

# Numerical Study on the Effects of Inner Crucible Window Heights on the Growth of Silicon in Continuous Czochralski Process



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## Introduction

- ◆ Czochralski (CZ) method is the main method to produce monocrystalline silicon. In order to further reduce the production cost, the continuous Czochralski (CCZ) method is developing rapidly.
- ◆ As a special structure in CCZ method, the window height of the inner crucible has an important influence on the heat and flow fields in the process of crystal growth.

## Model detail

- ◆ A global 2D model is carried out to investigate the effects of inner crucible window heights on the growth of single-crystalline silicon in a continuous Czochralski process.
- ◆ As shown in Fig.1, the main components of CCZ furnace include furnace shell, double crucible, insulation, support, heater, water cooling jacket and thermal shield. Each region is discretized by structured or unstructured grids.

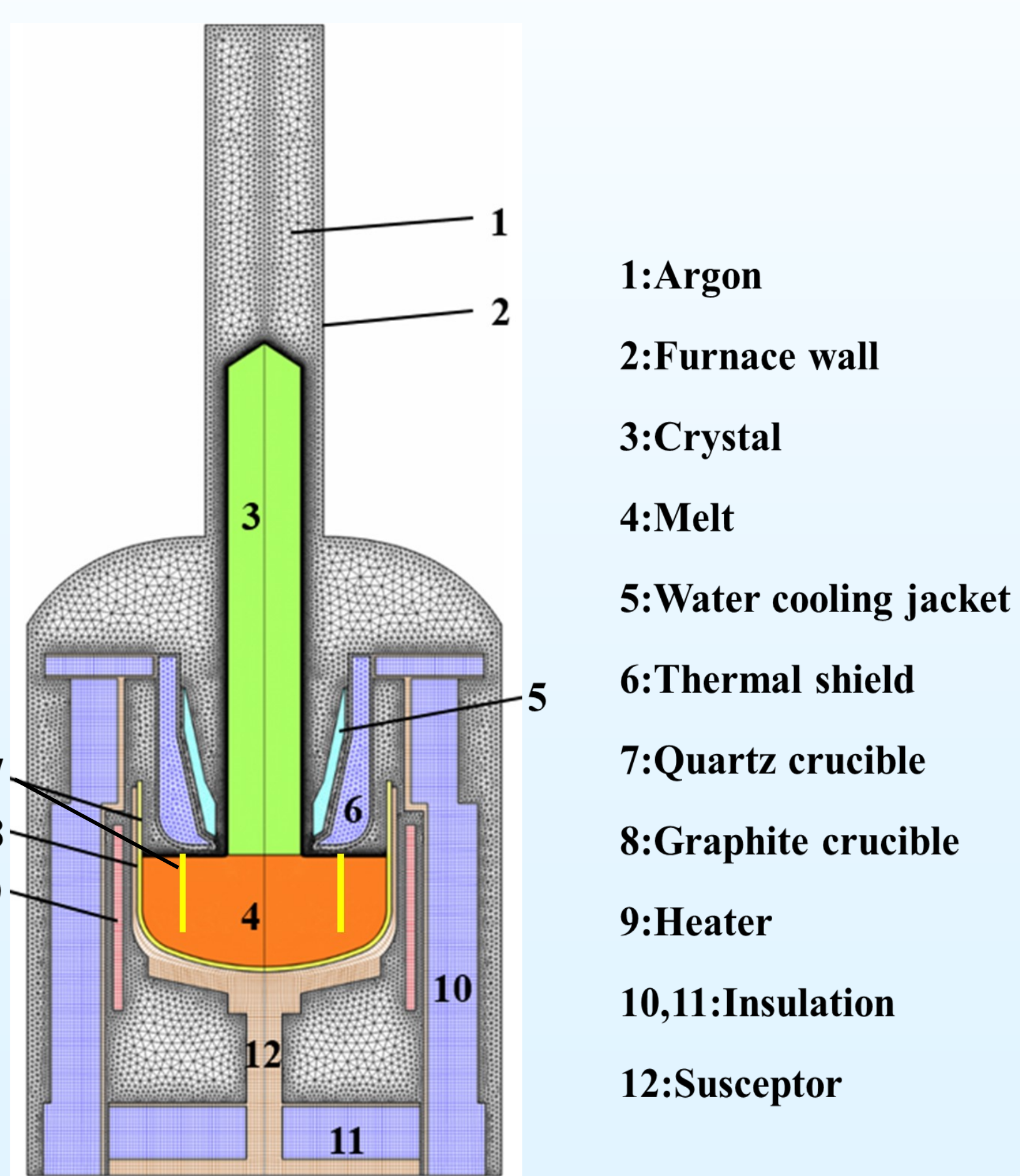


Fig. 1 Schematic diagram and calculation grids of industrial CCZ furnace

## Assumption

- ◆ All the radiative surfaces are assumed diffuse gray.
- ◆ Argon gas in the furnace is ideal and incompressible.
- ◆ The furnace shell is set as the normal temperature boundary.

## Result and discussion

- ◆ The inner crucible limits the heat transfer inside the silicon melt, and this effect is significantly enhanced as the window height decreases.

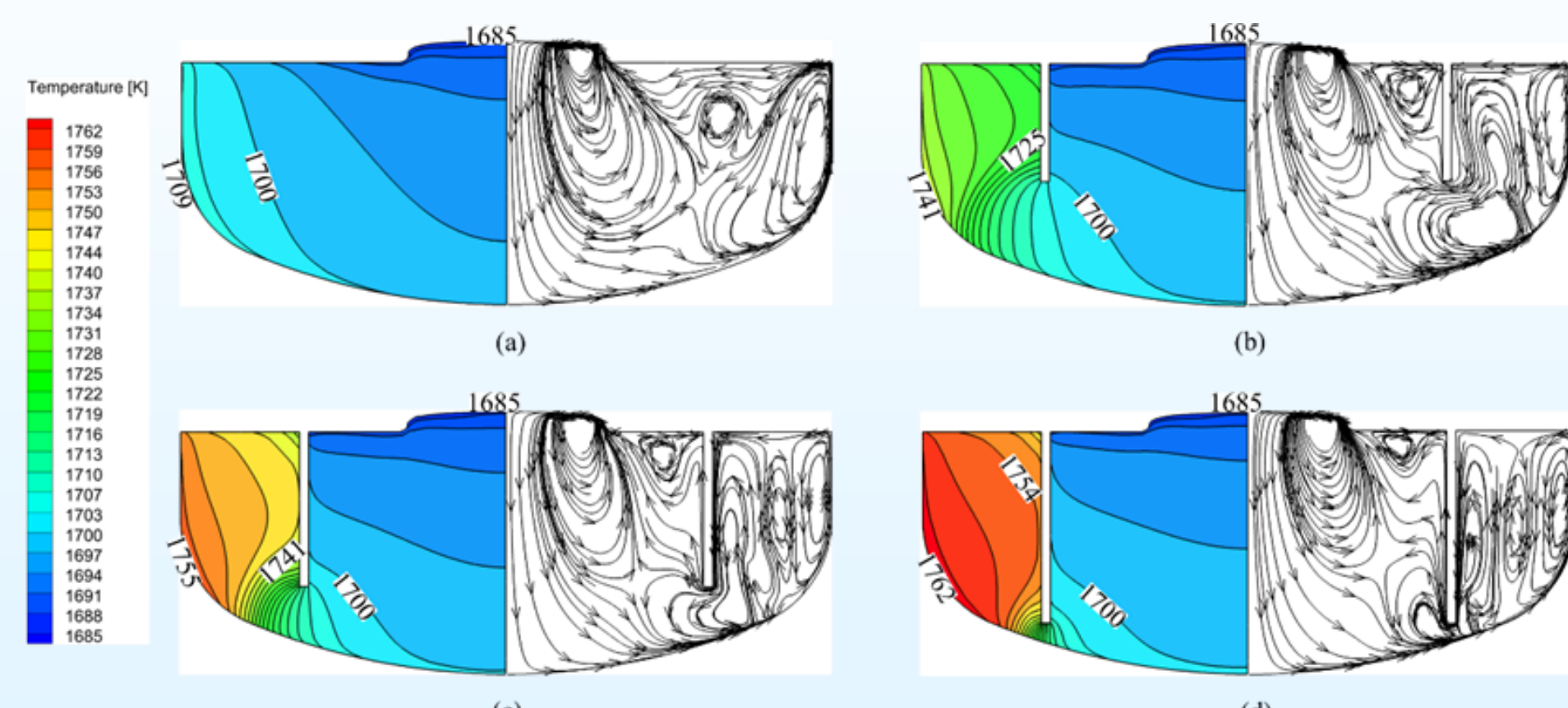


Fig. 2 Temperature field (left) and flow field (right) of silicon melt at different  $\Delta H$ : (a) Single crucible, (b)  $\Delta H=100$  mm, (c)  $\Delta H=60$  mm, (d)  $\Delta H=20$  mm

