Sensors and Materials, Vol. 35, No. 3 (2023) 691–701
MYU Tokyo

S & M 3204

Using ANSYS Fluent Finite Element Method to Simulate Effect of Opening Angle of Argon Inlet Channel in Polysilicon Directional Solidification System

Wenqiong Zhang,[1] Yu-Yi Lin,[2] Chao-Ming Hsu,[2*]
Xiaoping You,[1] and Cheng-Fu Yang[3,4**]

[1]Xiamen University Tan Kah Kee College - Xiamen HPRT Electronic Advanced Printing Technology Innovation Laboratory, Xiamen 363105, PR China
[2]Department of Mechanical Engineering, National Kaohsiung University of Science and Technology, Kaohsiung 807, Taiwan
[3]Department of Chemical and Materials Engineering, National University of Kaohsiung, Kaohsiung 811, Taiwan
[4]Department of Aeronautical Engineering, Chaoyang University of Technology, Taichung 413, Taiwan

(Received September 12, 2022; accepted October 25, 2022)

Keywords: ANSYS Fluent, simulation, finite volume method, argon gas inlet flow channel

In this study, a numerical analysis method was used to simulate the solidification growth process of polysilicon ingots in a DSS450 prototype directional solidification crystal growth furnace produced by GT Advanced Technology. Finite element modeling was carried out using the finite volume method, which is contained in the commercial software package ANSYS Fluent. In the simulation, many actual parameters during production, including those of the heat transfer model, flow field model, and thermal radiation, should be employed in addition to the opening angle of the argon inlet channel. This opening angle was taken as the main parameter to simulate the effect of different angles (20, 60, 140°) on the temperature variation at different positions in a directional solidification crystal growth furnace. The settings of the simulation parameters referred to the actual growth process of the polysilicon directional solidification system. The temperature of each part in the crystal growth furnace was set at 1685 K, and the temperature in the molten silicon crucible was set at 1750 K. Finally, the growth state of the crystal silicon ingots was simulated in a transient manner, and the variation of the temperatures of melting polysilicon ingots at different positions (points) was discussed on the basis of the simulation results. The results show that for different opening angles of the argon inlet channel, different temperature fields are obtained in the furnace body during the solidification and growth processes of the crystal silicon ingots.

1. Introduction

Computational fluid dynamics (CFD) is a complete system for studying fluid flow problems, which is a combination of traditional theoretical analysis methods and experimental measurement methods.(1) CFD is an important technology in the field of fluid mechanics.(1–3)

---

*Corresponding author: e-mail: jammy@nkust.edu.tw
**Corresponding author: e-mail: cfyang@nuk.edu.tw
https://doi.org/10.18494/SAM4108

The CFD numerical solution mainly uses discrete principles to govern the relative equations (the heat transfer model, flow field model, and thermal radiation) to predict flow fields and computing flows. According to the discrete principle used, the CFD numerical solution can be divided into three analysis techniques: the finite differential method (FDM), finite element method (FEM), and finite volume method (FVM). The FVM is a discretization method that has developed rapidly in recent years, and it is characterized by high computational efficiency. In this study, the FVM was used in the main theoretical model for numerical and analytical control. The simulation results show that for different opening angles of the argon inlet channel, different temperature fields are obtained in the furnace body during the solidification and growth processes of crystal silicon ingots.

Fluent is CFD software developed by the US company Fluent in 1983.(4) It is still one of the world's leading commercial CFD software and is an analysis software mainly based on the FVM. In terms of mesh characteristics, when Fluent is used as the processing CFD software, structured or unstructured meshes can be chosen by users. Fluent itself has a powerful post-processing function, which can integrate and export large amounts of data. After processing, a complete set of databases can be obtained, which is convenient for users processing the data for further analyses. Fluent is mainly based on the C language, and users can also write their own programs to modify the software according to their needs.

To obtain high-quality silicon ingots, many factors must be considered in the manufacturing processes. The common ones are the thermal field, argon flow, and the control of the solid–liquid interface and impurity concentration. Therefore, how to effectively improve the crystal silicon growth process is a challenging problem for factories performing crystal growth. Currently, crystalline silicon is the main internal component of solar cells, which can be divided into single-crystalline silicon and polycrystalline silicon. Owing to their lower manufacturing cost, solar cells processed using polycrystalline silicon have a market share of more than 50%.(5,6) In 2009, Wacker Company of Germany used the block casting method to form polycrystalline silicon ingots. Later, two different processing methods were developed for growing polycrystalline silicon ingots using the casting method. For example, the Crystal Systems Company in the US investigated the heat exchange method (HEM)(7) and the Solarex crystallization method,(8) which were based on the casting method. A popular method of growing polycrystalline silicon ingots used in manufacturing is the directional solidification method, because the growth of polycrystalline silicon ingots in a fixed direction can avoid the growth of disordered grains. There are three main directional solidification methods, namely, the casting method, the electromagnetic casting method, and the Bridgman method.(9) By these growth methods, a large volume of crystal silicon ingots can be produced at the same time, thereby achieving a low cost, high productivity, and commercialization.

