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# Modeling and Simulation of Silicon Epitaxy Growth in the Atmospheric Chemical Vapour Deposition Reactor

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## Introduction

It is critical to control the uniformity of silicon thin film in the silicon epitaxy growth process. As the structure of the epitaxy reactor is complex, the temperature distribution on substrate surface is not uniform, which contributes to the uniformity of epitaxy growth. Due to the complex thermal field structure and high temperature reaction conditions of epitaxy growth reactor, it is difficult to measure the thermal field of substrate surface. Although there has been some research focusing on simulation of silicon epitaxy, the substrate surface mostly adopts a constant temperature boundary condition, which is not accurate enough. To solve this problem, we propose a CFD model aiming to improve the uniformity of silicon epitaxy in trichlorosilicon-hydrogen system.

## Modeling descriptions

As shown in Fig.1, The three-dimensional geometry model of the atmospheric chemical vapour deposition reactor is established, including reacting chamber, wafer, susceptor, infrared lamp arrays, inlet and outlet.

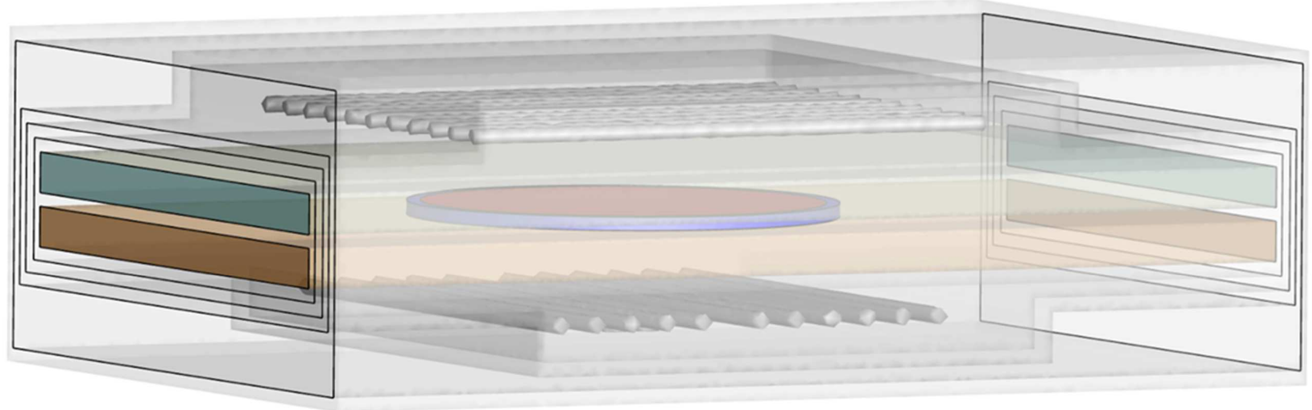


**Fig. 1 Geometry model of the chemical vapour deposition reactor.**

The global model accounts for heat transfer(convective, conductive, and radiative), species transport (convective and diffusive), and chemical reactions on the surface of substrate. The chemical reaction model of trichlorosilicon-hydrogen system is adopted based on the work of Habuka et al.(1994). The reaction is employed as:

$$SiHCl_3 + H_2 \rightarrow Si + 3HCl.$$

The activation energy, E, is assumed to be $1.38 \times 10^5$ Jmol$^{-1}$. The pre-exponential factor, A, is $2.65 \times 10^3$. The rate of reaction is therefore followed as:

$$k = 2.65 \times 10^3 \exp\left(1.38 \times 10^5/RT\right)\left(m^4 mol^{-1} s^{-1}\right).$$

The reactor chamber is under atmospheric pressure. The flow rate of trichlorosilicon-hydrogen system is 70 SLM. And the power of reactor is supplied by the infrared lamp arrays, which is controlled by PID algorithm to maintain constant temperature of four monitoring points around the susceptor.

