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DOI
10.1109/SSLChinaIFWS60785.2023.10399702

Publication date
2023

Document Version
Final published version

Published in
China International Forum o Solid State Lighting: International Forum on Wide Bandgap Semiconductors China (SSLChina: IFWS)

Citation (APA)
Tian, J., Tang, Z., Tang, H., Fan, J., & Zhang, G. (2023). Simulation of Epitaxial Growth of Silicon Carbide in a Horizontal Hot-wall CVD Reaction Chamber. In *China International Forum o Solid State Lighting: International Forum on Wide Bandgap Semiconductors China (SSLChina: IFWS)* (pp. 14-17). IEEE. https://doi.org/10.1109/SSLChinaIFWS60785.2023.10399702

2023 20th China International Forum on Solid State Lighting & 2023 9th International Forum on Wide Bandgap Semiconductors (SSLCHINA: IFWS) | 979-8-3503-8537-3/23/$31.00 ©2023 IEEE | DOI: 10.1109/SSLCHINAIFWS60785.2023.10399702

Simulation of epitaxial growth of silicon carbide in a horizontal hot-wall CVD reaction chamber

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Abstract

The silicon carbide (SiC) epitaxial growth process is crucial in chip manufacturing. The growth rate and uniformity of epitaxial film are two critical evaluation criteria of epitaxial process. In order to obtain a higher growth rate and more uniform epitaxial film, it is necessary to improve the SiC epitaxial growth process. The traditional method to improve the epitaxial growth process is the "trial and error method", but this method will consume a lot of time and economic costs. Therefore, it is necessary to find an efficient way to simulate the epitaxial growth process of SiC. This work uses computer aided Multiphysics simulation method to study the growth of SiC epitaxial films in a horizontal hot-wall chemical vapor deposition (CVD) reaction chamber. Firstly, a three-dimensional model of a horizontal hot-wall CVD reaction chamber is established, in which the MTS (methyltrichlorosilane)/H_2 is used to deposit SiC epitaxial films on large-area substrates. The effects of temperature, gas flow distribution ratio, and pallet speed on the growth rate and uniformity of SiC epitaxial films are studied. The results show that: 1) In the range of 1500K-1600K, the higher temperature brings the higher growth rate of SiC epitaxial film. 2) The gas flow ratio of three groups of air inlets can simultaneously affect the growth rate and uniformity of the SiC epitaxial film. With the greater the airflow at the middle air inlet, the higher growth rate and the lower film uniformity will be obtained. 3) The tray rotation speed does not affect the film growth rate, but the higher of film uniformity will be achieved under the higher tray rotation speed. The simulation results agree well with the experimental results, which proves that the Multiphysics simulation method is feasible and can be used for further optimization of the epitaxial growth process of SiC.

Keywords: SiC; Epitaxial growth; CVD; Multiphysics simulation

1. Introduction

SiC is an important material widely used in electronics, optoelectronics, energy and other fields[1]. Its chemical vapor deposition (CVD) process plays a vital role in the preparation of high-quality SiC epitaxial films and devices. As technology develops, understanding and optimizing the SiC CVD process becomes increasingly important. However, due to the complex experimental conditions and high cost, analyzing the SiC CVD process through experimental research is not only time-consuming and labor-intensive but also difficult to obtain comprehensive physical and chemical information.

In recent years, the use of simulation models to study and optimize the CVD process has become more and more popular. By establishing appropriate mathematical models and simulation methods, we can deeply understand the interaction and influence mechanism of various parameters in the CVD process, and predict the deposition rate and film uniformity under different process conditions[2].

Simulation technology can provide an effective method to study and optimize the SiC CVD process. Among them, the simulation model of the chemical vapor deposition process is the key to achieving this goal. In this process, the choice of source gas plays an important impact on the accuracy and reliability of the simulation results. In this study, we chose MTS (methyltrichlorosilane) as the source gas for the SiC CVD process, which is a commonly used precursor gas[3]. By simulating the SiC CVD process, we hope to gain an in-depth understanding of the basic mechanism and influencing factors of the process, and provide guidance and reference for optimizing the preparation of SiC epitaxial films.