Teng *et al.* used the simulation software CGSim and the FVM to simulate the temperature fields, oxygen impurities, carbon impurities, and so forth, in a directional solidification system (DSS) furnace.(10) The simulation results showed that the convection in a molten silicon crucible is mainly caused by buoyancy, and the shape of the convection changes with the growth process. Therefore, the design of the thermal field in the furnace can be used to improve the strength of convection. Gao *et al.* also used a simulation method to compare the distributions of oxygen and carbon concentrations for different argon flow rates and pressures in the silicon crystal growth process for a DSS furnace.(11) Dai *et al.*(12) and Li *et al.*(13) used ANSYS Fluent software to simulate the solidification and growth processes of crystal silicon ingots. Their simulation processes combined the parameters of turbulence, heat transfer, and phase change modules and used the FVM for calculation. The simulation results showed that a flow of argon in combination with a large flow rate during the solidification growth process results in a silicon crystal growth process with a short duration. The control of the argon flow rate in the curing process avoids over-convexity and an unstable solid–liquid interface shape at the center of the molten silicon crucible and thus determines the shape of polysilicon ingots and improves their quality.

When the DSS is used to grow molten materials, many sensors need to be used to detect the flow conditions of the growth materials. For example, an ultrasonic transducer can be attached at the bottom wall of a fluid container to achieve acoustic coupling between the fluid and sensors.(14) Sensor technology can also be used exploit the large difference in the electrical resistivity of the solid and liquid phases to determine the growth rate $V(t)$ and the current position $X(t)$ of the solidification front.(15) However, a simulation method can reduce fabrication costs, including those of the materials and sensors, during the growth of high-quality silicon ingots. Many factors affect the results of silicon ingot growth in a DSS furnace.(12,13) In this study, the main factor is the opening angle of the argon inlet channel, which is set to 20, 60, and 140°. Other simulation factors, including the heat transfer, flow field, and thermal radiation, are considered. First, the temperature of each part in the crystal growth furnace is set at 1685 K, and the temperature in the molten silicon crucible is set at 1750 K. Then, the growth state of the crystal silicon ingots is simulated in a transient manner, and the changes in the temperature fields of the silicon ingots are discussed from the results.

2. Simulation Process and Parameters

There are five stages in the polycrystalline silicon solidification growth process: heating, melting, growth, annealing, and cooling in sequence. In the melting process, because of the relatively short distance between the crucible wall and the heater in the furnace, the temperature in the ambient area of the molten silicon crucible is higher than that at the center. The molten silicon in the crucible is disturbed by the convection caused by this phenomenon. Therefore, producers must always pay attention to the melting conditions from the argon inlet channel to check whether there is incompletely melted silicon material floating in the molten silicon crucible. The turbulence generated by a flow of argon can indirectly remove the surface impurities in the molten silicon crucible; thus, argon plays an important role in the growth of polycrystalline silicon ingots. Therefore, the amount and shape of the flow and the turbulence generated by the argon flowing over the surface of the molten silicon crucible are also key factors affecting the performances of solar cells.

Figure 1 shows meshing graphs used to compare the number of elements and the maximum skewness between the 2D and 3D models. For 2D and 3D models, the numbers of elements are 4×10^4 and 3.5×10^6 and the maximum skewnesses are 0.65 and 0.88, respectively. In this study, a 2D geometric model is used for numerical analysis to reduce the total number of meshes and

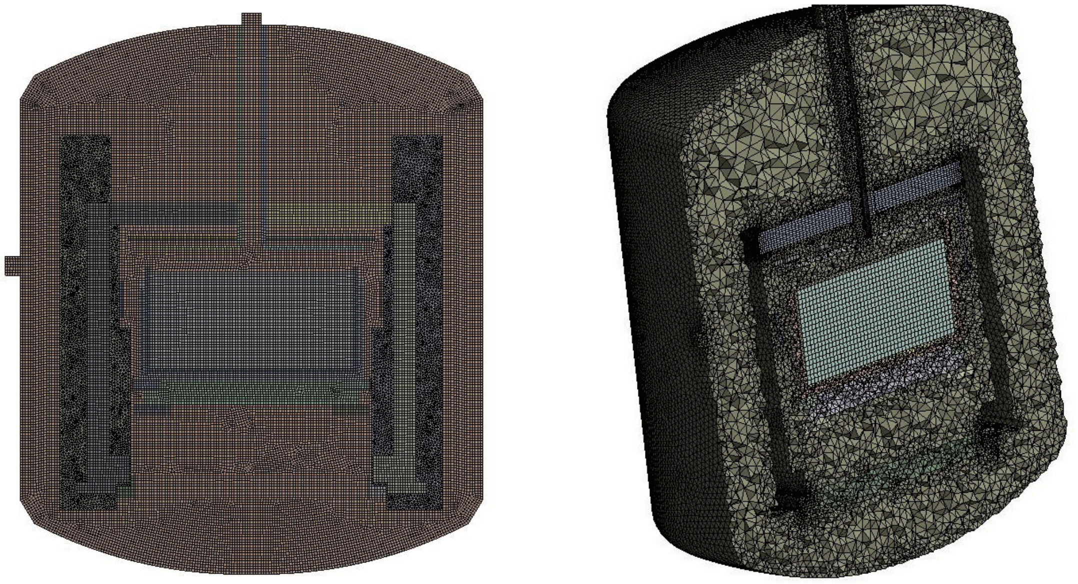

(a) (b)

