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Temperature Field Simulation and Optimization for Horizontal 6-inch 4H-SiC Epitaxial CVD

Reactor by Induction Heating

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Abstract

Silicon carbide (SiC) epitaxial process is a key step in the fabrication of power devices, and the temperature field inside the reactor chamber plays an essential role in this process. In this paper, the temperature field in the horizontal chemical-vapor-deposition reactor chamber used for growing homo-epitaxial 4H-SiC material is studied using the finite-element method. A threedimensional time-dependency model is built for the accuracy of simulation, and the effects of 11 relative coil locations (-50, -28, -18, -10, -4, 0, 4, 10, 18, 28, and 50 mm) on heating efficiency and temperature uniformity of the substrate are analyzed. Results indicate that the suitable relative location between the center of coil and that of the substrate to achieve optimum temperature uniformity is -4 mm, and 18 mm to obtain the highest heating efficiency. To increase the heating efficiency and temperature uniformity of the substrate, the structure of the reactor was analyzed and optimized. It is observed that both heating efficiency and temperature uniformity can be effectively improved by adding a graphite pillar inside the down susceptor.

1. Introduction

Silicon- (Si) based power devices are currently reaching their physical limits. As one of the representative semiconductor materials with a wide band gap, Si carbide (SiC) has many promising properties, such as high thermal conductivity, high electric breakdown field, and high carrier saturation velocity, and it has thus received widespread attention as a suitable next-generation material for high-voltage power devices [1,2]. The chemical-vapor-deposition (CVD) method, which is used to grow SiC epitaxial layers on homogeneous substrates, is an essential technique and process employed to produce SiC-based power devices. When using the CVD method, to maintain reactor cleanliness and high heating efficiency, induction heating is always considered the most effective way of providing the heat for the epilayer growth process. In CVD reactors, the heating system affects the temperature field and consequently determines the flow field. The temperature profile on the substrate has huge impacts on the thickness uniformity, surface morphology, growth rate, and reaction process of the epitaxial layer [3-5]. From the perspective of designing an induction heating reactor, the parameters of the induction coil will directly determine the temperature profile in such reactors. Thus far, researchers studying reactor design usually depend on "trial-and-error" experience and numerous experimental iterations to optimize such reactors. Under these conditions, numerical simulation of the reactor temperature field is a cost-saving and efficient solution to determine the optimal temperature profile in the reactor design process.

Numerous related studies of induction heating have been conducted in last several years. Janzen *et al.* [6] simulated the temperature field for a horizontal hot-wall SiC CVD reactor, and predicted the thin-film growth process. Meziere *et al.* [7] investigated the relationship between the heating mode, gas flow, reactor geometry, and the epitaxial layer properties in a horizontal hot-wall CVD reactor. Huang *et al.* [8] studied the effect of the number of coil layers on the temperature uniformity on the susceptor. Chen *et al.* [9] revealed the geometric effect on thermal field in a horizontal CVD reactor. Several studies of the influence of parameters of coil for temperature distribution in a vertical GaN metal-organic CVD reactor

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based on two-dimensional (2D) asymmetric models have been undertaken [10,11], but few investigations have been carried out on how the temperature field of a horizontal SiC CVD reactor is affected when changing the relative location of the coil.

In this study, a 3D time-dependency temperature field model of the reactor was built using the finite-element method (FEM). The heat radiation, heat conduction, and water cooling were considered in this model to ensure the accuracy of the simulation. The temperature distribution on the substrate of the relative location between the coil and the center of the substrate was investigated. Moreover, based on simulation results, a way to improve heating efficiency and temperature uniformity of the substrate is proposed.

2. Computational Modeling

(a) **3D** modeling of reactor

Figure 1 shows a sectional view of the structure of a SiC CVD reactor, in which the down and up susceptor is made of dense graphite and heated by an induction coil. Susceptors are semicircular and hollow inside in order to form an eddy current. Graphite susceptors are surrounded by insulation material inside a quartz tube. The quartz tube and rectangular shape induction coil have double layers, and the hollow area in the middle of both are filled with deionized water as a coolant. The induction coil, which is continuously wound around the outside of the double-layer quartz tube, produces an alternating magnetic field to generate an eddy current in the graphite area. The susceptors are significantly heated, leading to an increasing temperature inside the reactor due to the resistance effect.



Fig. 1 Sectional view of reactor structure.

(b) Mathematical model

When establishing the heat-transfer model, the following assumptions are made. (1) The rotation of the susceptor and flow field in the reactor is not considered. (2) Thermal radiation and thermal conduction are considered in the model. (3) The up susceptor, down susceptor, and hydrogen inside the reactor are considered to be a gray body, and the surface-to-surface radiation is imposed at the core area of the reactor. The radiative heat flux Q_{radi} can be expressed by the following radiative integral equation [12] for a gray and diffuse surface:

$$\frac{Q_{radi,j}}{\varepsilon_j} - \sum_{k=1}^N F_{j,k} \frac{1 - \varepsilon_k}{\varepsilon_k} Q_{radi,j} = \sigma T^4{}_j - \sum_{k=1}^N F_{j,k} \sigma_{SB} T_k{}^4, \quad (1)$$

where $F_{j,k}$ is the factor from parts j to k of the reactor, ε_j is the emissivity of the radiative surface, and σ_{SB} is the Stefan-Boltzmann constant (5.67 × 10⁻⁸ W/m²K⁴).