Mollick *et al*. simulated the CVD process of SiC growth using MTS/H_2, proposed a simplified two-step reaction mechanism in a hot-wall tube reactor, and analyzed the effects of total flow rate and wall temperature on deposition rate[4]. In order to make the SiC epitaxial film grow more uniformly, they set a constant rotation speed on the substrate, but did not consider the relationship between the specific rotation speed and the uniformity of the film. Bijjargi *et al*. proposed a new integrated CFD model and investigated the effects of operating pressure, temperature, H_2/Ar ratio, and total flow rate on the growth rate and film uniformity of SiC in CVD[5]. Fukushima *et al*. established a reaction model for CVD of SiC in MTS/H_2 vapor system through multi-scale analysis and basic reaction simulation, and analyzed the effects of temperature and residence time on the deposition rate of SiC[6]. Ogawa *et al*. proposed a simple SiC growth model for MTS/H_2 CVD of SiC, which consists of two gas-phase thermal decomposition reactions of MTS and one surface growth reaction of SiC. They analyzed the effects of process parameters such as temperature, residence time, H_2 ratio on the decomposition reaction of MTS, and analyzed the effect of temperature on the growth rate of SiC[7]. Generally, in order to obtain a more uniform SiC epitaxial film, multiple sets of air inlets are set up in the reaction chamber. Therefore, the air flow ratio of each set of air inlets has an impact on the growth rate and uniformity of the SiC epitaxial film. However, previous research has barely touched on this.

This study aims to simulate the CVD process of SiC epitaxial growth, focusing on the impact of deposition

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temperature, tray rotation speed, air flow distribution ratio and other process parameters on SiC deposition rate and film uniformity. By adjusting and optimizing these process parameters, it can achieve efficient and uniform SiC film growth and provide more comprehensive theoretical support for the preparation and application of SiC epitaxial materials.

2. Chemical reaction modeling

This study uses the commercial software COMSOL Multiphysics to model the geometric structure of the horizontal hot-wall CVD reaction chamber as shown in Fig. 1. The overall geometric model is a rectangular parallelepiped, with the air inlet located on the left side. The air inlets are divided into three groups, 5 on the left, 16 in the middle, and 5 on the right, for a total of 26. There is a rotatable tray in the middle of the chamber, where the deposition reaction of SiC occurs, and the reacted gas is discharged from the outlet on the right.

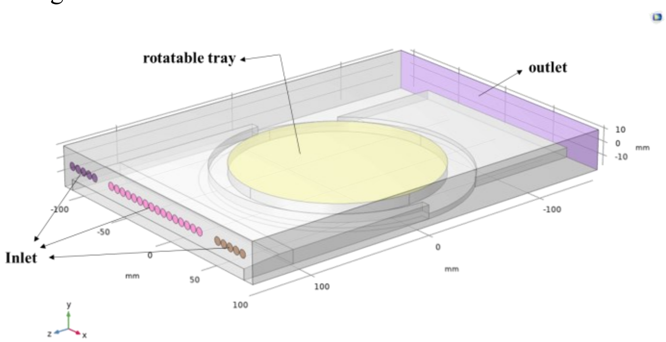

Fig. 1 Geometric structure of the horizontal hot-wall CVD reaction chamber.

The chemical reaction model used in this study is listed in Table 1[8]. After MTS gas injects to the reaction chamber from the left air inlet, a decomposition reaction occurs to generate effective active gas phase components $SiCl_2$ and C_2H_2, which are then adsorbed on the substrate surface to generate surface substances $SiCl_2$_s and CH_s, and finally forms SiC epitaxial film.

Table 1 Chemical reaction model

CH_3SiCl_3	→	**CH_3+SiCl_3**
$SiCl_3+H_2$	→	**$SiCl_2+HCl$**
$2CH_3$	→	**$C_2H_2+2H_2$**
$SiCl_2$	→	**$SiCl_2$_s**
C_2H_2	→	**2CH_s**
$SiCl_2$_s+CH_s+1/2H_2	→	**SiC_b+2HCl**

*_s means the surface species in solid phase.

*_b means the deposited solid phase material.

The reference pressure level in the reaction chamber is set to 1 atm, the initial temperature is set to 800 K, and the total growth time is set to 60 minutes. The total gas flow rate of the three groups of air inlets is set to 150 l/min, the input MTS concentration is 0.05 mol/m^3, and the H_2 concentration is 0.5 mol/m^3. Argon with a concentration of 0.05 mol/m^3 is used as a carrier gas and shielding gas.

3. Results and discussion

When a SiC film is grown in a reaction chamber, due to factors such as the structure of reaction chamber and the direction of air inlet, the film thickness are usually unevenly distributed, as shown in Fig. 2. Therefore, in order to make the film grow more uniform, the substrate material is usually placed on a rotatable tray, and the rotation of the tray makes the film grow more uniformly. As the tray rotates, the distribution of film thickness will take on the shape of a set of concentric rings as simulated and shown in Fig. 3.

