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SIMULATION OF SILICON CASTING PROCESS FOR PHOTOVOLTAIC (PV) APPLICATION

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Abstract

Directional Solidification System (DSS) is the commonly used casting station in the solar industry. In order to better understand the casting process, we use a commercial software ProCAST, primarily used in casting process simulation to predict the temperature distributions. As the software is based on first principles, it can be adapted to simulate the transient temperature field of the DSS station and the solidification process, including grain growth. The focus of this paper will be the temperature distribution, its corresponding solidification process and grain structure. The simulation results will be compared with cast silicon ingots.

Introduction

Global solar photovoltaic (PV) market installations reached a record high of 2,826 megawatts (MW) in 2007, representing a growth of 62% over the previous year. Meanwhile, production reached a consolidated figure of 3,436 MW in 2007, up from 2,204 MW a year earlier [1]. More than 90% of commercial PV modules are made from crystalline silicon, with the majority share of silicon grown as multi-crystalline ingots. Directional solidification of multi-crystalline silicon is the industrial production technique with the largest market share of solar silicon representing approximately 60%.

The quality of crystal grown by directional solidification is largely determined by the thermal field, which directly affects both the yield of good silicon from an ingot and the solar cell performance of resulting wafers. Because of the long cycle time and inability to directly observe the inside of the furnaces, numerical simulation was developed as a powerful tool to help understand the temperature distribution inside the growth furnace and to optimize the casting process.

In the past decades, several successful efforts were made in the simulation of silicon growth. More attention was recently gained in this area due to the fast development of the industry. A German group demonstrated the simulation of different types of silicon growth for PV from temperature, impurity segregation, dislocation density, and grain structure [2, 3]. Wu et al. compared two major types of casting stations, DSS and HEM, from the aspects of thermal field, crystal quality and shear stress [4]. The relative movement of various parts of furnace was considered in a global 3D time-dependent numerical simulation by Delannoy et al. [5]. The effects of melt convection on temperature distribution and growth front interface shape have also been studied [6, 7]. Liu et al. developed a transient code with a global model for the casting process, and carried out calculations of concentration of different impurities in a multi-crystalline silicon ingot [8, 9]. Besides temperature, stress and dislocation generation were investigated also

by simulations [3, 10, 11]. Grain structure directly determines the electrical performance of the cell. Some references reported the simulations of crystallization and grain structure of silicon ribbons and cast ingots [2, 12]. However, this analysis method is still far from being used in practical applications [2].

In this paper, a commercial software, ProCAST, predicts the transient 3D temperature distributions of a directional solidification cast silicon ingot during the solidification process. The relative movement of different parts in the furnace will be considered. Based on the temperature results, solidification fraction, crystallization and grain structure will be simulated and compared with grown silicon.

Growth Process and Software

The Directional Solidification System (DSS) station manufactured by GT Solar is widely used for manufacturing Silicon PV ingots. Heat is extracted through the bottom of the crucible in order to initiate solidification. Therefore, the crystal-liquid interface moves upwards from the bottom of the crucible. By adjusting the relative position of the crucible and insulation along with varying the heater power, the temperature gradient and growth rate are carefully controlled to favor the growth of a high quality crystal structure. Generally, the goal is to obtain vertically aligned grains which indicate good directional growth. This nearly unidirectional grain growth will avoid high thermal stress and reduce the dislocation density in the multi-crystalline ingot [2]. Dislocations will act as a recombination center and affect the electrical performance of solar cell. One of the other advantages of directional solidification is that the metal impurities will be pushed away from the crystal due to their small segregation coefficients. Therefore, the majority of the silicon ingot will have a quality suitable for a solar cell. The density of solid silicon is about 10% less than its liquid, which means that the volume of silicon will expand about 10% during growth. The directional solidification also provides the space for this expansion.

A schematic of a DSS station with opened insulation is shown in Figure 1. After the crucible with silicon charge is loaded in the station, the insulation is closed. The entire system is heated until the silicon charge is completely melted. To initiate silicon growth, the side insulation is moved up while all the other components remain stationary. The heat exchange block will therefore lose heat to the cold environment primarily by radiation. This causes high heat extraction from the bottom of crucible, initiating nucleation. The insulation remains open during the growth process, then is closed for annealing.