- ◆ As the height of the inner crucible window decreases, the heat transfer of the silicon melt on the outside of the inner crucible to the silicon melt on the inner side becomes more difficult, making the natural convection here more intense, resulting in a gradual increase in the turbulent viscosity of the silicon melt on the outside of the inner crucible.

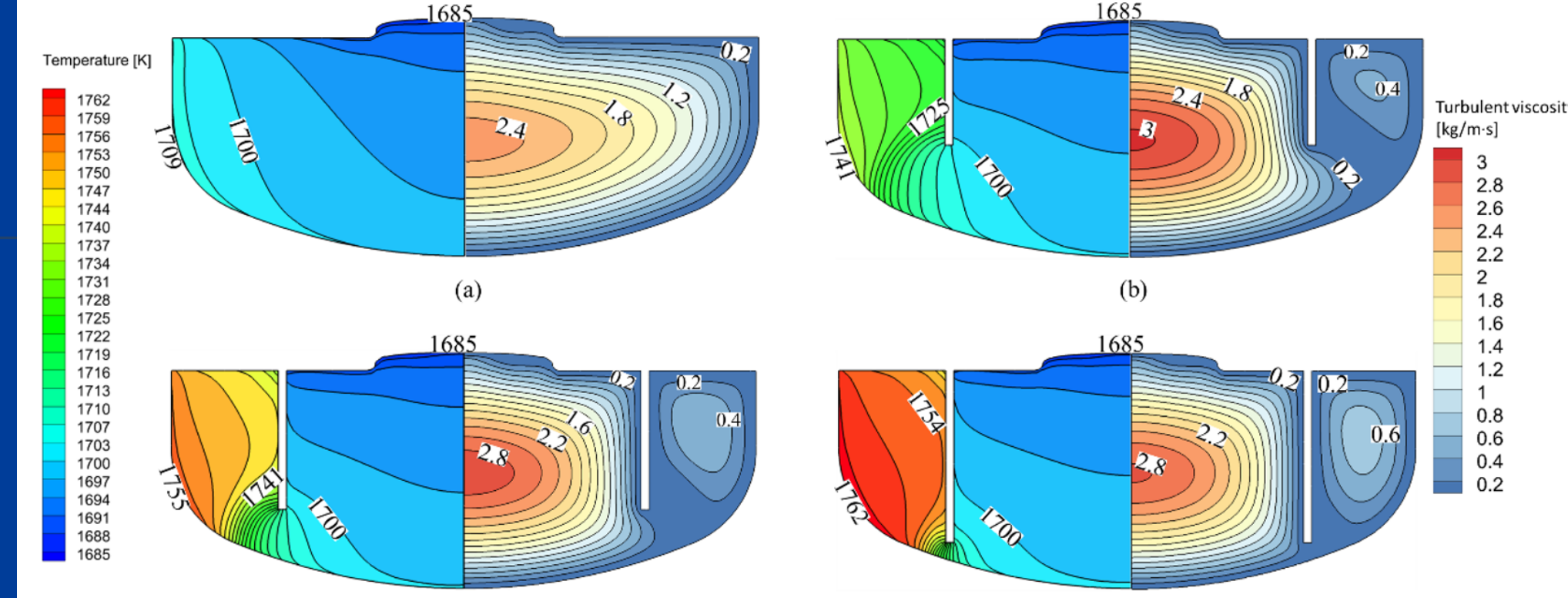


Fig. 3 Distributions of temperature and turbulent viscosity of silicon melt at different  $\Delta H$ : (a) Single crucible, (b)  $\Delta H=100$  mm, (c)  $\Delta H=60$  mm, (d)  $\Delta H=20$  mm

- ◆ Fig.4 shows the temperature distribution of different inner crucible window heights from the center of the crucible bottom to the (outside) crucible wall with the free surface.

