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Modelling of physical phenomena on Si melt during crystal growth process by Directional solidification method

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Abstract: Numerical simulation is a comprehensive tool in modern process development which is extensively used for promotion of crystal growth processes. Multi-crystalline silicon is an important material with advantages of low-production cost and high conversion efficiency of PV solar cells. The control of grains as well as the grain boundaries is particularly important to the crystal quality and thus the solar cell efficiency. The understanding transport of heat, mass and momentum is an especially essential in bulk crystal growth processes. Flow in the molten phase is indispensable for transport of heat and mass convection in bulk crystal growth systems. The computations are carried out in 2D model by the finite-element numerical technique._The fluid flows and their heat transfer characterstics like temprature distribution, stream line flow and velocity field are accurately simulated to analyze the various Rayleigh numbers. In this work stationary parametric dimensional model of crystal growth by the directional soldifictaion method has been developed. The convergence is handled by monitoring residuals of non-linear Navier-Stokes and energy equations.
key words: physical modelling; heat transfer; crystal growth; directional soldification.

Introduction:

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 mechanisms inside furnace, theoretical analyses and numerical simulation with these models has been an attractive topic in the circles of applied physics, materials science, and applied mathematics [1, 2]. With the awareness of global warming and the shortage of fossil energy, photovoltaic industry has been growing very rapidly in recent years. The majority of the solar cells are made from silicon. Especially, due to its low cost and high throughput in production, multi-crystalline silicon (mc-Si) produced by directional solidification (DS) has attracted much attention[3]. In the present investigation, numerical simulations were performed to study flow and thermal fields of non-Newtonian fluids in silicon melt of rectangular cruibles. 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[4] . The melt flow inside the crucible is complicated due to buoyancy and surface tension. 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. 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]. Here, the effects of buoyancy on the melt flow and heat transfer were studied for directional solidification process using the numerical technique.

Modelling:

The rectangular crucible with silicon melt is taken to the computational domain which is used for the local 2D-simulations. The Si melt flow is described by conservation equations written as momentum (Navier-Stokes equation) and continuity of an incompressible, Newtonian fluid with the application of the Boussinesq approximation[6].

Navier-Stokes equation with Boussinesq approximation

$$-\nabla.\eta[\nabla\vec{u}+(\nabla\vec{u})^T]+\rho\vec{u}.\nabla\vec{u}=-\nabla P+\rho g\beta(T-T_{ref}) \qquad (1)$$

where the variables 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

$$\nabla.(-k\nabla T+\rho C_P T\vec{u})=0 \qquad (2)$$

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.