Fig. 1. (Color online) Comparison of mesh quality: (a) 2D model and (b) 3D model.

improve the mesh quality, which greatly reduce the time spent on numerical calculations. Figures 2(a)–2(d) show the prototype furnace and furnaces with opening angles of the argon inlet channel of 20, 60, and 140°, respectively.

The simulation process is roughly divided into three stages: pre-processing, numerical calculation, and post-processing.(12) After the design diagram was drawn and before the design was meshed, the Design Modeler module in Workbench software was used to perform Boolean operations on each area of the geometric model. Then, the specified area was used to perform the union, difference, and intersection operations to obtain the actual working area. Finally, the flow field was defined and the boundary conditions for the inlet, outlet, furnace wall, and insulating cage wall of the crystal growth furnace were set. When the SIMPLE method is used, a given predicted pressure must be set, then it can be used to calculate the various pressure and velocity components from the original value. Because the predicted pressure is an assumed value, the obtained velocity field may not satisfy the continuity equation. Therefore, it is necessary to correct the predicted pressure value, and then the corrected pressure can be used to obtain the new values of the pressure and velocity; these steps are repeated until the convergence condition is reached. The actual temperatures at the simulation points of the DSS450 prototype directional solidification crystal growth furnace shown in Fig. 3 were detected by using thermocouples as sensors. The process to obtain the simulation results is as follows:

1. The predicted pressure is set.
2. The momentum equation is used to find a new value of the pressure.
3. The corrected pressure and velocity are obtained through the modified equation to solve the boundary conditions.

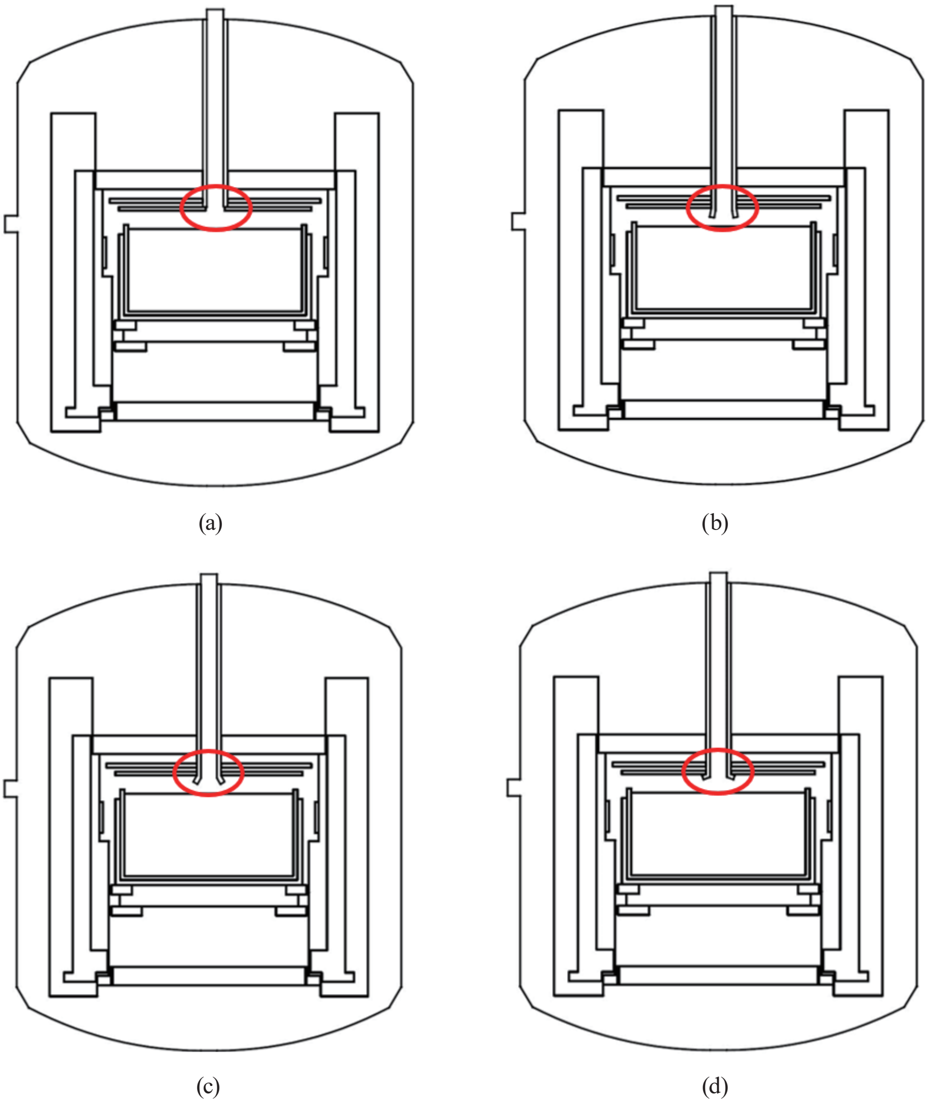


Fig. 2. (Color online) Models of (a) prototype furnace and furnaces with opening angles of the argon inlet channel of (b) 20°, (c) 60°, and (d) 140°.