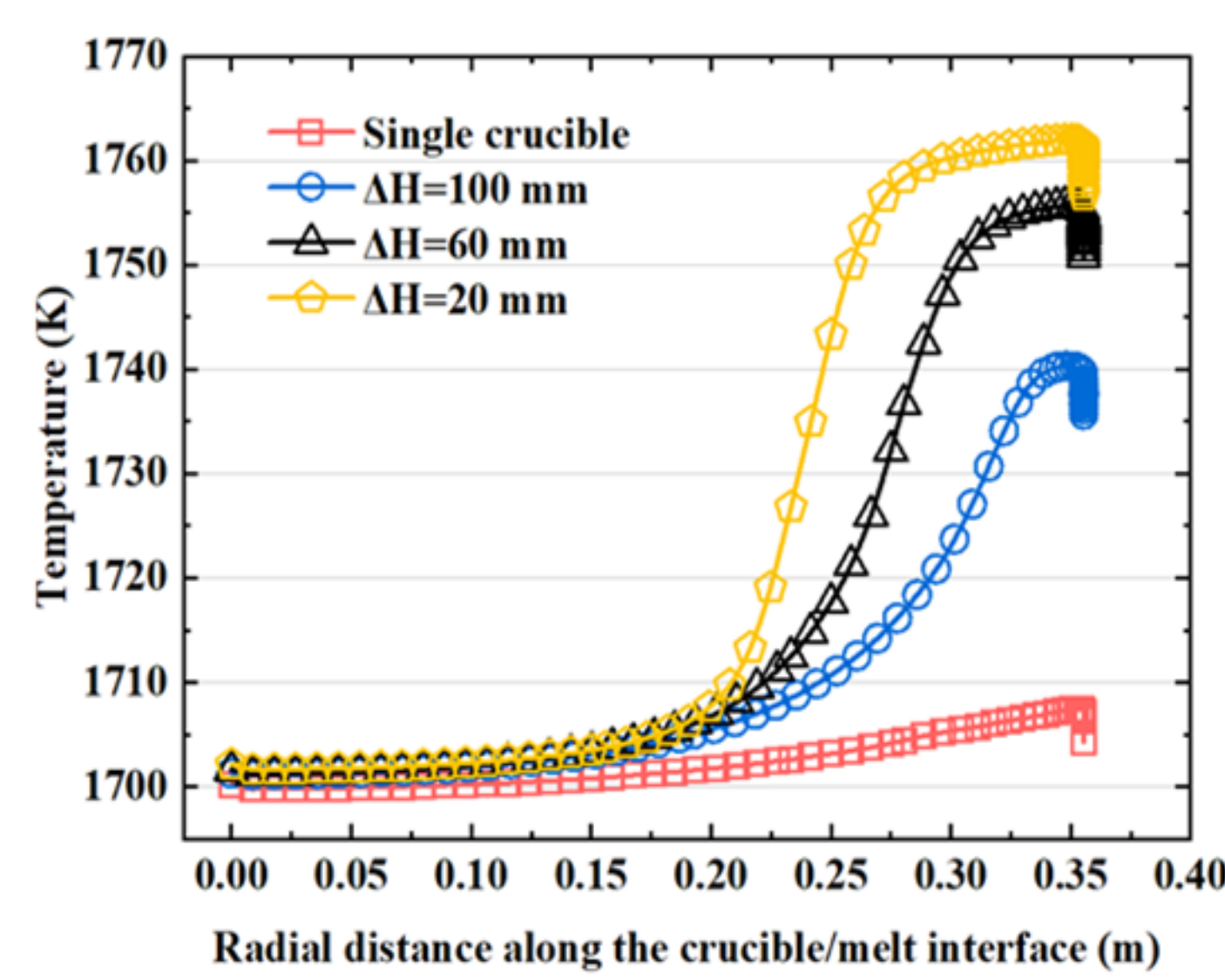


Fig. 4 Temperature distribution of (outer) crucible/silicon melt interface

- ◆ The temperature in the L1 position is higher in the double crucible method, and the temperature difference is greater as the height of the inner crucible window decreases.