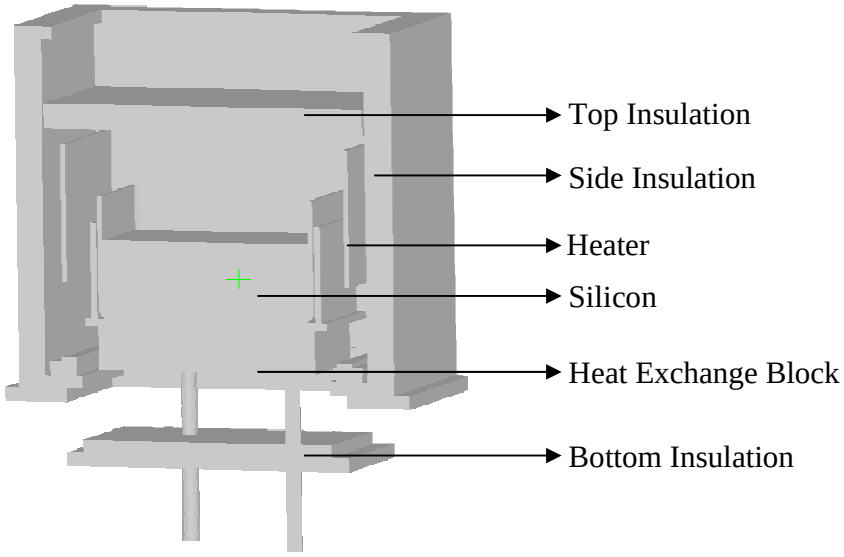


Figure 1. Schematic of DSS station with open insulation.

The commercial software ProCAST was chosen to simulate the 3D transient casting process and corresponding grain growth. While ProCAST is typically used for metal shape casting processes, the first-principles approach to the various physics solvers and flexibility in user input allows the DSS process and silicon ingot solidification with crystal growth to be accurately simulated.

The simulation begins with a "macroscopic" finite element simulation of the thermal transients during solidification based on the conditions of the process. Included in this calculation are both true view factor radiation effects as well as moving volumes for the raising of the insulation. The radiation view factors are updated with the movement to provide the directional solidification intended in the process, as well as to maintain high accuracy in the solution.

These temperatures and fractions solid are then transferred to the CAFE solver to determine the "microscopic" nucleation and crystal growth. This "CAFE" method, or Cellular Automaton Finite Element method, efficiently bridges the gap between micro- and macro-scopic level results, providing simulations of the crystalline structure formation of a given solidifying material. Users can view the crystal orientations, nucleation sites, crystal boundaries and growth with the benefit of understanding and estimating the quality of the resultant casting.

CAFE essentially uses Finite Element (FE) analysis as the macroscopic analysis method, in order to generate thermal, fluid, stress or other typical transients. Overlaid in the FE space is also an orthogonal grid of cubic cells, which are of much smaller size than the finite elements. The temperatures are then mapped from the FE nodes to CA cells, and, over time, produce the simulated grain formation calculated by the CA cells. The interaction of FE nodes and CA cells is not limited to a simple mapping of temperature history. A "fully" coupled interaction provides FE temperature and CA latent heat release coupling at each thermal calculation iteration during the given time step. A "weakly" coupled interaction is performed once per step. Finally, an "uncoupled" mode is provided which creates the temperature history independently from the CA grain nucleation and growth. The "fully coupled" method provides highest accuracy; while the "uncoupled" mode provides fastest solve time.

The nucleation evolution is controlled by a simple Gaussian distribution based on the undercooling in the liquid, as developed by Oldfield for continuous nucleation distribution, where the grain density increase is induced by an increase in the undercooling. A grain of random orientation is positioned at the nucleation site, and is now ready to grow [13, 14].

Growth kinetics may be described in a few different methods, which are all based on the advancement of the solidification front. The model typically used is a simple cubic polynomial, where the coefficients can be adjusted based on calibration techniques. As the grain tips grow at random orientations, they intersect and a grain selection is performed, where the tip that reaches the intersection location first continues, and the late-arriving tip is terminated [14].