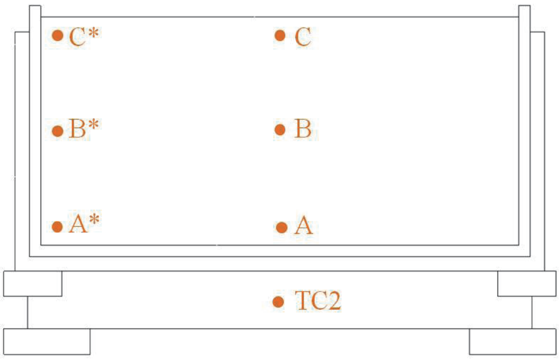


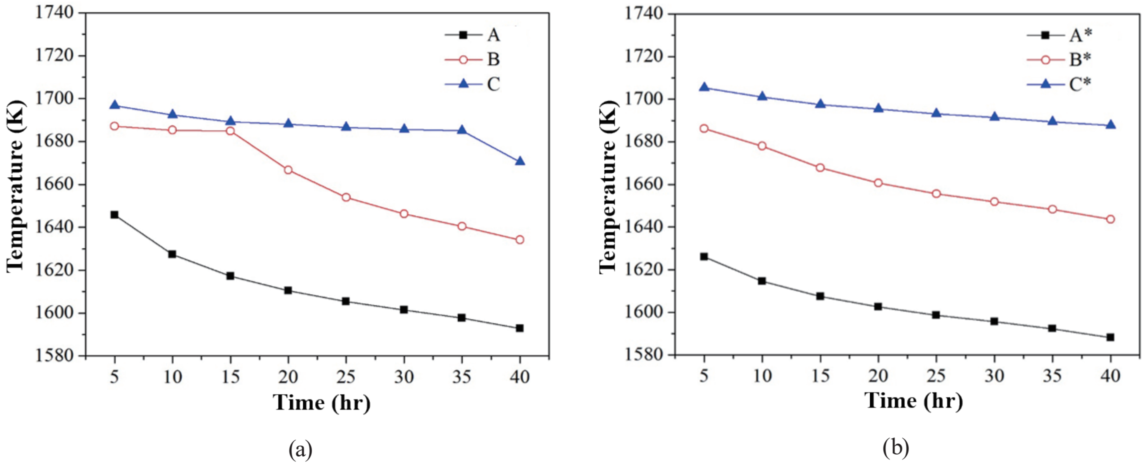
Fig. 3. (Color online) Schematic diagram for the data extraction points of the furnace.

4. The corrected pressure and velocity are incorporated into the momentum equation to find the relationship between the pressure correction term and the velocity correction term, and the values are incorporated into the modified equation to find the new velocity.
5. The new velocity is incorporated into the continuous equation to find the new pressure.
6. The new pressure and velocity are used to solve the governing equations.
7. The new pressure is used as the newly predicted pressure, and step 2 is repeated until the convergence condition is met.

3. Simulation Results and Discussion

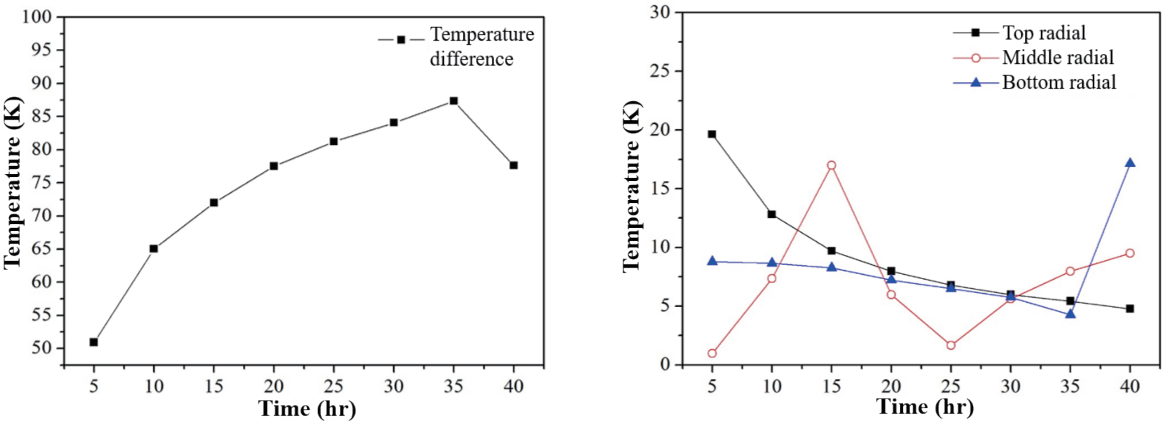
Figures 4(a) and 4(b) show temperature–time curves of the prototype furnace at points A, B, and C and points A*, B*, and C*, respectively. These curves are the simulation results for the six points in the molten silicon crucible, and the vertical distance between each data line is the temperature difference between different points. When the spacing is larger, the axial temperature gradient is larger, which can lead to the vertical upward growth of silicon grains. Extraction point C is higher than points A and B, and the molten silicon at point C is closest to the heater. Thus, the cooling rate at point C is the lowest, and about 36 h is required for the latent heat to be completely released during the growth process at this point. Point A is the lowest point, and the cooling rate is higher than that at other points; at this point, it takes about 0.6 h for the latent heat to be completely released. The growth rate of silicon raw materials is highest at the beginning of the process and gradually decreases after the middle stage. Because points A*, B*, and C* are closer to the wall in the molten silicon crucible than points A, B, and C, their cooling rates are higher than points A, B, and C at the center of the molten silicon crucible.

