4ème Conférence Internationale des Energies Renouvelables (CIER-2016)
Proceedings of Engineering and Technology – PET
Vol.15 , pp.115 - 121

Numerical Modeling *of* Silicon Ingot Growth *by* Directional Solidification

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Abstract

Directional solidification is widely **used** to **obtain m**ulti-crystalline **silicon ingots for photovoltaic solar ce**lls. I**n this technique, heat is extracted from the bottom of the crucible in order to initiate the solidification of silicon** melt. T**herefore, the crystal-liquid interface moves upwards**. B**y carefully adjusting the position of the bottom insulation and varying the heater power, the growth rate is controlled so as to favour the solidification of a highly oriented crystal.** In **the present study, we developed a numerical model to determine the temperature distribution, as well as the velocity field in the molten phase of silicon.**

KEYWORD: *DIRECTIONAL SOLIDIFICATION, SILICON, MULTIPHYSICS MODELLING*

INTRODUCTION

Directional solidification is set to become the preferred technique for producing multi-crystalline silicon (mc-Si) ingots [1-2]. After melting the initial silicon feedstock placed in a silica crucible, heat is extracted from the bottom (FIG.1-2) in order to initiate the crystallization of molten silicon. During growth, the melt phase is in the top, thus minimizing the negative effects of convection. Compared to high cost experiments, numerical simulation is an effective tool to predict and optimize the heat transfer in the furnace, in order to improve the crystal quality. Due to the complexity of the phenomena involved, numerical simulation becomes a precious toolso as to improve the process [3-8]. Heat and mass transfer during the solidification process are important for controlling both the solid-liquid interface and the impurities distribution in the ingot. To accurately track the solid-liquid interface, an enthalpy formulation methodology is adopted to model the phase change during the process [9].

The present study focuses on the determination of the temperature distribution and interface shape in the central part of the furnace, which includes the crucible containing silicon the graphite heat exchange block, the insulation parts, and heaters. Solidification of Silicon from the melt is modeled using a definite temperature of fusion, implying that the solid and liquid phases are separated by a sharp interface. Compared to the high cost experiments, numerical simulation is an effective tool to predict and optimize the heat transfer in the furnace, in order to improve the crystal quality. An open and closed thermal insulation was used to improve the DS process. It was beneficial because of its low heat loss, shorter growth cycle and efficient oriented solidification.

In this paper, we present a tractable simulation model of the temperature distribution in the growth furnace solved by Comsol Multiphysics. The model includes the latent heat of fusion in the apparent heat capacity.

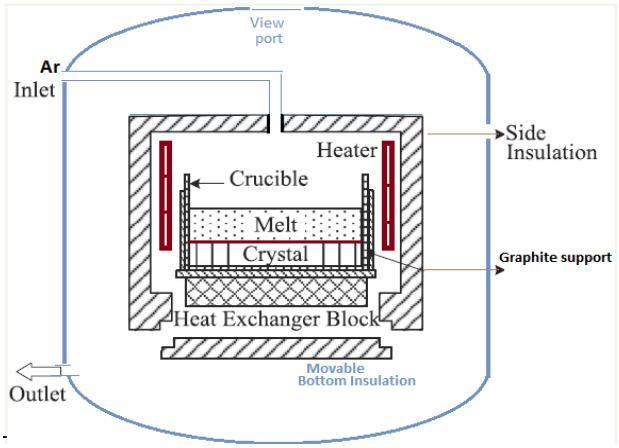

FIG.1: Interior of HEM furnace –*.Si-ingot is obtained in Si_3N_4 coated quartz crucible to prevent adhesion to its walls. The process steps are the following: -heating, melting,-Generation of appropriate thermal gradients in the melt,-Growth,-Annealing*