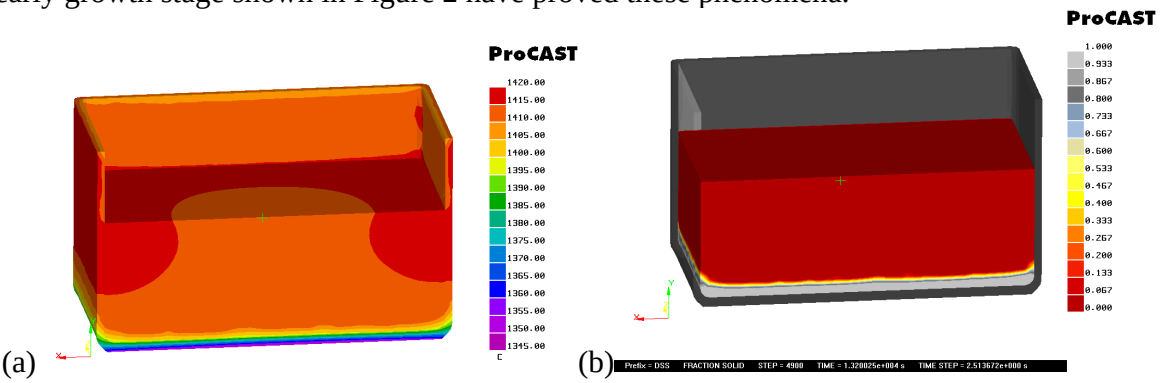
CAFE analysis is used in a wide variety of applications. Grain formation in single crystal (SX) and directionally solidified (DS) castings provide a microscopic level of insight into the relationship between solidification conditions and grain selection and growth. CAFE is widely used in metal casting to simulate grain structures and strains [13, 15, 16]. As computer hardware continues to advance in processing speed and memory storage, it is possible that a grain-based look at the casting process will be the standard method of processing, thereby providing an extremely detailed and accurate analysis of the casting process.

While CAFE is mostly used in dendritic growth, it may be adapted to the silicon casting process. The primary silicon grain growth direction is along the direction of maximum temperature gradient, which is similar to dendritic growth. Silicon growth preference is also given slightly to the favored silicon lattice growth directions. With a higher temperature gradient, dendritic growth is more dominant. This initial trial applies the CAFE model on a silicon casting. Additional work is needed to simulate silicon grain growth more accurately within the CAFE system.

Ingot Solidification Process

As described previously, the casting process starts with a crucible filled with silicon "chunks" and heated to a temperature well above the silicon melting point. This process takes a significant amount of time, and thus the internal components of the station are thoroughly heated to a steady-state temperature and the silicon is a "pool" of nearly uniform temperature. This heat-up process as been simulated and these steady-state temperatures have been used as the beginning temperatures for the solidification portion of the process.

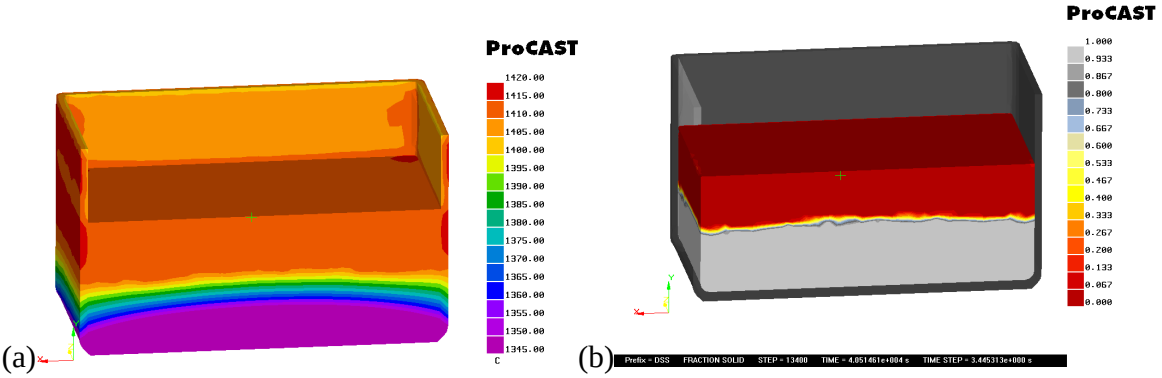
During the solidification portion, the side insulation is raised to expose the heat exchange block and bottom of the crucible to a "cold zone". This cold zone extracts a large amount of heat, and thus solidification is initiated from the bottom of the crucible. At the beginning stages of solidification, the side of the heat exchange block and the crucible bottom corner will "see" the cold zone directly, while the center part will "see" the top of bottom insulation. As significant time is required for the bottom insulation to lose heat to the cold environment, the bottom corner of the crucible may be slightly colder than the center part. This will produce a "U-shaped" isothermal line and solidification front. The temperature distribution and solidification fraction at the early growth stage shown in Figure 2 have proved these phenomena.