Figure 5(a) shows the temperature difference between points A and C, which represents the change in the axial temperature in the crucible. During the solidification process, in the 5th hour, the molten silicon crucible at point A solidified into solid silicon. However, the temperature at point C is still higher than 1685 K at this time, and the silicon is still liquid. This result is due to



(a) (b)

Fig. 4. (Color online) Temperature–time curves of the prototype furnace at (a) points A, B, and C and (b) points A*, B*, and C*.



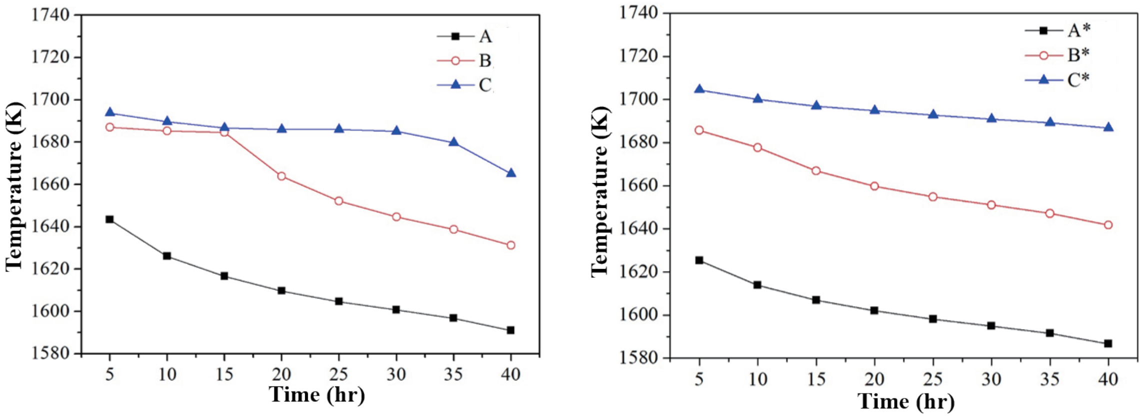
(a) (b)

Fig. 5. (Color online) (a) Axial temperature difference and (b) horizontal temperature differences of the prototype furnace.

the fact that the heat transfer characteristics of solid silicon are better than those of liquid silicon and the heat dissipation of the bottom silicon is faster. The temperature difference between the two points before solidification at point C gradually increases, and the maximum temperature difference is 39.41 K. The temperature difference gradually decreases after the solidification of point C, which is around the 36th hour.

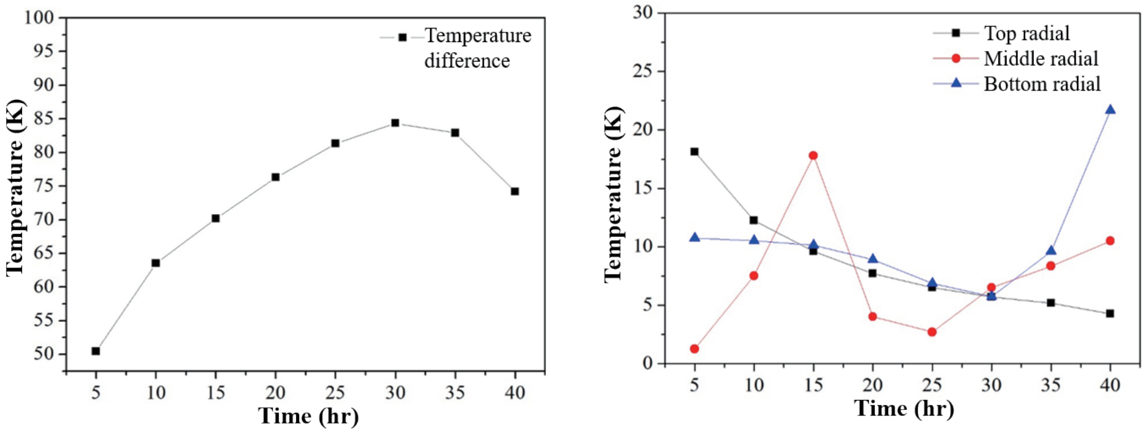
Figure 5(b) shows the changes in the horizontal temperature during the curing process. The curves show the temperature differences between the points at the center (points A, B, and C) and those on the wall (points A*, B*, and C*). As shown in Fig. 4(a), the change in the horizontal temperature at the top is that the silicon at point C starts to solidify in the 36th hour owing to the influence of the argon flow. However, point C* is closer to the heater than point C, and its temperature is kept at 1685 K; thus, the temperature difference gradually increases. The change in the horizontal temperature at an intermediate height is that the silicon at point B* solidifies first in the 5th hour, then the silicon at point B solidifies in the 16th hour. The maximum temperature difference between the two points is 16.05 K, and when the silicon at point B solidifies, the horizontal temperature difference between points B and B* decreases. The change in the horizontal temperature at the bottom is that the silicon at point A* solidifies instantaneously in the early stage of silicon ingot growth, and the silicon at point A solidifies after 0.6 h. The horizontal temperature difference gradually decreases after the 5th hour, and the maximum temperature difference between the two points is 8.76 K in the 5th hour.

