Modeling on control of melt convection during mc-Si growth process under the influence of magnetic field

M. SRINIVASAN*, G. ARAVINDAN, P. RAMASAMY

SSN Research Centre, SSN college of Engineering, Chennai-603110, India.

Numerical simulations have been performed on directional solidification furnace with magnetic induction coils. The rotating magnetic field was applied by using magnetic coils to influence the melt stirring and melt-crystal interface shape. The velocity of the melt flow and distribution of the stream function were improved by placing the magnetic induction coils inside as compared to outside of the insulation which may be used to control the melt flow patterns. The value of velocity field in silicon melt flow is 2E-5 m/s when the magnetic coil is placed inside the insulation. The value of velocity field in silicon melt flow is 2E-4m/s when the magnetic coil is placed outside the insulation. And, the resistive heaters are replaced by the inductive heaters to produce the heat and magnetic fields simultaneously. The results are compared with the magnetic coils placed inside the insulation.

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1. Introduction

The global increase of energy consumption leads to increasing environmental problems caused by greenhouse gasses. It can only be resolved if the power generation from renewable energy sources can be strongly raised in the future. The electric power generation by conversion of sun light via solar cells is one of the assuring options of renewable energy sources. In 2014, the cumulative photovoltaic capacity is increased by around 40 GW or 28% and reached at least 178 GW by the end of the year. A global total new solar PV capacity of 55 GW was added in 2015. Growth forecast for 2016 is 21% rise (to 66 GW). Silicon is the second most abundant element in Earth's crust by weight whose forbidden band is quite narrow, about 1.1 eV. Due to its semiconducting and most abundant nature silicon is preferred as a most predominant material in PV industries. Currently, around 90% of industrial solar cells are made from silicon ingots. To produce photovoltaic (PV) silicon wafers, two main techniques have been involved. One is Czochralski method, which gives high-quality mono-crystalline silicon material and another one is the directional solidification process which is used to produce multi-crystalline silicon ingots at low cost[1]. During the directional solidification process, melt convection is an important one which affects the crystallization occurred in the molten silicon. The conversion efficiency of the directionally solidified material is lower when compared to monocrystalline silicon wafers because of the less favorable crystalline structure of mc-Si ingot. Therefore, considerable efforts are needed for improving the quality of mc-Si ingot in DS process. During the crystallization process, the silicon is contaminated with non-metallic impurities such as C, O and N and the metallic impurities like Fe, Co and Ni which affect the electrical and mechanical behavior of the mc-Si

wafers. Therefore, understanding the complexity of these impurity sources and their impact on the material quality is very important [2]. Defects and dislocation clusters act as recombination centers, which affect the conversion efficiency. The quality of the crystal depends on the lifetime of minority carriers. If the resulting product of mc-Si ingot has low minority carrier lifetime, the solar cell wafers will become poor in efficiency[3-4].

Researchers have put considerable effort on the optimization of the directional solidification of process parameters. Nakajima et al., [5] have controlled the dendrite arrangement in the dendrite casting method by the cooling pad with different thermal conductivity. Also, they have reported the enhanced cooling conditions [6]. Li et al., controlled the grains to get a high-quality mc-Si by introducing the notched - crucible [7]. Zhou et al., have shown that the final dislocation density can be reduced by the modified cooling process in mc-Si ingot production [8]. Xi Yang et al., have investigated the effect of temperature distribution, melt convection, c-m interface and thermal stress of mc-Si growth process in the DS process [9]. The thermal distribution, c-m interface shape and energy consumption and heat loss from different portions of the system have been analyzed [10]. T.Y. Wang et al., have reported the cooling spot furnace for the higher cooling rate at the center portion of the crucible than the other parts of the charge [11]. Last two decades, 2D and 3D simulation modeling was seriously performed for DS process by many researchers especially, C. Tanasie, J. Bauer, K. Kakimoto, C.W. Lan, K. Kutsukake, K. Fujiwara, etc[12-17]. Specifically, they are involved in reducing the formation of multi-nucleus and the recombination defects such as grain boundaries, twins and dislocation density which may affect the lifetime of minority carriers[18]. Now a days, research is focused on the application of vibrations, growth rate and crucible