(a) (b)

Figure 2. (a) Temperature distribution, (b) fraction solid early in the growth process.

As seen in Figure 3, when the solidification is approximately at the mid-height of the "pool", the shape of isothermal line and growth front becomes essentially flat to slightly inverted, i.e. convex. As the solidification continues, the temperature of bottom insulation will decrease significantly. The center of the heat exchange block has a large view factor with the bottom insulation, thus the majority of heat extraction will be from the center part of the heat exchange block. The cooling of the silicon will mainly be from the center of the solidified ingot via good contact with the crucible and heat exchange block. Also, at a higher position of the silicon, it will couple better with heater. These effects will make the silicon next to the crucible wall slightly warmer than the internal silicon.



(a) (b)

Figure 3. (a) Temperature distribution, (b) fraction solid approximately half-way through solidification.

The final stages of solidification shows the full inversion, where the initially "U-shaped" front has modified to an upside-down "U-shape" (Figure 4). The final liquid pools reside in the corner as the corner is the hottest spot in the silicon "pool". Due to the configuration of the station, the corners of the crucible are exposed to two sides of the heater. Therefore, this hottest spot will be the location of last solidification.

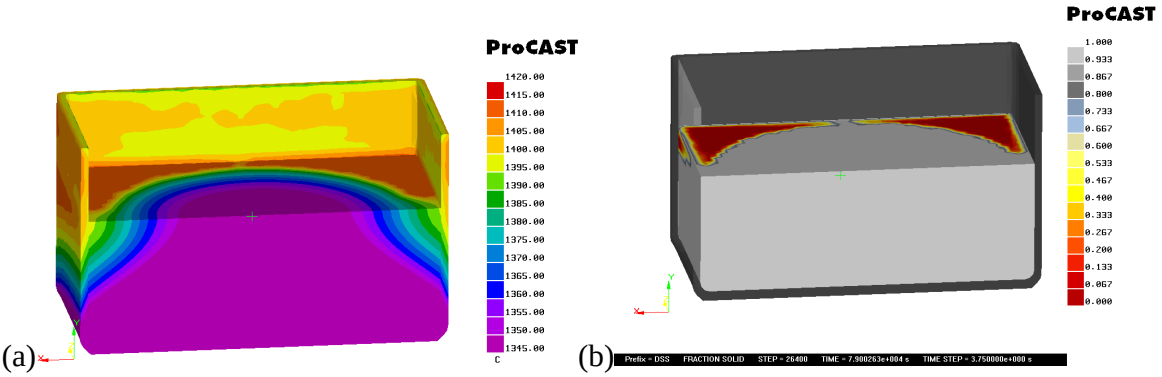


Figure 4. (a) Temperature distribution, (b) fraction solid at final moments of solidification.

Since the center part will be solidified earlier than the corners, the remaining silicon melt will be pushed to the corner. As previously noted, silicon exhibits expansion during solidification. When the corners solidify, there is not much space to expand and must accommodate the majority of late expansion. For this reason, the corners will show obvious signs of expansion and be higher than the center of the ingot.