The smallest opening angle of the argon inlet channel of the crystal growth furnace in this study is 20°, as shown in Fig. 2. When argon starts to pass over the molten silicon surface, turbulence occurs on the surface due to the shrinkage and change of the used air inlet with different angles, and the temperature field in the furnace is affected. The angle of the argon inlet channel also affects the grain growth due to the change in the temperature field in the furnace, which directly affects the solid–liquid interface of the crystal silicon ingots. In addition, the turbulent argon lifts up impurities on the surface of the molten silicon and pumps them out of the furnace through the argon outlet. Figures 6(a) and 6(b) show temperature–time curves of the



(a) (b)

Fig. 6. (Color online) Temperature–time curves of the furnace with the opening angle of the argon inlet channel of 20° at (a) points A, B, and C and (b) points A*, B*, and C*.



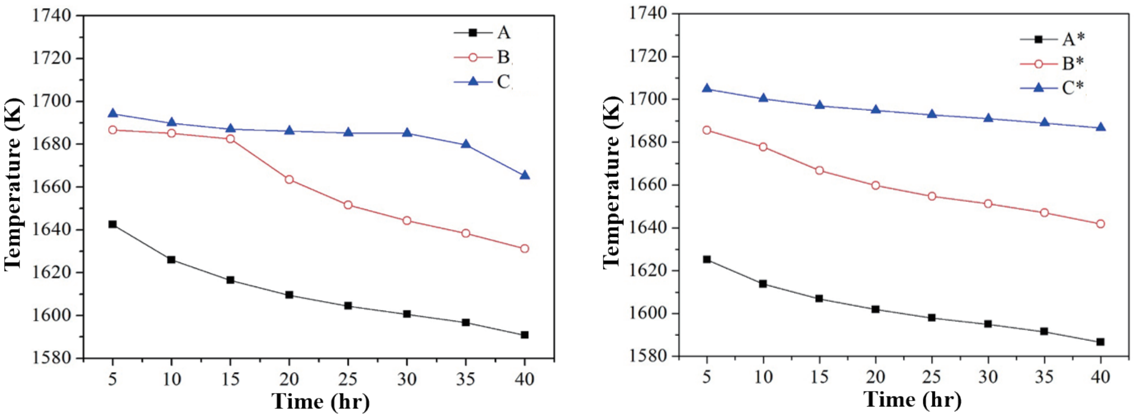
(a) (b)

Fig. 7. (Color online) (a) Axial temperature difference and (b) horizontal temperature differences of the furnace with the opening angle of the argon inlet channel of 20°.

simulated process in the furnace for an opening angle of the argon inlet channel of 20°. Figure 7(a) shows the temperature difference curve between points A and C, which represents the change in the axial temperature. When the opening angle of the argon flow channel is 20°, the maximum temperature difference between the extraction points A and C during the 5th hour of the curing process is 36.35 K, which is 3.06 K lower than that of the prototype furnace. This result demonstrates that the opening angle of the argon inlet channel affects the growth of silicon ingots.