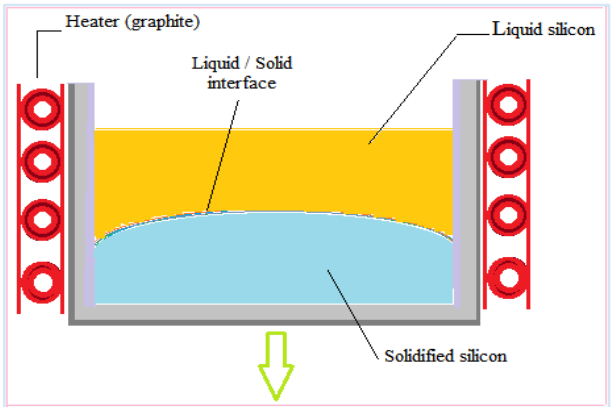

FIG. 2: **Principle of Directional Solidification technique**

2. Silicon ingot Growth

A reliable method for producing multi-crystalline silicon is the directional solidification. In this method, molten silicon is solidified in controlled conditions to achieve a quasi-planar solidification front between the solid and liquid phases.

ISSN 2356-5608

In HEM (*Heat Exchanger method*), *H*EX BLOCK is seated at the bottom of the crucible through which there is a localized heat evacuation. The process results in a homogeneous distribution of large columnar grains. Initially used to produce single crystals, this technique was adapted to get larger Si-ingots [10].

In DSS system, the crucible is kept stationary and the heat flow is controlled by the insulation movement. This technique results in shorter process times and a relatively planar solid-liquid interface [11-12]. Solidification takes place thanks to the axial temperature gradient in the furnace, and the goal is to produce a single nucleus from which a crystal will propagate and grow. Crystallization occurs by opening the isolation and slowly moving down the crucible containing the melted silicon out of the heated zone in the furnace.

During one experiment, we deliberately stopped the run for five minutes in order to fix the shape of the solidification front. A longitudinal cross-section photo of ingot is shown (FIG. **3**). The interface was clearly revealed to be slightly convex, which is typically a favorable case for the silicon crystal growth. In the corner we observed a linear grain growth due to the huge heat extraction in these areas. After recovering the experiment, we observed that the growth process is running while maintaining the same form of interface.

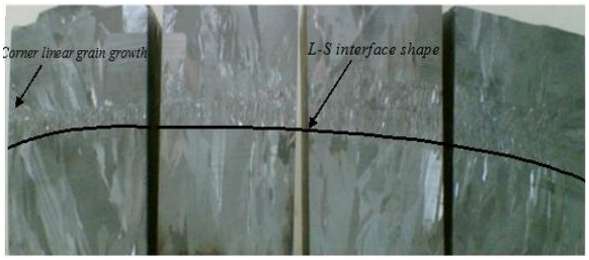

FIG. 3: **Photo** *of* the **L**-S interface as revealed

3. PHYSICAL MODEL

In this work, the melt is considered as Newtonian fluid, and the inert argon gas was treated as ideal. Physical parameters of the materials are indicated (TAB. I).

Table1: **PROPERTIES** OF MATERIALS USED IN SIMULATION

Physical properties. Silicium		
Melting temperature, T_m *(K)*	**1687**	+
Density, ρ*(kg* m^{-3}*)* , *L, S*	**2530**	**2330**
Thermal conductivity, $k(W\ m^{-1}K^{-1})$	**61**	**17**
Specific Heat capacity, $C_p(J\ kg^{-1}\ K^{-1})$	**1040**	**915**
Latent heat of fusion, $L_f\ (J.\ kg^{-1})$	**1.87 10^6**	
Dynamic viscosity, μ *(Pa.s)*	**7.57 10^{-4}**	
Thermal expansion $\beta_T(K^{-1})$	**1.4 10^{-4}**	

	$\rho(kg\ m^{-3})$	$C_p.(J\ kg^{-1}K^{-1})$	$k(W\ m^{-1}K^{-1})$
Graphite Heater	**1830**	**710**	**100**
Quartz Crucible	**2650**	**750**	**1.5**
Hex block	**1790**	**1800**	**140**

• Governing Equations

– Liquid phase

Governed by the NAVIER STOKES *equations: (1, 2)*

$$\begin{cases} \rho\frac{\partial \boldsymbol{u}}{\partial t} + \rho(\boldsymbol{u}.\nabla)\boldsymbol{u} = \nabla\left(-pI + \eta(\nabla\boldsymbol{u} + (\nabla\boldsymbol{u})^T)\right) + \overrightarrow{F} \\ \nabla\boldsymbol{u} = 0 \end{cases}$$

$\boldsymbol{u}$: Velocity vector, p the pressure, μ is the viscosity, ρ is the density, C_p the heat capacity. The velocity field that is calculated in common with the pressure field only within molten silicon is, in general, very difficult to obtain. As *Re* number is sufficiently low, it may be considered linear. Provided that the fluid is incompressible, its behavior can be described by N-S (1), supplemented with the continuity equation (2).