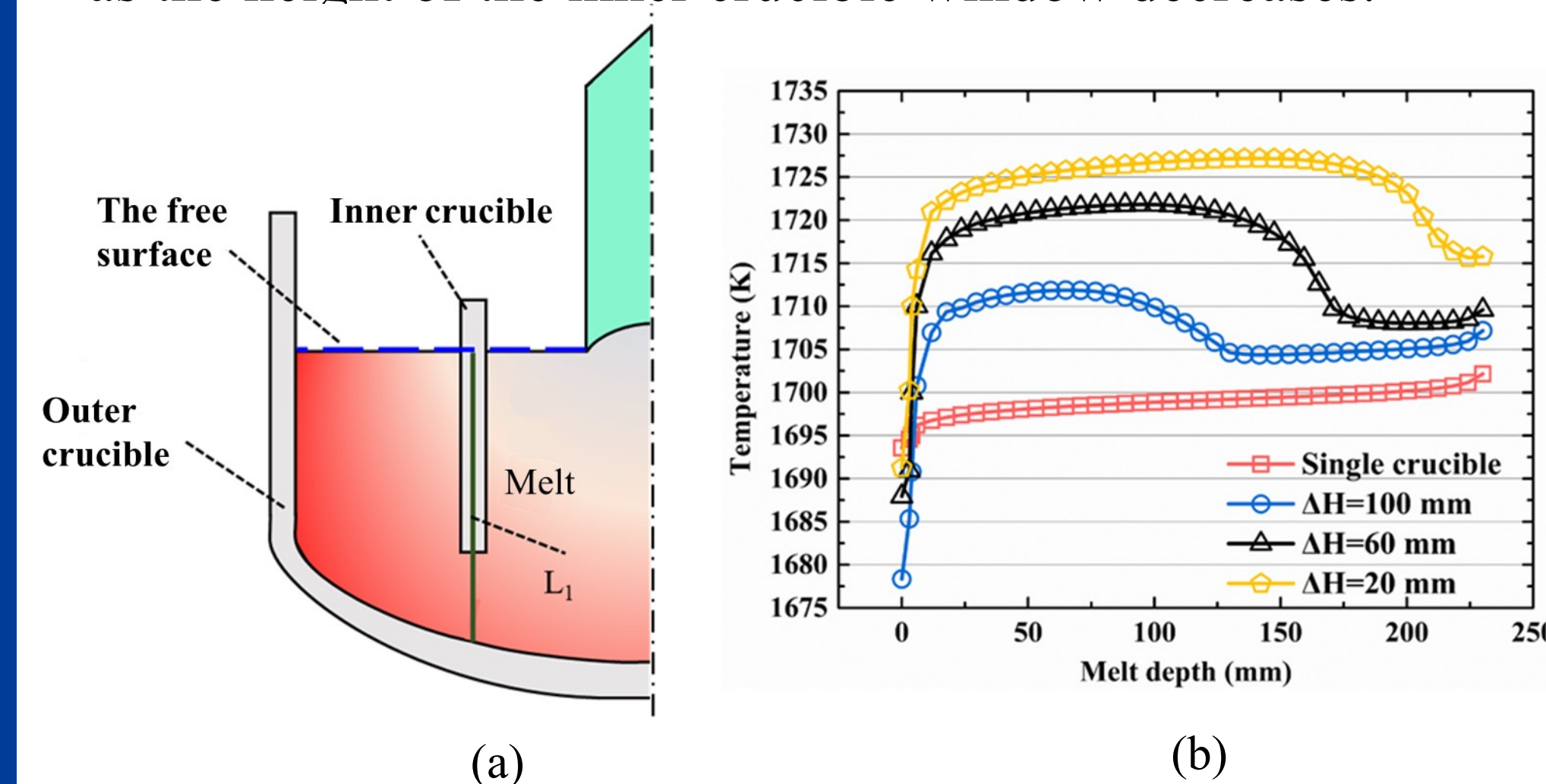


Fig. 5 (a) Schematic diagram of L1 position and (b) temperature distribution along L1

- ◆ The internal crucible inhibits the heat transfer on both sides, and the heat transfer on the melt side at the crystal-melt interface is weakened, thereby reducing the convexity of the crystal-melt interface under the double crucible structure, which is also the reason for increasing the crystal growth rate.