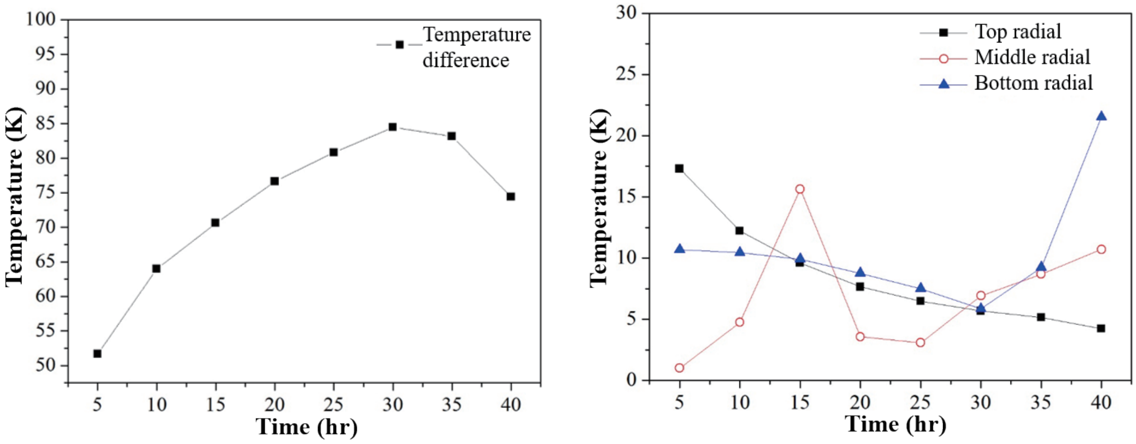
Figure 7(b) presents the changes in the horizontal temperature for the same furnace, which are the temperature differences between the points at the center and the wall. A low horizontal temperature difference can prevent the pre-growth of grains from the crucible wall. The horizontal temperature change at the top is that the silicon at point C solidifies first in the 36th hour due to the strong effect of the argon flow. Point C* is closer than point C to the heater in the furnace, and the temperature there is maintained at 1685 K; thus, the temperature difference between points C and C* gradually increases. The change in the horizontal temperature at an intermediate height is that the silicon at point B* solidifies first in the 5th hour, and the silicon at point B solidifies after the 16th hour. The maximum temperature difference between the two points for the furnace with the opening angle of the argon channel of 20° is 16.53 K, which is 0.48 K higher than that for the prototype furnace. The change in the horizontal temperature at the bottom is that the silicon at point A* solidifies instantaneously in the early stage of growth, whereas the silicon at point A solidifies after 0.6 h. The horizontal temperature difference here gradually decreases after 5 h, at which the maximum temperature difference between the two points is 10.73 K, which is 1.96 K higher than that of the prototype furnace.

Figure 8 presents the temperature–time curves of the simulated process for the different positions for the molten silicon crucible with the opening angle of the argon inlet channel of 60°. Figure 9(a) shows the temperature difference curve between points A and C, which represents



(a) (b)

Fig. 8. (Color online) Temperature–time curves of the furnace with the opening angle of the argon inlet channel of 60° at (a) points A, B, and C and (b) points A*, B*, and C*.



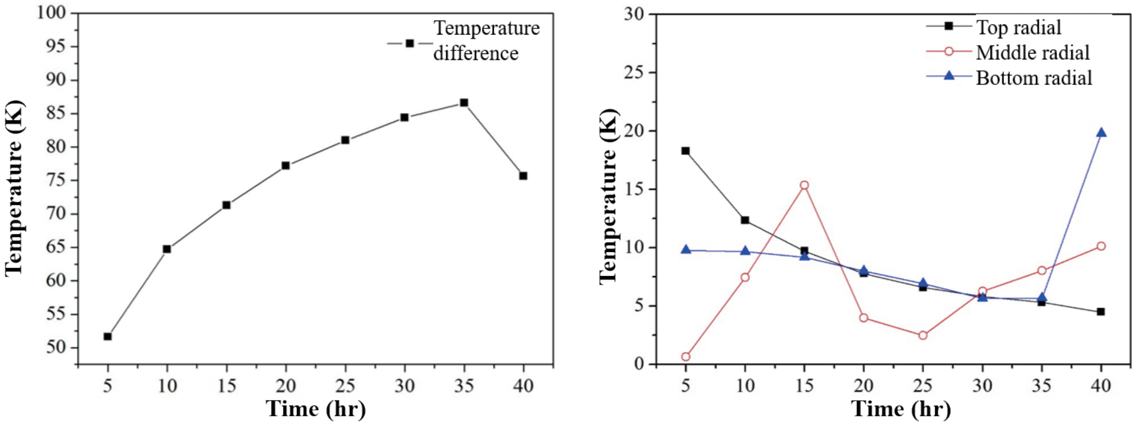
(a) (b)

Fig. 9. (Color online) (a) Axial temperature difference and (b) horizontal temperature differences of the furnace with the opening angle of the argon inlet channel of 60°.

the axial temperature change. The maximum temperature difference between the data extracted from points A and C is 37.3 K and occurs after 5 h, which is 2.1 K less than that for the prototype furnace.

Figure 9(b) shows the horizontal temperature change curves during the curing process. The horizontal temperature change at the top is that the silicon at point C solidifies first in the 36th hour due to the effect of the argon flow. Point C* is closer than point C to the heater, and the temperature there is maintained at 1685 K; therefore, the temperature difference gradually increases. The change of the intermediate horizontal temperature is that the silicon at point B* solidifies first in the 5th hour, and the silicon at point B solidifies after the 16th hour. The maximum temperature difference between these two points is 14.62 K, which is 1.42 K less than that for the prototype furnace. These results suggest that when the silicon at point B solidifies, the horizontal temperature difference decreases. The horizontal temperature change at the bottom is that the silicon at point A* solidifies instantaneously in the early stage of silicon ingot growth, and the silicon at point A solidifies at 0.6 h. The maximum temperature difference between the two points is 10.73 K in the 5th hour, an increase of 1.96 K compared with that for the prototype furnace, after which the temperature difference decreases.