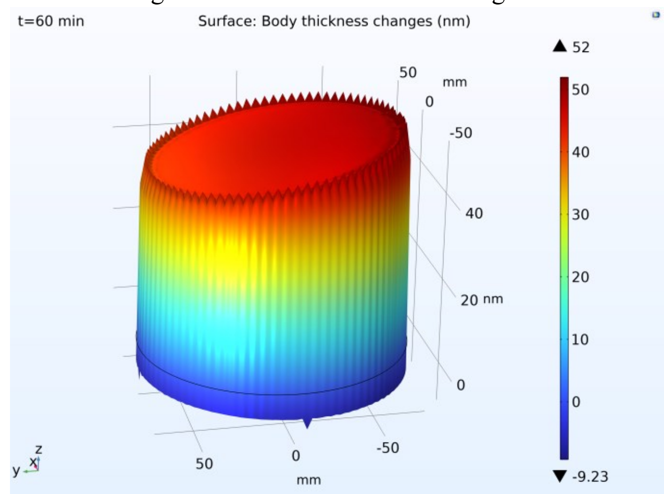

Fig. 2 The thickness distribution of SiC epitaxial layer when the tray does not rotate.

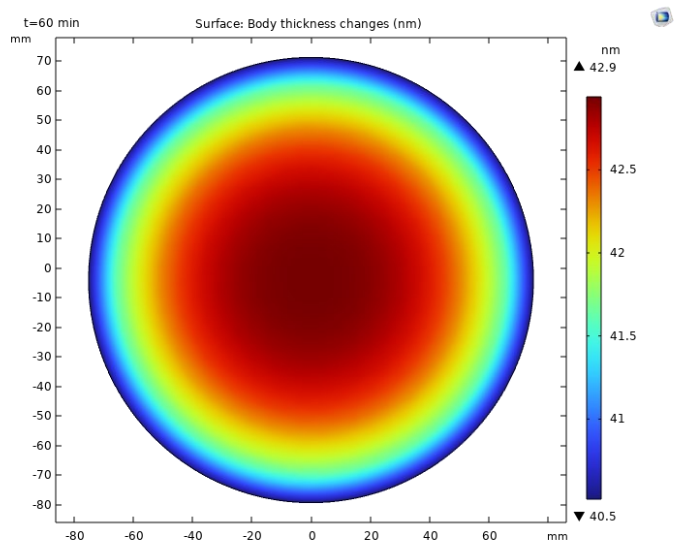

Fig. 3 The thickness distribution of SiC epitaxial layer when the tray rotates

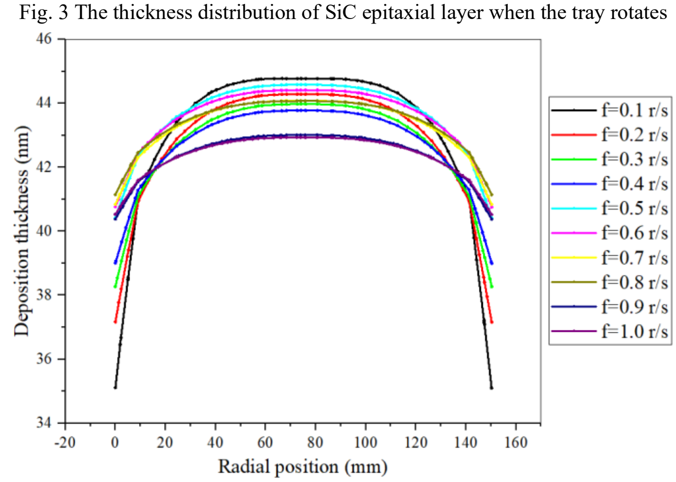

Fig. 4 Radial distribution of SiC thickness at different rotational speeds.

To study the relationship between growth rate and the uniformity of SiC epitaxial film and the rotation speed of tray, the rotation speed of tray was set as gradually increasing from

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0.1 revolutions per second to 1 revolution per second. The thickness distributions of SiC epitaxial film in the radial direction were simulated and shown in Fig. 4. The distribution of SiC epitaxial film in the radial direction presents the shape of " ∩ ". When the rotation speed is small, the thickness difference between center and edge is obvious, and with the increase of the rotation speed, the thickness difference between center and edge shows a decreasing trend and the thickness becomes more uniform.

