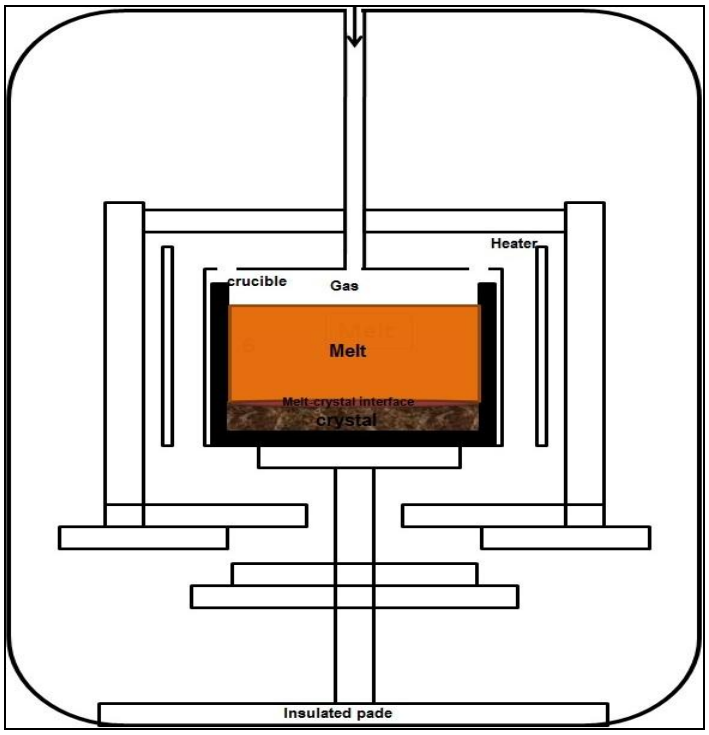


Figure .1 Schematic diagram of the DS furnace

The schematic diagram of industrial-scale DS system is shown in Figure 1. The system is used for growing mc-Si ingots traditionally for solar cell application. 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: Figure.1 shows the DS furnace for growing multi-crystalline silicon. A directional solidification apparatus consists typically of a rectangular–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.

Mathematical equations:

The rectangular silica crucible with molten silicon is considered to the computational domain which is used for the local 2D-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 [9]

Momentum (Navier-Stokes) equation

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

Continuity equation

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

Navier-Stokes equation with Boussinesq approximation

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

where η, ρ,u, p, g, β,T. are dynamic viscosity , density, velocity vector, pressure, acceleration due to gravity, thermal expansion and reference temperature respectively.

Conduction-convection equation

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

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 rectangular 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[10].

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

$$Ra = (g\beta TL^3)/(\eta\rho^{-1}K\,CL^{-1}) \quad (5)$$

The Prandtl number(Pr) denotes the ratio of momentum and thermal diffusivities

$$Pr = (\eta\rho^{-1})/(K\,CL^{-1}) \quad (6)$$

Here, υ is Kinematic viscosity L is the length of the system.

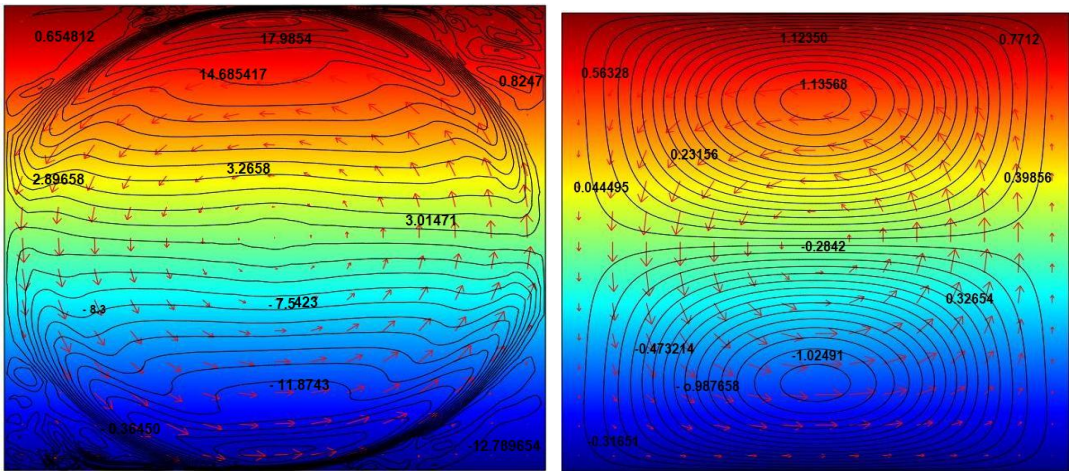
Numerical Method:

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. 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 computations are performed using the two-dimensional(2D) 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[11].