The simulation results for the furnace with the opening angle of the argon inlet channel of 140° were also obtained. Figure 10(a) shows the temperature difference curve between points A and C, which represents the variation of the axial temperature. For the furnace with the opening angle of the argon inlet channel of 120°, the maximum temperature difference between points A and C is 39.96 K, which occurred in the 5th hour of the curing process and is 0.55 K higher than that for the prototype furnace. Figure 10(b) shows the differences in the horizontal temperature during the curing process. The horizontal temperature change at the top is that the silicon at point C solidifies first in the 36th hour due to the effect of the flow of argon. Point C* is closer than point C to the heater, and the temperature there is maintained at 1685 K; thus, the temperature difference gradually increases. The horizontal temperature change at the bottom is that the silicon at point A* solidifies instantaneously in the early stage of silicon ingot growth,



(a) (b)

Fig. 10. (Color online) (a) Axial temperature difference and (b) horizontal temperature differences of the furnace with the opening angle of the argon inlet channel of 120°.

and the silicon at point A solidifies after 0.6 h. The maximum temperature difference between the two points is 9.79 K in the 5th hour, which is 1.01 K higher than that for the prototype furnace.

4. Conclusions

The simulation results have demonstrated that the opening angle of the argon inlet channel affects the solidification and crystal growth of silicon ingots. An argon inlet channel with a small opening angle in the early stage of growth of polycrystalline silicon ingots is conducive to pushing out the impurities in the polycrystalline silicon ingots to the surroundings and improving the purity of polycrystalline silicon ingots. After the middle stage of growth, the opening of the argon flow channel can be enlarged, which is beneficial for the overall crystal growth of the silicon ingots and reduces the processing time to reduce costs. In this study, when the furnace had an opening angle of the argon inlet channel of 20°, it had the highest axial temperature difference, which accelerates the growth of silicon crystal ingots. In the later stage, a furnace with an opening angle of the argon inlet channel of 60° has the lowest radial temperature, which can prevent the grains of the polycrystalline silicon ingots from growing out of the crucible wall. The simulation process can be used to find the optimal opening angle of the argon inlet channel, making it beneficial for actual production.

Acknowledgments

This work was supported by project numbers MOST 110-2622-E-390-002, MOST 110-2221-E-390-020, and Xiamen University Tan Kah Kee College Pre-research Project YY2019L03.

References

1 J. Blazek: Computational Fluid Dynamics: Principles and Applications (Elsevier, 2015) 3rd ed.
2 H. Lomax, T. H. Pulliam, D. W. Zingg, and T. A. Kowalewski: Appl. Mech. Rev. **55** (2002) B61.
3 K. Kuhlmann, C. Sinn, J. M. U. Siebert, G. Wehinger, J. Thöming, and G. R. Pesch: Eng. Appl. Comput. Fluid Mech. **16** (2022) 1706.
4 Fluent, Inc.: https://www.bloomberg.com/profile/company/FLNT:US (accessed April 2021).
5 H. Matsuo, R. B. Ganesh, S. Nakano, L. Liu, K. Arafune, Y. Ohshita, M. Yamaguchi, and K. Kakimoto: J. Cryst. Growth **311** (2009) 1123.
6 L. Liu, S. Nakano, and K. Kakimoto: J. Cryst. Growth **310** (2008) 2192.
7 D. B. Joyce and F. Schmid: J. Cryst. Growth **312** (2010) 1184.
8 W. H. Bloss and G. Grassi: 4th E. C. Photovoltaic Solar Energy Conf. (1982) 858–867.
9 M. Fernanda, S. Ganschow, D. Klimm, S. Serrano-Zabaleta, Á. Larrea, and R. I. Merino: J. Eur. Ceram. Soc. **34** (2014) 2051.
10 Y. Y Teng, J. C Chen, C. W. Lu, H. I. Chen, and C. Y Chen: J. Cryst. Growth **318** (2011) 224.
11 B. Gao, X. J. Chen, S. Nakano, and K. Kakimoto: J. Cryst. Growth **312** (2010) 1572.
12 J. Dai, Y. C. Yang, C. M. Hsu, H. W. Tseng, P. Wang, and C. F. Yang: Sens. Mater. **33** (2021) 2577.
13 X. Li, Y. C. Yang, C. M. Hsu, H. W. Tseng, J. Zhang, and C. F. Yang: Sens. Mater. **33** (2021) 2607.
14 D. Räbiger, Y. Zhang, V. Galindo, S. Franke, B. Willers, and S. Eckert: Inter. Symp. Liquid Metal Processing & Casting (2015) 1–7.
15 M. Brunčko, A. C. Kneissl, and I. Anžel: Int. J. Mater. Res. **102** (2011) 25.