Figure 5 is a finished ingot grown from DSS station. Even though the station is essentially quarter-symmetric, the final ingot is not totally symmetrical. This may be related to off center loading and/or aging of different parts in furnace. The majority of the top ingot surface is flat; however, the corners are raised. This effect can be well explained by the simulation results.

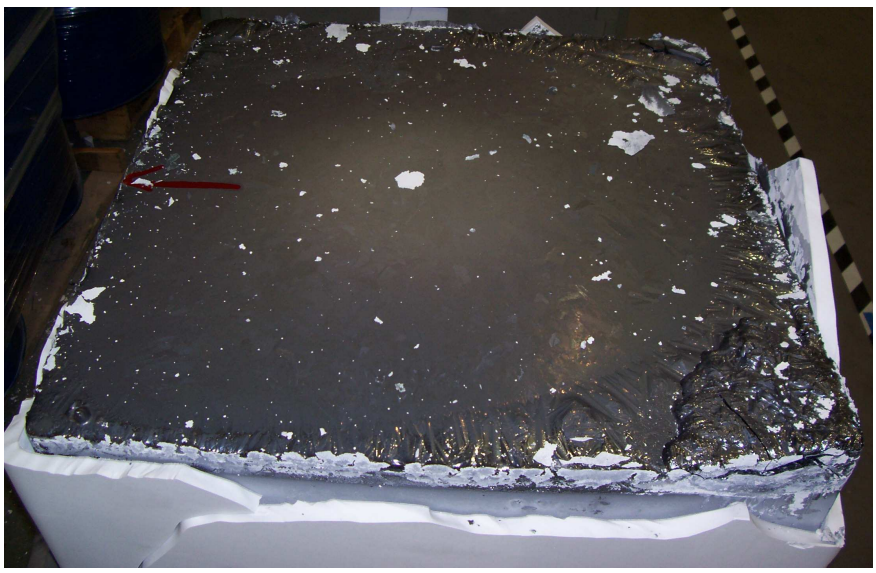


Figure 5. Finished ingot from DSS station

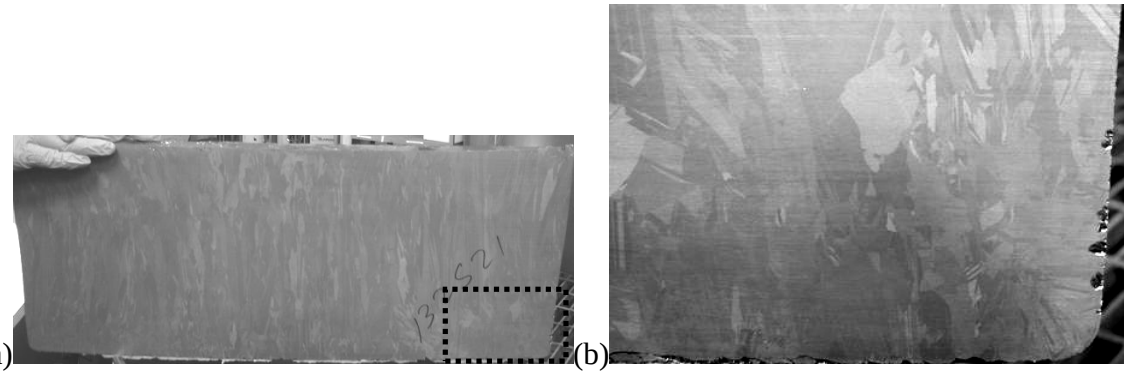
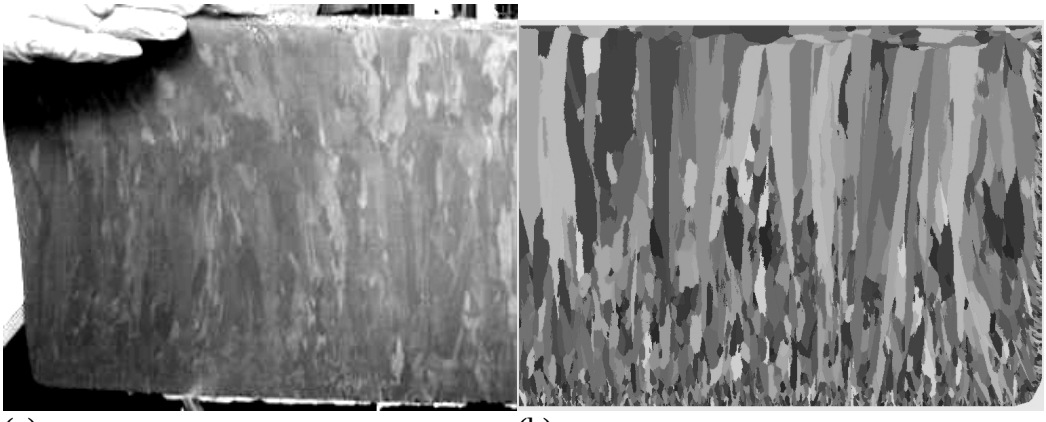