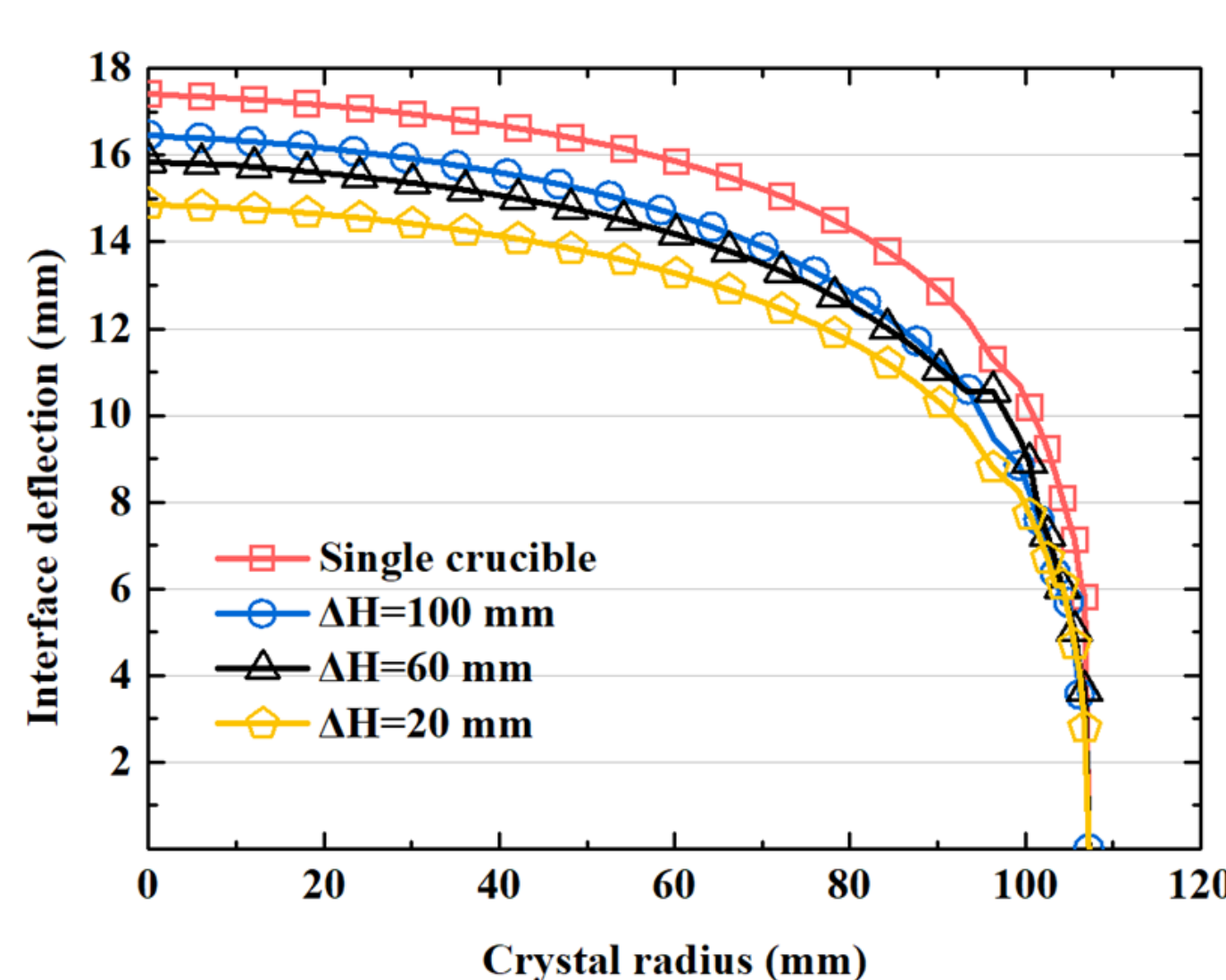


Fig. 6 Variation of crystal-melt interface shape melt at different  $\Delta H$ : (a) Single crucible, (b)  $\Delta H=100$  mm, (c)  $\Delta H=60$  mm, (d)  $\Delta H=20$  mm

- ◆ From Fig.4(a), under the double crucible structure, the radial temperature difference near the free surface of the melt is negative, which means that the temperature near the inner wall of the inner crucible is lower than the temperature in the center of the silicon melt. From Fig 4(b), the axial temperature difference of the silicon melt in the double crucible structure is smaller.