The body force $\overrightarrow{F}$ is composed by the forces supported by the fluid, i.e. due to natural convection: $\left(f_B = \rho\, \boldsymbol{g}\, \beta_T (T - T_M)\right)$. Additional forces are the solidification f_d, and the thermo-capillary force (surface tension).

$$f_d = -C\frac{(1-f)^2}{q+f^3}\boldsymbol{u}\ ;\ \vec{\boldsymbol{\sigma}}_{\boldsymbol{\tau}} = -\boldsymbol{\gamma}_T \cdot grad_\tau T \quad (3)$$

C is a characteristic constant of the growth interface (must be sufficiently high to extinguish velocities in the solidified cells), .f is the fraction of cell volume in the liquid state; q being a small computational constant to prevent division by zero.

- Heat transfer.

Steady state is assumed during the crystal growth process. Under this assumption, the thermal energy conservation may be written:

$$-\mathrm{div}\left(\mathrm{k(T)}\overrightarrow{grad T}\right) + \rho C_p u.\overrightarrow{grad T} = \mathrm{Q_{th}} \quad (4)$$

$\mathrm{Q_{th}}$: *Heat losses density*. (4)-*Energy conservation equation*

A set of boundary conditions must be formulated for the thermal problem. Heat flux conservations are kept at all interior boundaries of adjacent domains. The radiation surfaces are assumed as diffuse-grey. *N-slip* condition is applied on walls of the crucible. In order to account for the phase change, an enthalpy method based on fixed grids was employed to model the evolution of the solidification front [14]. Moreover, since we are interested in how the material melts and solidifies, the standard heat equation is modified by introducing an enthalpy formulation*. The heat and momentum transfer conditions at the interface are incorporated into the governing equations via introducing a pertinent source term.

**During the phase transition, a significant amount of latent heat is released. In addition, the specific heat capacity also changes considerably. To account for, we replaced C_p in the heat equation with $(C_p+\delta\Delta H)$, where ΔH is the change in enthalpy. δ is a Gaussian curve.*

4. *SIMULATION RESULTS*

A modeling work using COMSOL has been developed for simulation of the crystal growth dynamics. In the calculation, temperature of the cooled chamber walls is imposed (=300K),

ISSN 2356-5608

while the thermal field in the system; the flow velocities and the melt-crystal interface are the computation results.

- HEAT TRANSFER

The heat transfer characteristics were calculated, and the results graphically depicted. The thermal field in the system is shown (Fig. 4), zooming inside the hot zone of the furnace.The simulations show a slightly concave interface shape at the beginning of the growth cycle. The interface is curved near the crucible wall and relatively flat at the central region.

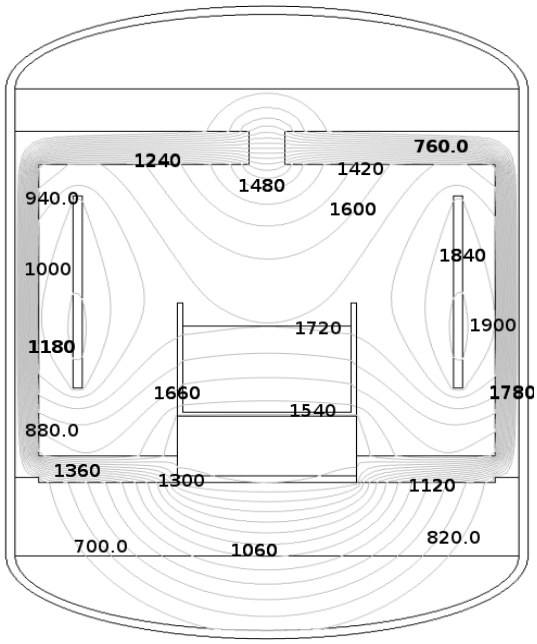

FIG. 4: Global Temperature distribution

- FLUID DYNAMICS

The aim in determining the melt flow pattern is to find a relation to the crystal growth behavior. Therefore, it is necessary to understand its origin and the dependency of the different forces acting on the molten zone.