rotation rate variations which are the techniques used in the directional solidification process to control the meltcrystal interface shape and melt convection[19-21]. Among these techniques, applying the external magnetic forces like a steady magnetic field and non-steady magnetic field have been shown to have beneficial effects [22]. Compared to steady magnetic fields, the non-steady magnetic fields such as traveling magnetic field, rotating magnetic field and alternating magnetic field have a high impact on the velocity flow fields and distribution of stream function of the melt during the crystallization process [23]. In our previous papers [26, 27], some of the dimensionless numbers such as Rayleigh number, Prandtl number, Peclet number based on heat transfer phenomena were discussed for controlling the melt flow velocity during the mc-silicon growth process. In this paper, a global modeling of heat transfer was performed to study the melt flow velocity and streamline function when subjected to the magnetic field on the crucible. The aim is to control the melt flow velocity and suppress the eddy formation in molten silicon for increasing the average grain size in grown mc-silicon ingot and reduce the impurities concentration. The study is performed in the framework of the incompressible Navier-Stokes equation in the Boussinesq approximation with convectionconduction equations. Also, Maxwell equations together with Ohm's law were used as body force. The computations are carried out in a two-dimensional (2D) axisymmetric model by the finite volume method. The influence of the magnetic field on molten silicon was simulated and analyzed. We report the distribution of stream function and velocity flow fields of the molten silicon under the influence of magnetic field by positioning the magnetic induction coils outside and inside the insulation of DS furnace. And the results were also obtained for the furnace using the inductive heaters which produce the heat and magnetic field simultaneously.

2. Description of DS model

The schematic diagram of industrial-scale DS system is shown in Fig. 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 and chamber wall. The silicon feed material is loaded into a silica crucible. The crucible walls are supported by graphite susceptors to avoid deformation at high temperature. The furnace is well sealed with a water-cooled wall and operates at a low pressure. The inert argon gas is used for purifying the growth environment in the system. A 2D modeling for DS furnace was carried out by using the finite volume method. In this paper, the numerical simulation results were analyzed by the applied magnetic field in different approaches. In one the magnetic coil is positioned outside the insulation(Fig.1a) and in another one the magnetic coil is placed inside the insulation (Fig.1b).



Fig. 1. Typical view of DS furnace (a) magnetic coils outside of the insulation (b) magnetic coils inside of the insulation and (c) inductive heaters.

Commonly, the researchers have used the magnetic coils outside the insulation in the laboratory scale. In industrial scale, due to the vast area, the strong non-steady magnetic field is required. Loss due to the thickness of insulation wall, heaters and the crucible wall have to be compensated. Such industrial application inductors are very expensive. High cost and field loss can be reduced by placing the magnetic coils inside the insulation, as close to the melt region. It may produce the required magnetic field. Fig. 1(c) shows the resistive heaters replaced by the inductive heaters. Such inductive heaters produce the heat and magnetic field simultaneously. A three-phase alternating current of frequency 50 Hz and phase shift 120^0 was applied to the inductive heaters for magnetic field generation. Thermo-physical parameters of DS components are given in Table 1.

Material	Variable	Value
Silicon (crystal)	Heat conductivity, k (W/m.K) Emissivity Density, ρ (kg/m ³) Latent heat, Δ H (J/kg) Heat capacity, C _p (J/kg.s) Poisson's ratio Young's modulus, E (Pa)	110.612-0.1507T+0.000109T ² -4.0094E- 008T ³ +5.668E-012T ³ 0.90160026208T 2339.5-0.03267 1800000 1000 0.217 1.653E+11
Silicon (melt)	Heat conductivity, k (W/m.K) Emissivity Density, ρ (kg/m ³) Melting point, T _m (K) Heat capacity, C _p (J/kg.s) Dynamic viscosity, μ (Pa.s) Latent heat, Δ H (J/kg)	66.5 0.3 3194-0.3701T 1685 915 0.008 1800000
Quarz	Heat conductivity (W/m.K) Emissivity Density, ρ (kg/m3) Heat capacity (J/kg.s)	4 0.85 2650 1232
Graphite	Heat conductivity, k (W/m.K) Emissivity Density, ρ (kg/m3) Heat capacity, C _p (J/kg.s)	146.8885-0.17687T 0.8 1950 710
Susceptor	Heat conductivity, k (W/m.K) Emissivity Density, ρ (kg/m3) Heat capacity, C _p (J/kg.s)	105 0.8 1720 1000
Insulation	Heat conductivity, k (W/m.K) Emissivity Density, ρ (kg/m3) Heat capacity, C _p (J/kg.s)	0.5 0.8 500 100
Argon	Heat conductivity, k (W/m.K) Heat capacity, C _p (J/kg.s) Dynamic viscosity, μ (Pa.s) Pressure (Pa) Molar mass (kg/k.mol)	0.01 521 8.466E-6+5.365E-8T-8.682E-12T ² 50000 40