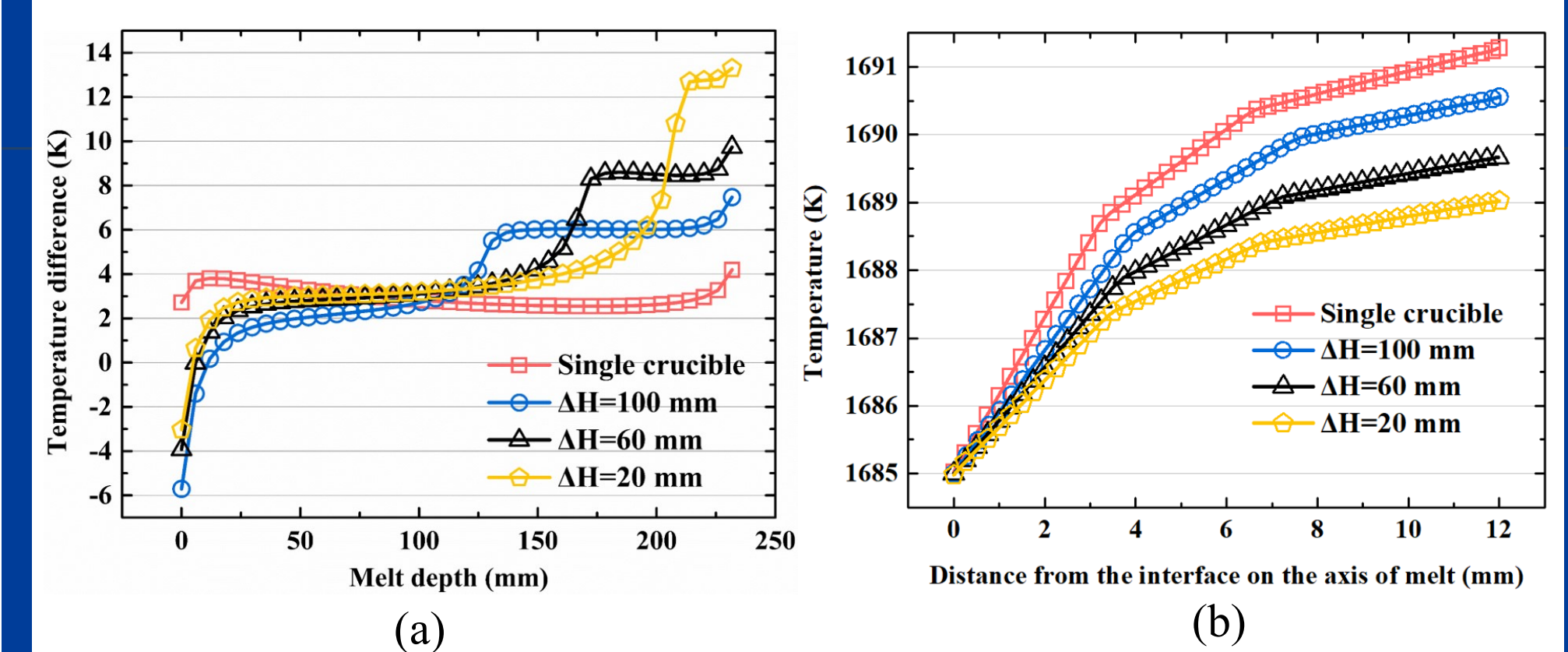


Fig. 7 Radial temperature difference of silicon melt inside crucible (a) and axial temperature distribution on the melt side near the crystal-melt interface (b)

- ◆ From Fig.8, as the height of the inner crucible window decreases, the maximum thermal stress at the crystal-melt interface decreases due to the uneven transfer of radial heat.