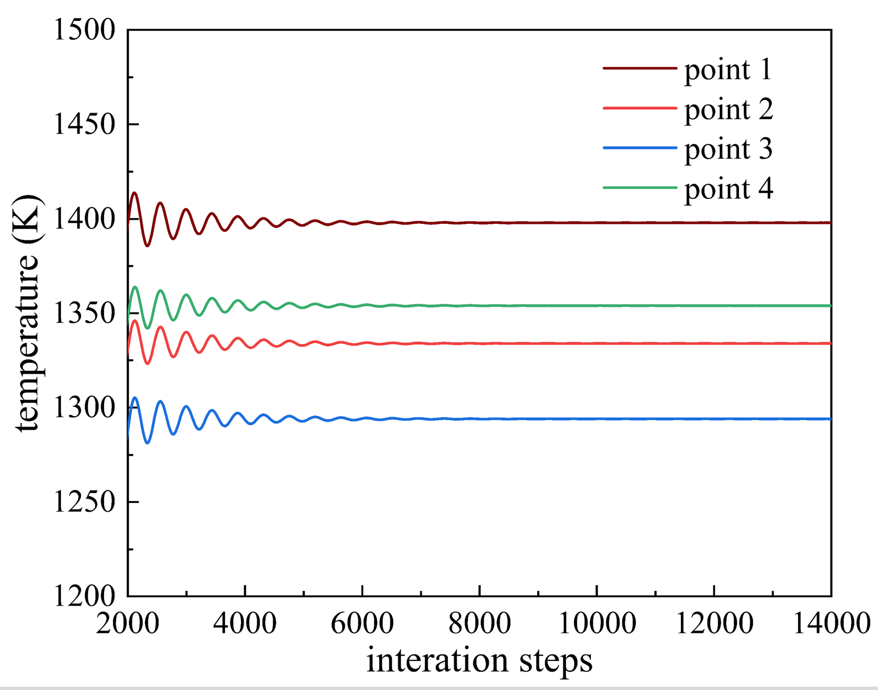
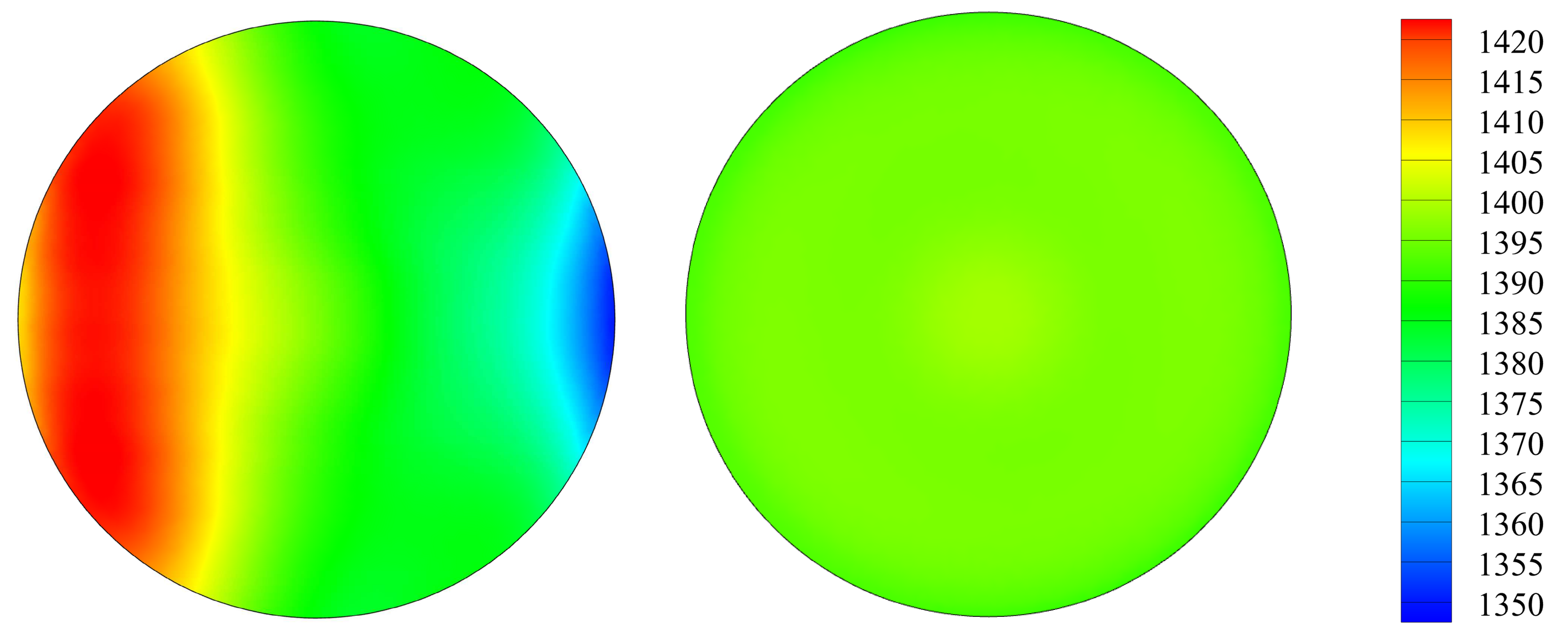