Table 1. Thermo-Physical properties of DS components

3. Mathematical modeling

The molten silicon is assumed as a Newtonian incompressible fluid and the joule dissipation is neglected. Under the influence of magnetic field in the DS furnace, the transport phenomenon of silicon melt was governed by continuity equation, Navier-Stokes equation with Boussinesq approximation, energy balance, species conservation and Maxwell equations together with Ohm's law [24].

Continuity equation:

$$\nabla \mathbf{.u} = \mathbf{0} \tag{1}$$

Navier-Stokes equation:

$$\rho\left(\frac{\partial u}{\partial t} + (u.\nabla)u\right) = \rho g - \nabla p + \mu \nabla^2 u + F_L \quad (2)$$

Boussinesq approximation:

$$\rho g = \rho_{ref} \left(1 - \beta T_{ref} \right) g \tag{3}$$

Energy balance equation:

$$\rho C_{P} \left(\frac{\partial T}{\partial t} + (u.\nabla)T \right) = \lambda \nabla^{2}T$$
(4)

Diffusion equation:

$$\frac{\partial C}{\partial t} + (u \cdot \nabla)C = D\nabla^2 C \tag{5}$$

Maxwell equations:

$$\nabla H = j \tag{6}$$

$$\nabla E = -\frac{\partial B}{\partial t} \tag{7}$$

$$\nabla . B = 0 \tag{8}$$

$$j = \sigma(E + (uB)) \approx \sigma E \tag{9}$$

$$B = \mu \mu_0 H \tag{10}$$

$$F_L = jB \tag{11}$$

The results were taken by varying the value of magnetic field with a frequency 50 Hz and a phase shift 120^{0} by using the following equation given in the software.

$$B = B_0 \left(\frac{r}{R_0}\right)^{p-1} \left(\vec{e}_r \cos(p(\varphi - 2\pi f t)) - \vec{e}_\varphi \sin(p(\varphi - 2\pi f t)))\right)$$
(12)

where, B, B₀, R₀, p, ϕ , and f represent the magnetic field, field intensity, radius of the crucible, pole pairs count and frequency respectively. The above governing equation represents the rotation magnetic field.

4. Results and discussion

In this work, numerical calculations were done using finite volume method to simulate the thermo - physical properties during the crystallization process of industrial size mc-Si ingots. Predicting the behavior of an industrial-scale melt crystal growth process requires a faithful depiction of furnace-scale heat transfer along with a detailed accounting for heat transfer, melt convection, and solid-liquid interface motion. Here, the problem is mainly focused on the utilization of finite volume technique to understand the influence of magnetic field and thermal characteristics on molten silicon during directional solidification process. The temperature distribution in the silicon melt is nearly same for the magnetic coils outside and inside of the insulation pad which is shown in Fig.2 (a) and (b). When resistive the heaters are replaced by inductive heaters, the temperature distribution differed from the DS furnace using resistive heaters which are shown in Fig. 2(c).