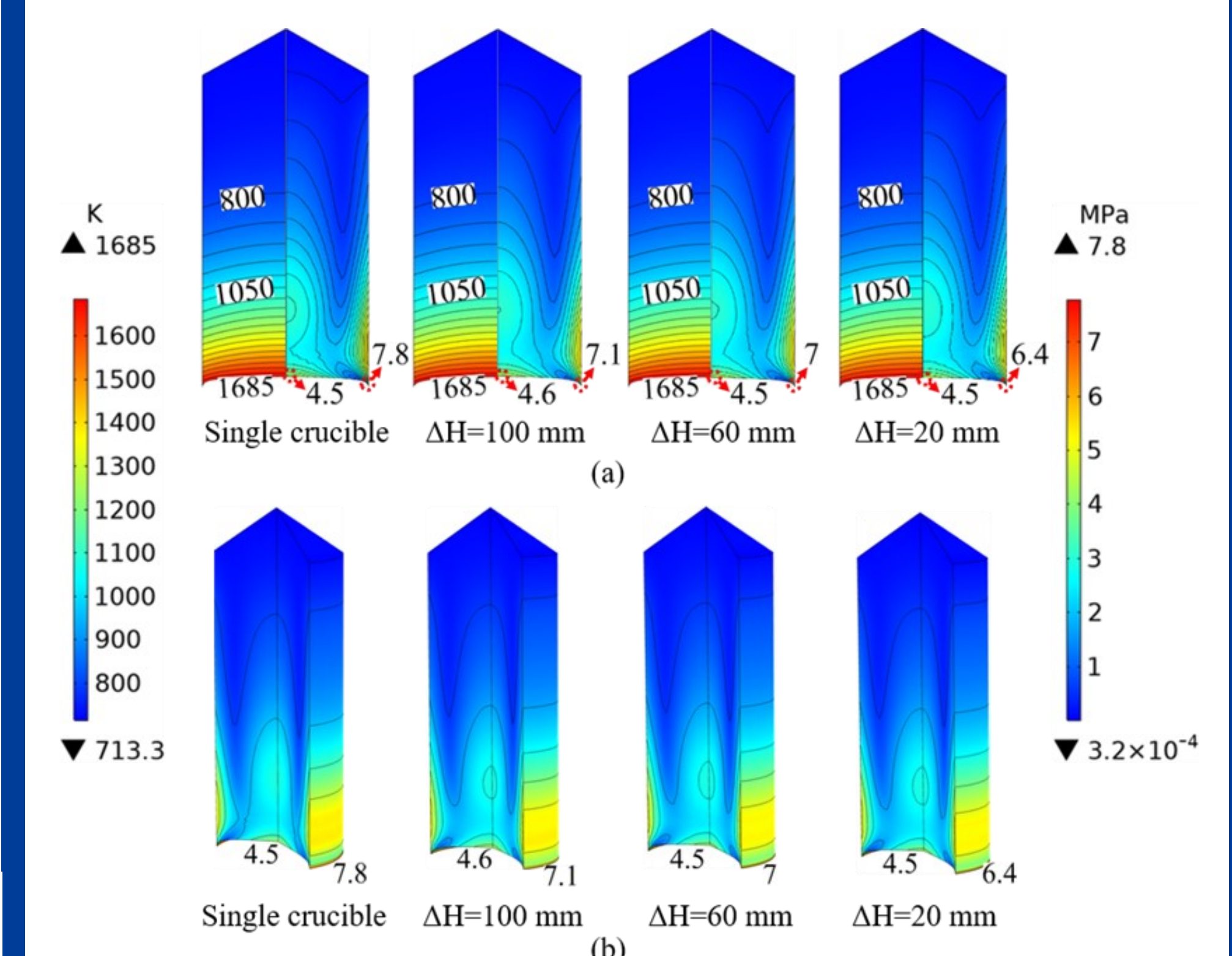


Fig. 8 Temperature and thermal stress distribution of crystal for single crucible structure and different  $\Delta H$ : (a) 2D, (b) 3D

## Conclusion

The effects of different inner crucible window heights on heat transfer, growth rate, crystal-melt interface and crystal thermal stress in CCZ-Si growth were numerically studied, and compared with the growth of CZ-Si under the same conditions.

- ◆ The decrease in the height of the inner crucible window weakens the heat transfer of the outer silicon melt of the inner crucible and increases the free surface temperature of the outer melt.
- ◆ With the decrease of the height of the inner crucible window, the convexity of the crystal-melt interface decreases, the maximum thermal stress decreases, and the crystal growth rate increases.
- ◆ The lower inner crucible window height is conducive to the growth of the CCZ-Si.

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