**Fig. 2 Temperature of monitoring points changes with the number of iteration steps.**

## Results & Discussion

The temperature distribution of substrate in different rotation speed is shown in Fig. 3. It can be concluded that when the rotation of wafer is taken into account, the difference of temperature in substrate surface is decreased greatly, and the temperature distribution uniformity of substrate surface is improved.



**(a) 0 rpm (b) 50 rpm**

**Fig. 3 Temperature distribution of substrate in different rotation speed. (unit: K)**

Fig. 5 shows the radial deposition rate distribution of substrate in different rotation speed. The distribution demonstrates that the deposition rate of substrate is more smoothing when wafer rotates.

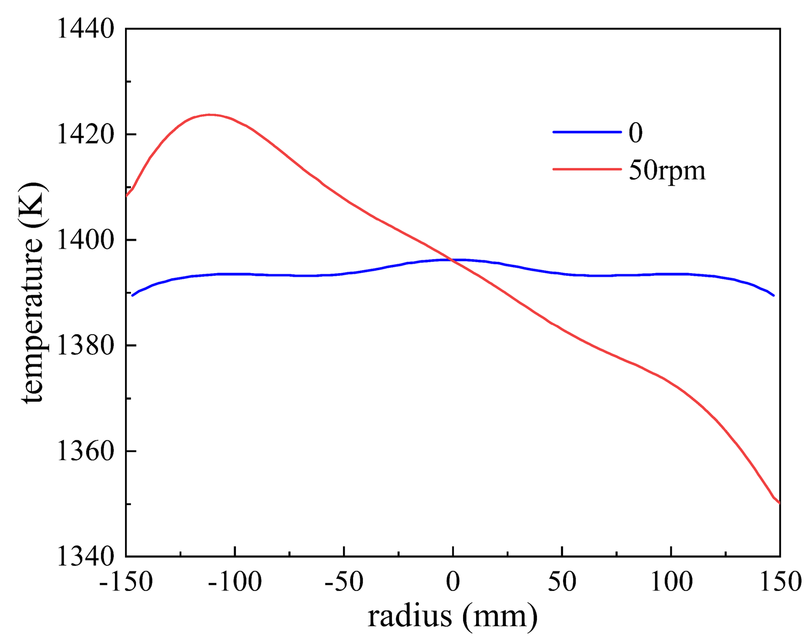



**Fig. 4 Radial temperature distribution of substrate with different rotation speed.**

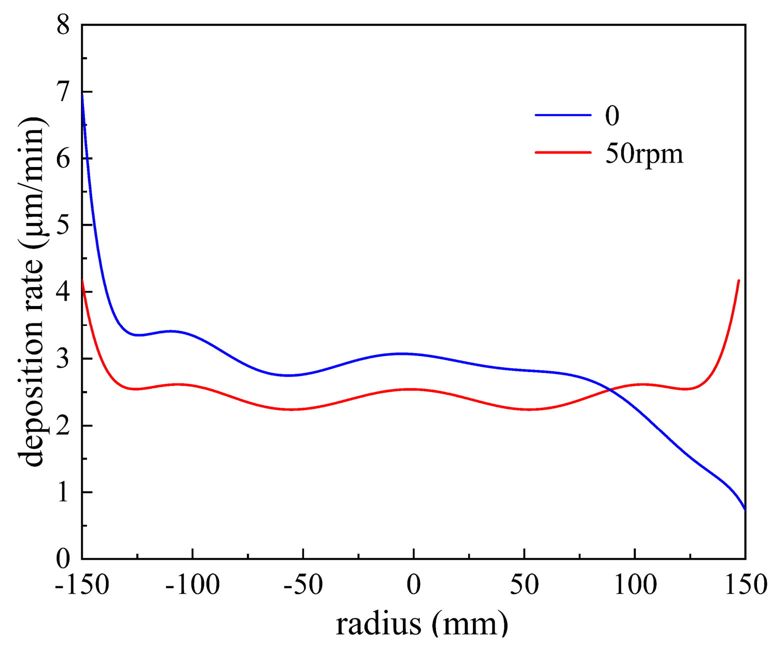



**Fig. 5 Radial deposition rate distribution of substrate with different rotation speed.**

The radial temperature distribution of temperature and deposition rate in substrate surface with different mole fraction of TCS is shown respectively in Fig. 6 and Fig. 7. It can be seen that with the decrease of mole fraction of TCS in the trichlorosilicon-hydrogen system, the uniformity of deposition rate is improved significant.