1) Flow driven by natural convection

First of all, it is necessary to know how the fluid moves only due to the natural convection, driven by the heat transferred from the walls of the crucible to the melt. In fig. 6, one can observe the radial and axial velocities of the melt. As expected, the flow moves upward along the crucible walls. This is because the melt expands and becomes less dense when heated by the walls of the crucible. It cools down and becomes denser while flowing along the surface. Next, it flows down again through the centre of the liquid region.

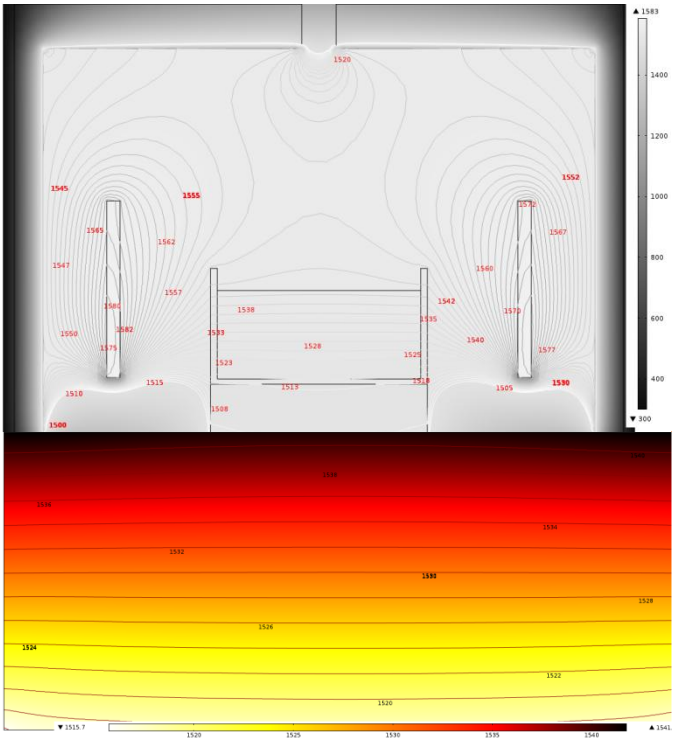

Fig. 5: isotherms in the silicon domainzoom inside the hot zone of the furnace (up).

There are two vortices in the silicon melt. Both of them are induced by the thermal buoyancy force. The upper vortex circulates inward along the melt free surface, while the lower one flows in the opposite direction. The main clockwise flow is stronger, as the horizontal temperature gradient and the corresponding thermal buoyancy force near the crucible side wall are larger.