Furthermore, as the rotation speed of tray increases, the standard deviation of film thickness shows a decreasing trend, as shown in Fig. 5. Due to the influence of the of chamber structure and the gas flow rate, the chemical reaction rates of different regions on the substrate surface are not the same, so the SiC epitaxial growth rate is different on the substrate. The effect of reaction rate difference at different positions on the uniformity of film can be greatly reduced by increasing the rotation speed of tray and the uniformity of SiC epitaxial film will be enhanced. When the tray rotation speed is set as 0.5 revolution per second, the averaged thickness of SiC epitaxial film reaches to maximum value, but it does not change much compared to other cases.

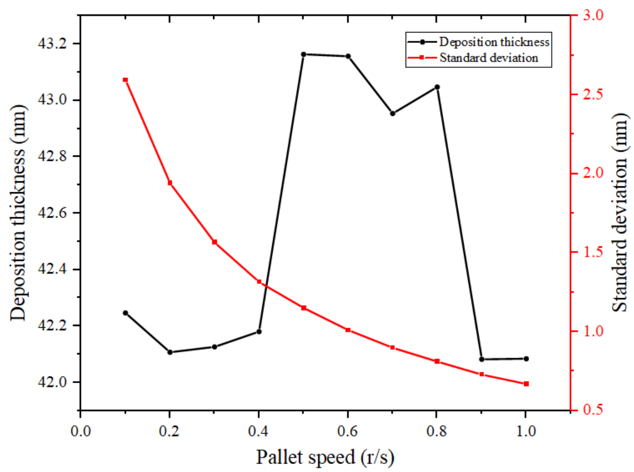

Fig. 5 The relationship between averaged and standard deviation of thickness with rotation speed.

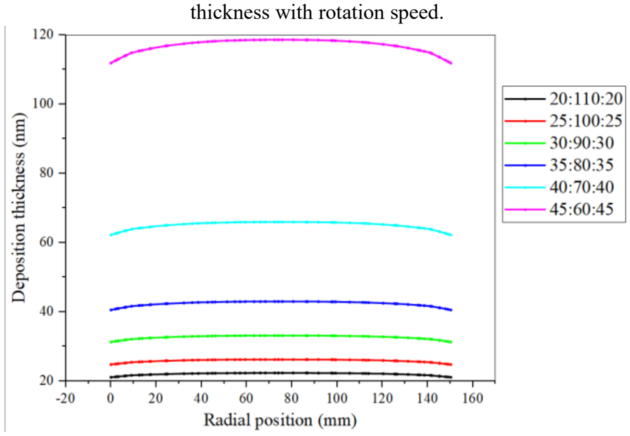

Fig. 6 Radial distribution of SiC epitaxial film thickness under different airflow distribution.

The total gas flow of three groups of air inlets was controlled to be 150 l/min. The effect of the proportion of gas flow on the growth rate and uniformity of the SiC epitaxial film was studied by changing the proportion of gas flow between three groups of air inlets.The air inlet in the middle of the gas flow rates were set to 60 l/min, 70 l/min, 80 l/min, 90 l/min, 100 l/min, 110 l/min, respectively, the thickness distribution of SiC epitaxial film on the radial were simuateed and shown in Fig. 6. It can be clearly seen that with the increase of gas flow at the middle air intake, the thickness of SiC epitaxial film gradually decreases.The mean value and standard deviation of SiC epitaxial film thickness decrease with the increase of gas flow at the middle inlet, as shown in Fig. 7. It is indicated that when the gas flow at the middle inlets increases, the growth rate of SiC epitaxial film decreases, while the uniformity increases.

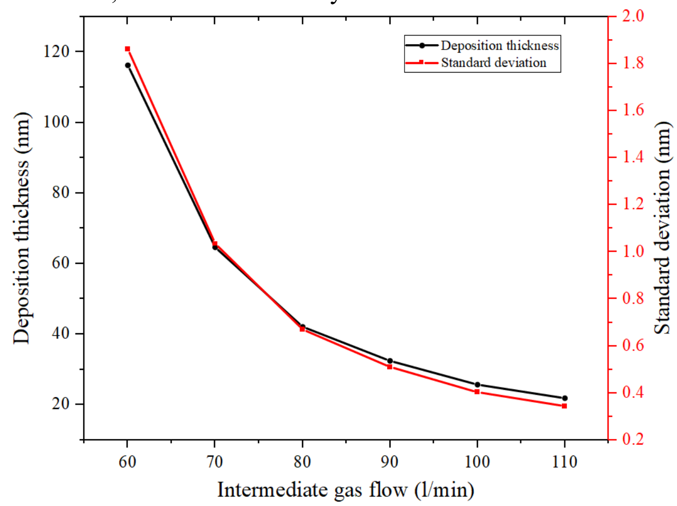

Fig. 7 The relationship between averaged and standard deviation of thickness with airflow distribution.