In addition, the water inside the double-layer quartz tube and the copper coil serve as a cooling system that can be simulated through high effective thermal conductivity and combined with a convective loss term:

$$Q_{waterincopper} = \frac{\frac{dM}{dt}C_{water}}{V_{waterincopper}}(T_{in} - T) \quad (2)$$

$$Q_{waterinquartz} = \frac{\frac{dM}{dt}C_{water}}{V_{waterinquartz}} (T_{in} - T)$$
(3)

where M is the water mass flow, C_{water} is the heat capacity of the water, and $V_{waterincopper}$ and $V_{waterinquartz}$ are the volume of the water inside the copper coil and inside the double-layer quartz tube, respectively. T_{in} is the temperature of the inlet water and T the current temperature. Under such conditions, the temperature distribution in the reactor can be obtained by using the following heat conduction equation (the first law of thermodynamics):

$$q_{eddy} + Q_{waterincopper} + Q_{waterinquartz} + \nabla \bullet$$

$$Q_{radiation} = \rho C_p \frac{\partial T}{\partial t} - \nabla \bullet (k \nabla T)$$
(4)

where ρ is the mass density, C_p is the specific heat capacity, and k is the thermal conductivity. In addition, we consider temperature-dependent material properties as much as possible, which can improve the accuracy and reliability of the simulation [13]. For the temperature accuracy of the graphite susceptors, we used following equation to present the electrical conductivities of the graphite:

$$\sigma = \frac{1}{\rho_0(1 + \alpha(T - T_{ref}))},\tag{5}$$

where $\rho_0 = 1.0 \times 10^{-5} (\Omega \cdot \text{m})$ is the graphite reference conductivity at $T_{ref} = 293$ K, and $\alpha = 5.0 \times 10^{-6} (1/\text{K})$ is the graphite temperature coefficient of graphite resistivity. We assume that the initial environmental temperature is 293 K. For the material parameters of graphite, H₂, the quartz tube, and SiC, the reader is referred to Ref. [14]; for those of the cooper coil and insulation material wafer, the reader is referred to Ref. [15].

A mesh of 380,000 elements was created for the entire reactor; the FEM meshing map is shown in Fig. 2. In addition, the mesh is refined over both the graphite and substrate areas since they are the areas of greatest importance when investigating the temperature profile. In reality, purified H₂ is used as a carrier and dilution gas in the growth process [16]. Other precursor gases, such as silane (SiH₄), ethylene (C₂H₄), and trichlorosilane (TCS), are highly diluted and can be neglected compared to H₂ [17,18]. In this case, only H₂ fills the entire reactor.



Fig. 2 FEM mesh of 3D model reactor.

3. Comparison and Results

Figure 3 shows the results of the temperature field simulation when the reactor reaches a steady equilibrium state. The temperature of both sidewalls is higher than the middle of the reactor.



Fig. 3 Temperature distribution of reactor at steady-state equilibrium.

The substrate temperature distribution of 11 relative positions (-50, -28, -18, -10, -4, 0, 4, 10, 18, 28, and 50mm) between the center of the coil and the center of the substrate was simulated, and the results are shown in Fig. 4. The figure shows that the higher-temperature area of the substrate moves from left to right as the coil location moves toward and away from the center of the substrate.



Fig. 4 Temperature distribution of the substrate when moving the induction coil.

Average temperature and temperature standard deviation of different coil locations is displayed in Fig. 5. Average temperature and temperature standard deviation represent heating efficiency and temperature uniformity on the substrate, respectively. It can be observed from the figure that the optimum temperature uniformity of the substrate is the coil located at -4 mm, and that the highest heating efficiency is the coil located at 18 mm.





It is found that the middle area of the SiC substrate has the relative lower temperature compared to the side area.

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It is necessary to increase the temperature in the middle area of the SiC substrate to improve the temperature uniformity, which is beneficial to the growth of highquality homo-epitaxial films. The conventional graphite down susceptor is hollow inside the circular area, as Fig. 6(a) shows. Figure 6 (b) shows a modified structure for the down susceptor. A pillar has been added into the semicircular area, and its role is to enhance the effect of heat conduction from outside the circular graphite to the middle area of the SiC substrate. When using the conventional down susceptor, the heat is transferred by heat radiation of H₂, and the thermal radiation efficiency is low. However, if the modified down susceptor is used, the temperature will be compensated by thermal conduction, the efficiency of which is higher than that of the thermal radiation.



Fig. 6 Schematic of (a) a conventional structure and (b) the proposed structure.

The radial temperature distribution for a conventional structure is a "V" shape (coil location at

-4 mm), and that for a conventional structure is a "W" shape, as shown in Fig. 7(a). The temperature distribution of the proposed structure on the SiC substrate is shown in Fig. 7(b). It can be observed from the figure that the temperature in the middle area of the substrate is increased by using the newly proposed structure. Furthermore, by using the conventional structure, the temperature uniformity (standard deviation) is 16.95°C and the heating efficiency (average temperature) is 1612.6°C on the substrate. However, the temperature uniformity and heating efficiency when using the proposed structure are 6°C and 1691.5°C, respectively.



Fig. 7 (a) Radial temperature distribution of the SiC substrate on conventional and proposed down susceptors;(b) temperature profile of the substrate with the proposed down susceptor structure.

4. Conclusions

The 3D time-dependency temperature field in an induction heating SiC CVD reactor was simulated using the finite-element method. The effect of the relative location between the center of the coil and the center of the substrate on temperature distribution and heating efficiency was investigated, and a new graphite susceptor structure (considering its influence on temperature distribution) proposed. After analysis of the results, the conclusions that follow were drawn. (1) Optimum temperature uniformity of the substrate is the

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coil at location -4 mm, and the highest heating efficiency occurred in the coil located at 18 mm. (2) Both heating efficiency and temperature uniformity can be improved by inserting a graphite pillar into the semi-circular area of the down susceptor.

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