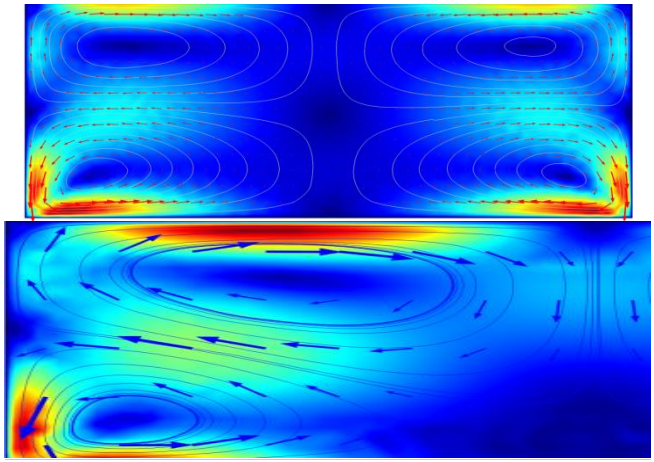

Fig. 6: Fluid velocity mapping and streamlines in the silicon melt

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2) MARANGONI CONVECTION

The velocity of fluid in melted silicon is significantly higher at the surface than in the volume. The fluid on the free surface *(hotter)* is moved to the low-temperature regions by the gradient of surface tension. The thermal map and the fluid velocity field in the melt (represented by vectors) are shown (Fig.7). As can be seen, four circulation zones *(vortices)* are generated in the fluid.The lower one is driven by the radial temperature gradient caused by the interface curvature. The upper one transports silicon fluid from the surface downwards into the melt volume at the center, and upwards at the crucible wall. In contrary, the silicon melt in the region of the lower vortex goes up in the center and descends near the crucible wall.

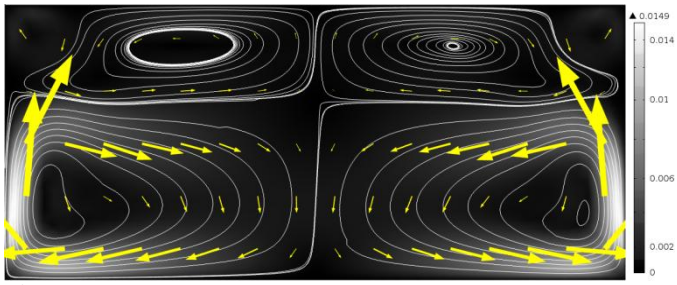

Fig.7: Fluid velocity mapping in the melt taking account MA-convection

3) Solidified silicon ingot

Near the meltingisotherm, the fluid convection is driven by the radial temperature gradient, caused by the interface curve. This leads to an increase of its convexity during the process.At the beginning of the solidification, there are two convection cells, with the most important being the one closest to the surface; this cell moves the melt from the side towards the center near the solidification front (Fig. 8). The control of the process must be very precise at the beginning of the solidification cycle. The melting velocity must be slowed down to reach an equilibrium state when molten silicon is complete.

The melt velocity and melt-crystal interface are shown.The fluid flow inside the melt is determined by natural convection; after establishment of the concave shape on the interface, the flow direction changes near the front. This feature is important for the distribution of impurities in the ingot. At half solidified fraction, the lower convection vortex has almost completely been replaced by the upper one.

The interface shape and the velocity field are easily affected by the latent heat at the final stage of solidification. There is only one vortex in the silicon melt compared with the two vortices flow pattern at the beginning stage of solidification, as is shown. The vortex flows outward along the melt free surface. Due to the smallest temperature gradient in the silicon melt, the intensity of the melt flow in is the smallest.

During the growth cycle, we noted the change of the solid-liquid interface from concave to convex shape, as seen from the liquid L-phase.In other words, the horizontal component of the temperature gradient changes gradually. This has beneficial effect on the final ingot quality by limiting the expansion of grains growing from the crucible walls, due to heterogeneous nucleation. According to representation of L-fraction in the crucible, the growth interface is slightly convex (favorable case)*;* convexity is maximum when the isotherm coincides with the corner of the crucible, then it is gradually flattened to become more planar at the end of the growth.

At slow growth rates, the m-c interface is relatively flat, which is beneficial for growing high quality silicon ingots. At high growth rates, the temperature distribution in the silicon melt makes the m-c interface convex to the crystal. Since the growth direction is vertical to the interface, poor quality silicon ingot will be produced in this case.

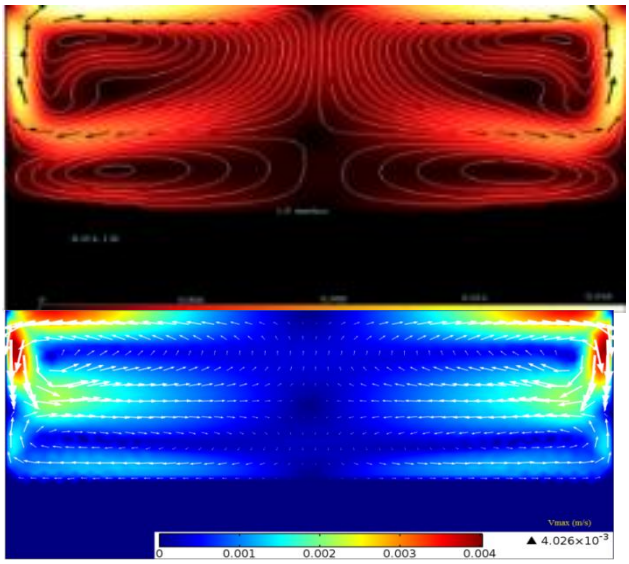

FIG. 8: **Evolution of velocities in the molten silicon** [m/s], streamlines inside the silicon domain at different stages of the Growth cycle.
Solid silicon is shaded in dark colour