(a) (b)

Figure 6. (a) Grain structure of a slab from a DSS ingot, (b) enlarged image of slab corner.

To better compare the simulation results and grown ingot, we can take a close look at the grain structure of a cut slab from a DSS ingot, shown in Figure 6. The majority of the grains are straight and columnar, especially at the middle part of the ingot. The isothermal lines in simulation are flat in the middle when they are close to the bottom (see Fig.2), which will result in columnar growth. The grains at the bottom corners of the slab grow slightly inward, so does the lower part of it next to the crucible. This indicates that the crucible is slightly colder than the middle of the silicon at the lower half (shown in Fig.2). At the top half of the slab, the grains grow slightly outwards. This is the result of convex interface shape, which is also shown in the simulation result Figure 4.

Ingot Crystal Nucleation and Grain Growth

CAFE simulation of grain growth is conducted based on the temperature. Due to computer limitations, a 5 cm window close to the side of ingot was selected as the scope of the calculation. The simulation result of the cross section of grain structure is shown in Figure 7(b). The grain size is small at the lower part of the slab. When silicon first nucleates, many nucleation sites are produced. As the growth continues, fast growing grains take over. The slowly growing grains will be terminated. The average grain size increases. The simulation also well reflects the temperature effects. We see corner grains grow slightly inwards and grains grow slightly outwards after about half way. If we put the cut off slab (Fig. 7a) and simulation result next to each other, we find that simulation result agrees well with reality.


(a) (b)

(c)

(d)

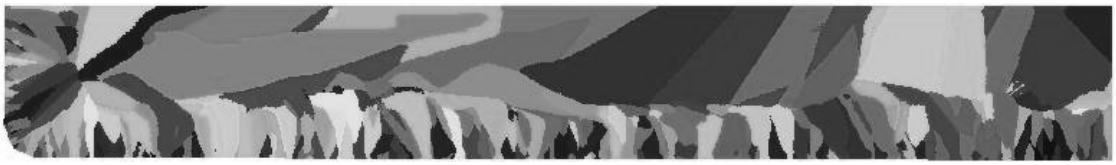


Figure 7. (a) Grain structure of the left half of the slab, (b) simulated grain structure of the right half, (c) grain structure of the top of a DSS ingot, (d) simulated grain structure of ingot top.

On the top surface of the ingot, dendritic growth can be observed next to the crucible wall, shown in Figure 7(c). In the temperature and solid fraction results shown in Figure 4, one can see that the silicon next to the crucible wall on the top surface solidifies relatively early. This solidification may lead to growth inwards from the crucible wall. It will be terminated by the majority of columnar grains at the center of the ingot. The grain simulation result (see Fig 7d) also shows the nucleation next to the crucible wall on the top surface. And the grain structure has reasonable agreement with real grains.

Conclusion

The commercial software ProCAST predicted the transient 3D temperature distributions of the DSS cast silicon ingot. Based on the temperature results, crystallization and grain structure were simulated by the same software. Simulation results agreed well with grown silicon.

The simulation tool fosters an understanding of the growth process and grain structure and also provides an opportunity to "view" and comprehend the dynamics inside the furnace. From here, the station configuration, growth process and grain quality may be optimized to produce high quality high efficiency silicon solar cells.

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