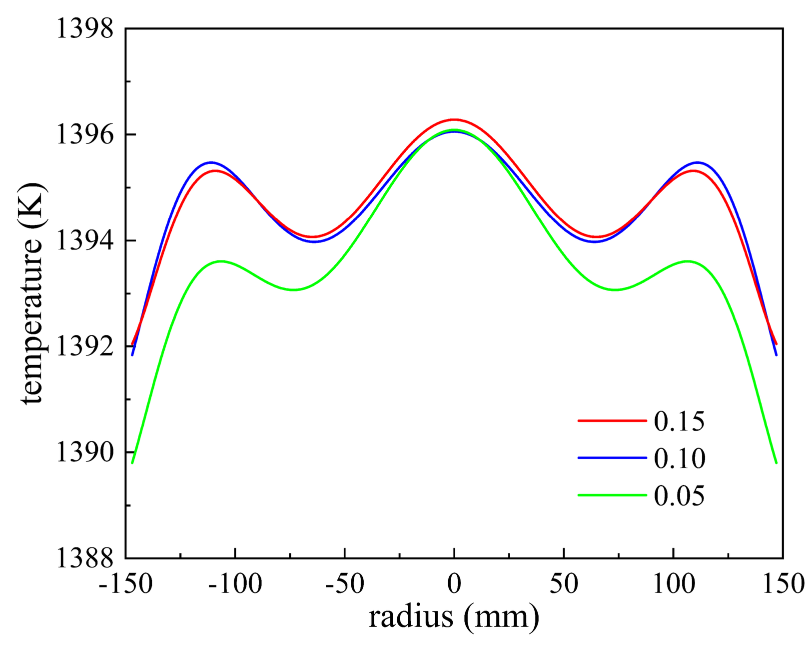



**Fig. 6 Radial temperature distribution of substrate with different mole fraction of TCS.**

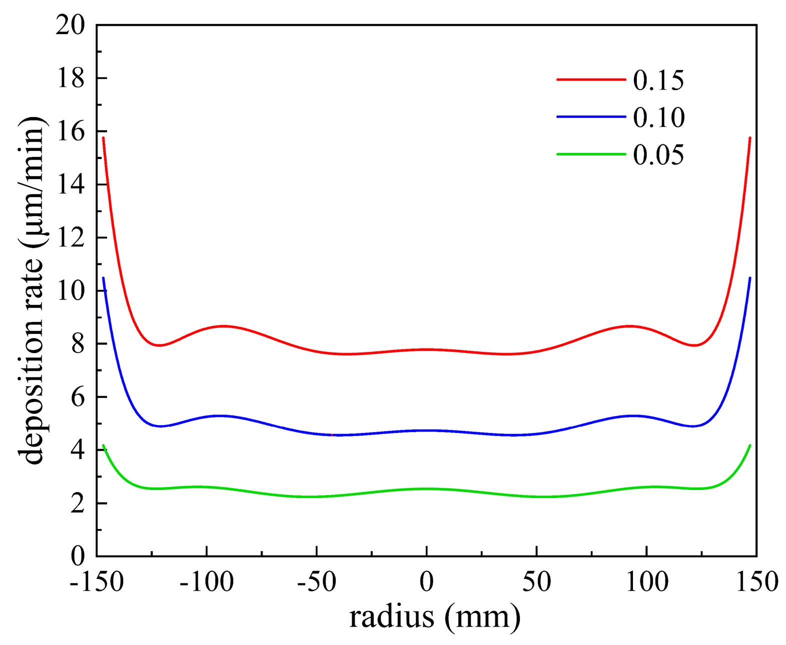



**Fig. 7 Radial deposition rate distribution of substrate with different mole fraction of TCS.**

## Conclusions

In this work, a three-dimensional CFD model for atmospheric chemical vapour deposition reactor is developed. The simulation results show that substrate rotation as well as low mole fraction of TCS gas has obvious improvement in uniformity of silicon epitaxy deposition rate.

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