CONCLUSION

We have performed a global simulation of heat transfer and fluid flow to study the solidification of silicon in a heat exchanger configuration. Thermal and velocity fields were calculated. The effect of temperature distribution on the melt convection patterns was pointed out. The silicon melt flow is in a laminar state dominated by the thermal buoyancy force.

The variations of interface type were attributed to variations in temperature gradients and to convection currents in the liquid phase. In the near future, the numerical simulation herein should provide useful information to improve the quality of multi-crystalline silicon ingot.

ACKNOWLEDGMENT

This work was completed thanks to the financial support from the National Fund of Research, DGRSDT/MESRS (Algeria)

ISSN 2356-5608

ISSN 2356-5608

REFERENCES

[1] X. Zhang, “Characteristics enhancement of cast Silicon ingots”, *Sol. Energy Mater. Sol. Cells*, 139, p. 27-33, 2015

[2] W. Shur, “Growth of multi-crystalline silicon by improved directional solidification process based on numerical simulation”, *Sol. Energy Mater. Sol. Cells*, 95, 3059, 2011.

[3] D. Frank, A. Muller, “Silicon ingot casting: process development by numerical simulations”, *Sol. Energy Mater. Sol. Cells*, 72, p. 83-92, 2002

[4] Optimization and Modeling of PV Silicon Crystallization Processes; Georg Müller, ISSCG 14 Dalian (2010)

[5] Xi. Yang, “Modified directional solidification system of Silicon based on optimizing Heat transfer”, *J. Crystal Growth*, 400, 7, 2014.

[6] L. Chen, Bing Dai, “Optimization of power consumption on silicon directional solidification system by using numerical simulations”. *J. Crystal Growth*, 354, pp .86-92, 2012.

[7] J. Chen, H. Chang; Numerical simulation of impurity transport under the effect of a gas flow guidance device in the growth of silicon ingots by the DS process, J. Crystal Growth 385, p. 1-8, 2014

[8] C. Prakash, M. Simonds, A. Signal, Int. J. Heat Mass Transfer 30, p. 2690-3, 1987

[9] C. Khattak, F. Schmid, "Directional Solidification of Multi-crystalline Silicon Ingots by HEM" *Proc. 22nd IEEE Photovoltaic Specialists Conference*, NY, 1991, p. 976-978

[10] N. Stoddard, R. Clark. Multi-crystalline silicon growth for pv application; J. Cryst Growth, 310, p.2178-2184, 2008

[11] D. Ciscato, M. Forzan, F. Dughiero: A new DSS furnace for energy saving in the production of multi-crystalline silicon. 35th IEEE Photovoltaic Specialists Conference (2010)

[12] D. Ouadjaout, et al., “Growth by the HEM method, and characterization of multi-crystalline silicon ingots”, *EUPVSEC* 20th, Barcelona. pp. 111-112, 2005

[13] R. Voller, C. Prakash. A numerical modeling methodology for convection-diffusion mushy region phase-change problems; Int. J. Heat Mass Transfer 30,p.1709-1719, 1987

[14] M SRINIVASAN, 'Modeling of physical phenomena on Si melts during crystal growth process by Directional Solidification method', International journal of Chem. Tech Research, 6 (2014)1585

[15] B. Devulpalli, S. Kulkarni, 'Modeling multi-Crystalline Silicon Growth in Directional Solidification Systems', ECS Transactions, 18 (1) (2009)1023–1029

[16] COMSOL MultiPhysics. v4.3a, 2012

ISSN 2356-5608