Fig. 8 presents that when the temperature increases, the growth rate of SiC epitaxial film will increase. Increasing the temperature will increase the kinetic energy of reactive molecules, thus the probability of collisions between molecules and increasing the reaction rate is enhanced. With the increase of temperature, the standard deviation of SiC epitaxial film thickness also increase, which means that the uniformity of epitaxial film improved, as shown in Fig. 9. At a certain temperature, the deposition rate of SiC epitaxial film increases gradually with the increase of temperature, and the deposition process is controlled by mass transfer. Therefore, with the increase of temperature, the concentration gradient of the reactants in the gas phase components gradually becomes larger, which leads to the deterioration of the uniformity of epitaxial growth .

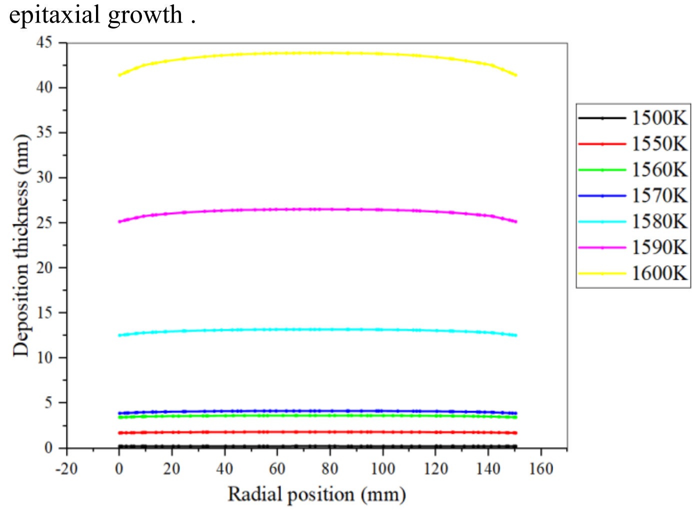

Fig. 8 Radial distribution of SiC epitaxial film thickness at different temperatures

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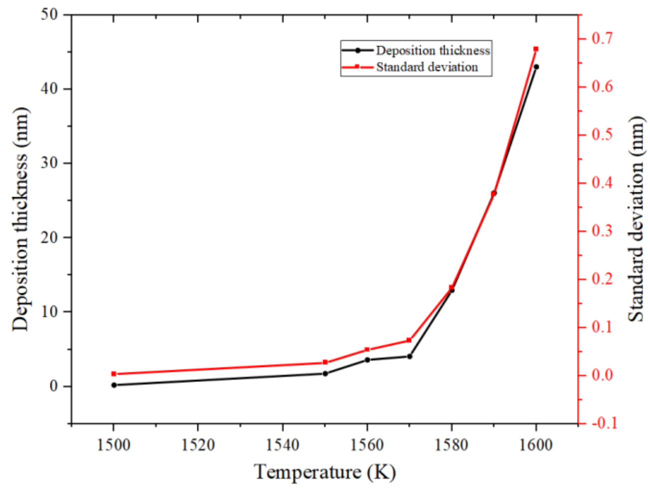

Fig. 9 The relationship between averaged and standard deviation of thickness with temperature

4. Conclusions

In this study, the SiC epitaxial growth process in a horizontal hot-wall CVD reaction chamber is investigated with Multiphysics simulations, in which the effects of tray speed, airflow distribution and temperature on the growth rate and uniformity of SiC epitaxial films are discussed. The findings can be concluded as: (1) Among them, increasing the tray speed can reduce the standard deviation of film thickness, that is, increase the uniformity, but has little effect on the film growth rate. (2) The airflow distribution has a great influence on the film growth rate. With the increase of gas flow at the middle air inlet, the film growth rate decreases and the uniformity increases. (3) Increasing the temperature can greatly improve the film growth rate, but it will also reduce the film uniformity. Thus, it is necessary to make a proper balance between the growth rate and uniformity of the film

Acknowledgments

This work was partially supported by National Natural Science Foundation of China (52275559), Shanghai Pujiang Program (2021PJD002), and Shanghai Science and Technology Development Funds (19DZ2253400).

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