Simulation Results:

Numerical analysis of the silicon melt in DS system were investigated based on assumption of a stationary state under a 2D axisymmetric model. Time independent simulations were performed in Si melt for various dimensionless numbers. In this study, we can analyze a wide range of assumptions using the parametric

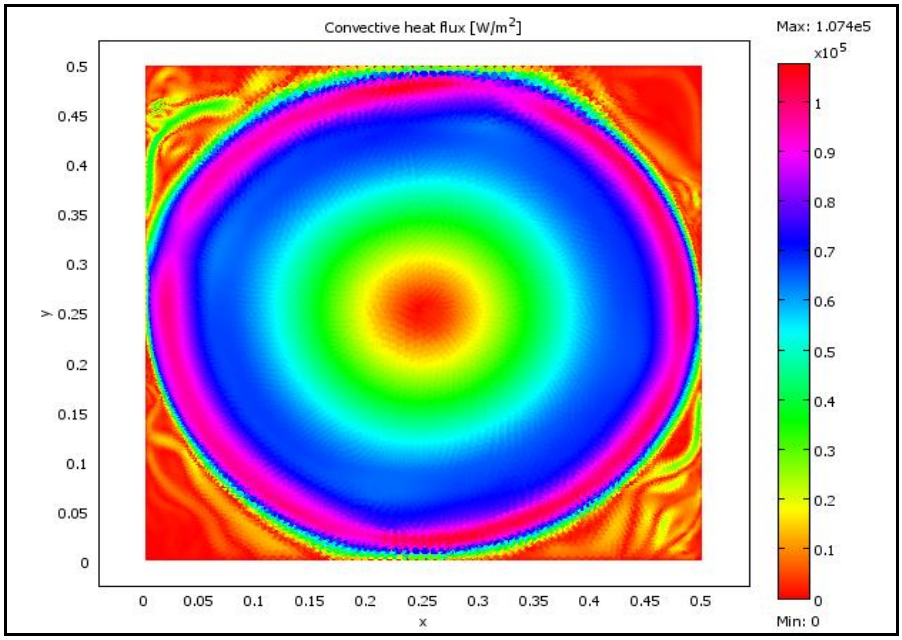
solver and sequencing through different values of Rayleigh numbers(Ra) with constant Prandtl number(Pr). The simulation results in Figure 1. which summarizes temperatures (surface), velocity fields (arrows), and y-velocities (contours) for two Rayleigh numbers.



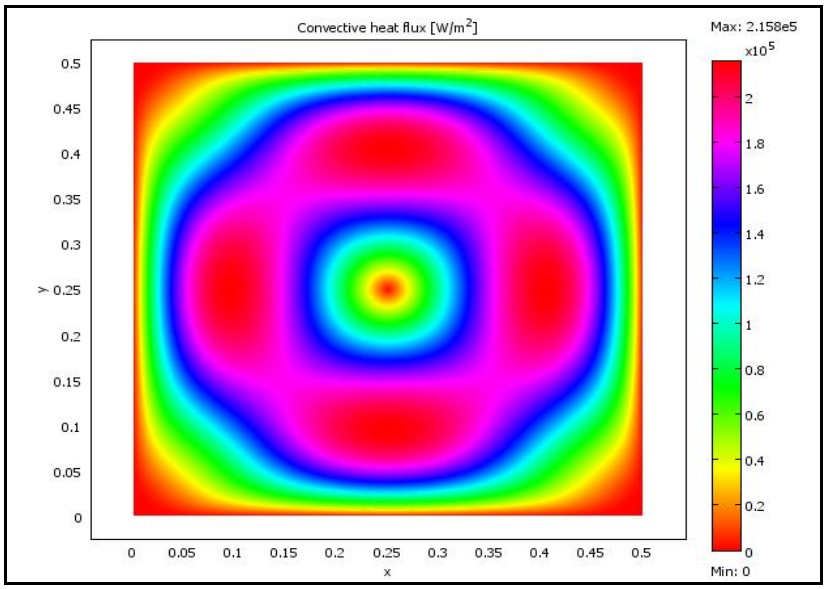
(a) Ra= 1000 **(b) Ra=1000000**

Figure 2: Dimensionless solution for buoyancy flow in the molten silicon system for two Raleigh numbers at constant Prandtl number: Temperature (surface plot), velocity field (arrows), and y-velocity (contours).

Figure 2. shows the developing velocity contour when increasing the Rayleigh number from 1000 to 1000000. The melt flow contour is split as two region when increasing Raleigh number. The results indicate in the Figure .1 how the vigour and complexity of the convection increase at higher value of Ra. Figure 3. demonstrates convective heat flux of molten system with two various Raleigh numbers(1000, 1000000). If Rayleigh number is increasing the convective heat flux also randomly increased in most of the melt. This convective heat fluxes are influenced to Marangoni convective flow. It may affect the growing crystal's homogeneity and impurity distributions. So, we can control the melt flow pattern when we optimize the Raleigh numbers of molten silicon during direction solidification.



(a) Ra = 1000



(b) Ra=10000000

Figure 3: Convective heat flux of silicon melt system for two Rayleigh numbers

Conclusion:

Our objective in the present work was to study the convective flows induced by a temperature gradient and understanding the fluid mechanism for various Raleigh numbers during directional solidification crystal growth process for PV application. Heat transfer characteristics like temperature distribution, velocity field, convective of molten silicon, during solidification of mc-Silicon growth process have been studied numerically using finite element technique. We have analysed the motion of the flow due to buoyancy effect in silicon fluids. The present analysis is focused on the influence of a limited number of dimensionless parameters. The Raleigh numbers ranging between 1000 < Ra < 10000000, are simulated at constant Prandtl number(0.011) and the results are given in the present paper only for Ra=1000 and Ra=1000000.

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