The stream function is defined for incompressible flows in two dimensions with an axisymmetry. The flow velocity components can be expressed as the derivatives of the scalar stream function. The stream function can be used to plot streamlines, which represent the trajectories of particles in a steady flow. Considering the particular case of fluid dynamics, the difference between the stream function values at any two points gives the volumetric flow rate or volumetric flux through a line connecting the two points. The volumetric flow rate is the volume of fluid which passes per unit time. Yu et al [25], proposed that the value of the flow of stream function in the Si melt region is -9.59×10^{-4} m³/s for the case without magnetic field. Fig. 3(a) and (b) show the distribution of stream function in the molten silicon when the magnetic induction coils are placed outside and inside of the insulation. The magnetic coils placed outside the insulation result in two large vortices induced in the melt region which is shown in Fig. 3a. The lower vortex occupies the most of the melt domain. The center portion of this vortex has separated as a two small vortices nearer to the bottom of corner of the crucible. This flow of the stream function of the lower vortex is about -2.2013×10⁻⁵ m³/s. Hence the distribution of stream function is denser near to the crucible side wall.



Fig. 2. Temperature distribution of Si melt (a) magnetic coils outside, (b) magnetic coils inside and (c) inductive heaters.



Fig. 3. The stream function of the Si melt (a) magnetic coils outside (b) magnetic coils inside and (c) inductive heaters.

By placing the magnetic induction coils near to the melt region, the flow pattern of the stream function has completely changed as shown in Fig. 3(b). There is no separate smaller vortex in the center portion of the lower large vortex which is the result of the magnetic field near to the melt region. The distribution of stream function is more uniform, about -4.3009×10⁻⁵ m³/s. The distribution of stream function has less density around the crucible side wall, while compared to the magnetic coils outside of the insulation. Fig. 3(c) shows the better streamline flow patterns when replacing the resistive heaters by inductive heaters, the whole melt was almost occupied by a single vortex. The flow of the stream line in the melt region is about -6.3860 \times 10⁻⁵m³/s. And, the distribution of stream function near the crucible side wall is more uniform than in the magnetic coils inside and outside the insulation.

The velocity field of the melts determine the melt flow as turbulent or laminar. For growing better quality crystals, the controlling of melt velocity is required to make the melt flow as laminar. The melt convection plays an important role in solid-liquid interface shape and in the distribution of impurities and dopants. If the velocity of the melt becomes lower, the influence of convection on the melt flow becomes lower. The better control of melt flow velocity has been achieved when applying the magnetic fields. Dadzis et al. have shown that the unsteady segregation process of carbon and oxygen impurities results in a non-uniform concentration distribution under magnetic field condition[28]. Liu et al. have shown the effects of different types of traveling magnetic field on the molten silicon mixing and the solid-liquid interface shape at different directional solidification stages. The abovementioned results indicate that magnetic fields have an important role in the shape of the solid-liquid interface and the vortex flow of molten silicon during the directional solidification process[25]. Also, the melt velocity value is very important to decide the crystal quality. So magnetic field is one of the tools to control the melt velocity. In our case, the results have proved that the velocity of the melt is damped by the magnetic fields very effectively. Fig. 4a shows the velocity flow field for the magnetic field(B) value 0.1T where the magnetic coils are placed outside the insulation.



Fig. 4. Velocity field of molten silicon (a) magnetic coil outside the insulation, (b) magnetic coil inside the insulation and (c) inductive heaters

The velocity field of the melt slightly decreases when the magnetic coils positioned near the crucible wall with the B value of 0.1T compared to the magnetic coils placed outside of insulation which are shown in Fig.4(a) &(b). For the inductive heaters, the velocity flow fields were more uniform than in the magnetic coils placed inside and outside of the insulation. If velocity field of molten silicon is low and uniform then the better quality of mc-silicon ingot can be grown by DS method. Therefore, our results demonstrate that modification of applied magnetic field in an industrial Si crystallizer may be used for growing better quality mc-Si crystals.

5. Conclusion

We have carried out the global simulation of heat transfer during directional solidification process under the influence of magnetic field. The simulation results were analyzed for stream function and the velocity field of the melt flow by applying the magnetic field with a different approach which means changing the position of magnetic induction coils and replacing the resistive heaters by inductive heaters. The uniform distribution of stream function, melt stirring and melt flow velocity were influenced by positioning the magnetic induction coils near to the melt region. Our simulation results proved that the magnetic field can be used to control the melt fluctuation and growth interface shape. It may be used to grow high-quality mc-Si ingot.

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*Corresponding author: srinisastri@gmail.com