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

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

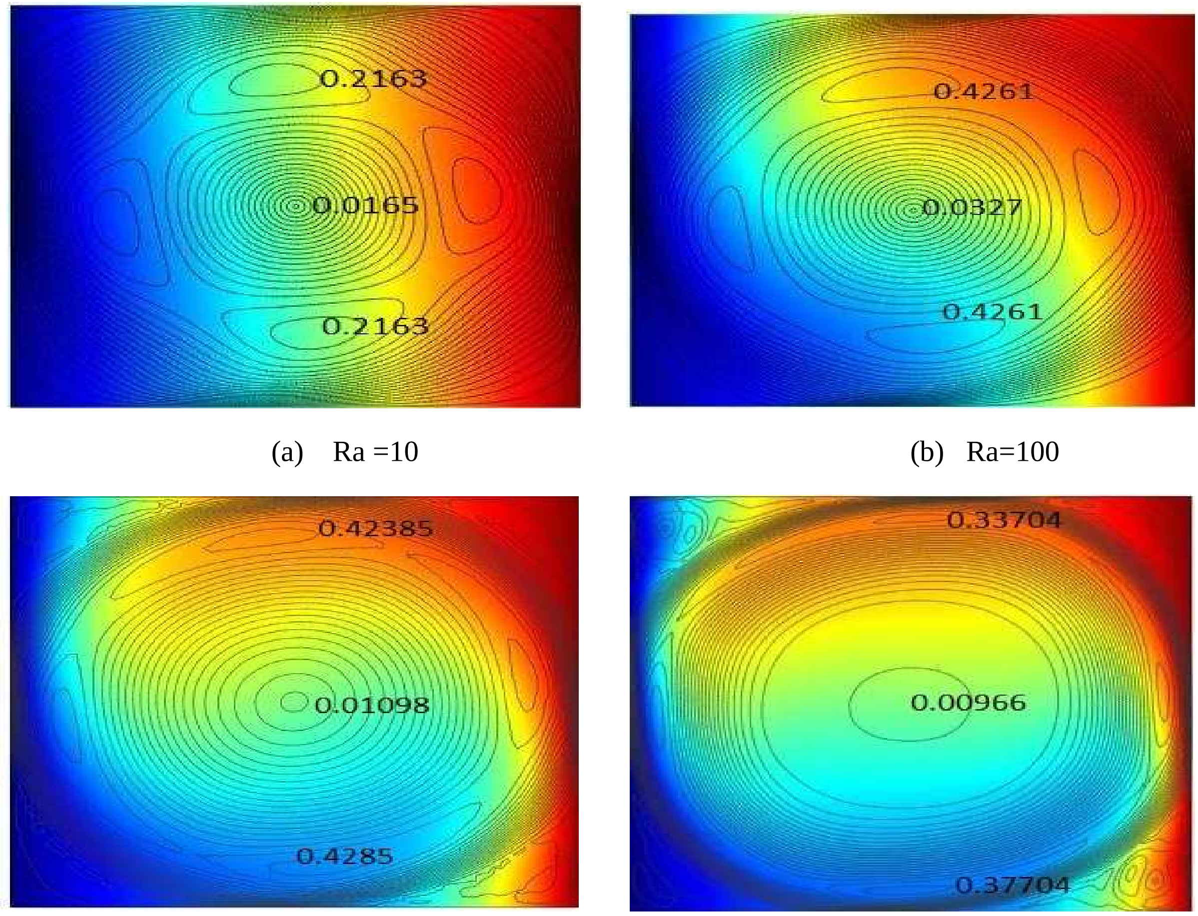
The Prandtl number(Pr) denotes the ratio of momentum and thermal diffusivities

$$Pr = (\eta\rho^{-1})/(K\ CL^{-1}) \qquad (4)$$

Here L is the length of the system.

Simulation Results:

Numerical simulations of the DS melt flow were based on an assumption of a stationary state under a 2D model. Time independent simulations were performed in Si melt for 4 different Rayleigh numbers and velocity field was also analysed. It can be observed in Fig. 1 that Ra increases as viscous forces decrease. Figure 1 show the developing velocity contour when increasing the Rayleigh number as 10, 100, 1000 and 10000 respectively. The results indicate in the figure .1 how the vigour and complexity of the convection increase at higher values of Ra.



(a) Ra =10 (b) Ra=100

(c) Ra-1000 (d) Ra=10000

Figure 1: Temperature distribution of Si melt and velocity field of contour for different Rayleigh numbers at constant Prandtl number (0.65).

Conclusion:

Flow and heat transfer in the melt, during directional 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 ranges of the parameters studied herein are: $10 < Ra < 10000$.

References:

1. Davis S H. Theory of solidification[M]. Cambridge: Cambridge University Press, United Kingdom, 2001.
2. Xu J J. Introduction to stability and dynamics of interface in solidification[M]. Beijing: Science Press, 2006.
3. Lan C W, Lan W C, Lee T F, Grain control in directional solidification of photovoltaic silicon, Journal of Crystal Growth., 2012, 360, 68–75.
4. http://www.comsol.co.in/support/books
5. Qisheng Chen, Yanni Jiang, Junyi Yan, Ming Qin, Progress in modeling of fluid flows in crystal growth processes, Progress in Natural Science., 2008, 18,1465–1473.
6. De Vahl Davis G and Jones I P, Natural convection in a square cavity—a comparison exercise, Int. J. Num. Meth. in Fluids., 1983, 3, 227–248.

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