Finite element analysis of the temperature field in a vertical MOCVD reactor by induction heating*

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Abstract: The temperature field in the vertical metalorganic chemical vapor deposition (MOCVD) reactor chamber used for the growth of GaN materials is studied using the finite element analysis method (FEM). The effects of the relative position between the coils and the middle section of the susceptor, the radius of the coil, and the height of the susceptor on heating condition are analyzed. All simulation results indicate that the highest heating efficiency can be obtained under the conditions that the coil distributes symmetrically in the middle section of the susceptor and the ratio of the height of the susceptor to that of the coil is three-quarters. Furthermore, the heating efficiency is inversely proportional to the radius of the coil.

Key words: MOCVD; finite element; temperature; suspector

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1. Introduction

As one of the III–V group compound semiconductor materials with wide band gaps, GaN has excellent optic, electric and thermodynamic characteristics. GaN and nitride compounds, which are representatives of the third generation semiconductors, are important subjects in the optoelectronic research field[1]. Presently, the MOCVD method, which is used to grow thin semiconductor film, is a key technique. Induction heating is used to create the temperature needed for reactions in the MOCVD reactor. The temperature distributions of the substrate are currently always assumed to be uniform, when the temperature and flow fields in the reaction chamber are studied[2–4]. But in a conventional vertical MOCVD reactor, the coils are around the outside of the walls of the reactor chamber. Due to the skin effect, the temperature distributions of the substrate are non-uniform. For studies of induction heating, Chen *et al.*[5] showed that, by keeping the current intensity constant in the induction coils, the maximum temperature increases as the electric current increases. Pu obtained the relationship between the turns of the coils and the joule heat[6]. Zhang showed the influence of different spaces between turns of the induction coil on the temperature distributions[7]. However, there are few studies on the effect of the relative position of the coils, the radius of the coils, and the height of the susceptor on the heating efficiency. In this paper, the relationship between the relative position of the coils, the radius of the coils, and the height of the susceptor on the heating efficiency is studied by using Ansys software.

2. Mathematical model and mesh generation

A numerical algorithm has been developed which consists of a calculation of the frequency time-harmonic magnetic field by induction heating and a calculation of the thermal field distribution. We use magnetic potential vector theory to model the induction heating and an axisymmetric conduction-radiation model to calculate the temperature distributions. The magnetic vector potential equation derived from Maxwell's equation is[5]

$$\nabla \times (\frac{1}{\mu}\nabla \times \boldsymbol{A}) + \varepsilon\frac{\partial^2 \boldsymbol{A}}{\partial t^2} + \sigma\frac{\partial \boldsymbol{A}}{\partial t} = \boldsymbol{J}, \quad (1)$$

where $\boldsymbol{J}$ is the current density in the coil, μ is the magnetic permeability, $\boldsymbol{A}$ is the magnetic vector potential, and σ is the electrical conductivity.

Since the electromagnetic field distribution is axisymmetric, the current density $\boldsymbol{J}$ in the coil and the magnetic potential vector $\boldsymbol{A}$ have only one angular component with exponential form

$$\boldsymbol{J} = \begin{Bmatrix} 0 \\ J_0 \exp \mathrm{i}\omega t + C \\ 0 \end{Bmatrix}, \ \boldsymbol{A} = \begin{Bmatrix} 0 \\ A_0 \exp \mathrm{i}\omega t + C \\ 0 \end{Bmatrix}, \quad (2)$$

where ω is the angular frequency, C denotes the complex conjugate, i is the complex unit, J_0 is the current density which is a scalar here, and A_0 is the magnetic scalar potential (J_0 and A_0 are functions of the position). Thus, the magnetic potential

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vector equation can be written as

$$\left(\frac{\partial^2}{\partial r^2}+\frac{1}{r}\frac{\partial}{\partial r}-\frac{1}{r^2}+\frac{\partial^2}{\partial z^2}\right)\left(\frac{A_0}{\mu}\right)-\mathrm{i}\omega\sigma A_0+\varepsilon\omega^2 A_0=-J_0. \quad (3)$$

The boundary conditions are

$$A_0=0 \text{ at } r=0 \text{ and } r^2+z^2\to\infty. \quad (4)$$

The temperature distributions in the susceptor can be obtained using a heat conduction equation:

$$c\rho\frac{\partial T}{\partial t}=\frac{1}{r}\frac{\partial}{\partial r}\left(k_i r\frac{\partial T}{\partial r}\right)+\frac{\partial}{\partial z}\left(\frac{\partial T}{\partial z}\right)+q, \quad (5)$$

where c is the specific heat, ρ is the density, k_i is the thermal conductivity of the material i, and q is the eddy-current-generated heat power density due to the induction which can be obtained as

$$q=\frac{1}{2}\sigma\omega^2 A_0 A_0^*, \quad (6)$$

where A_0^* is the complex conjugate of A_0.

A coupled convection-radiation boundary condition is applied on the outer surfaces of the susceptor,

$$-k_i\frac{\partial T}{\partial n}=h(T-T_c)+\varepsilon\sigma_{\mathrm{sb}}(T^4-T_{\mathrm{c}}^4), \quad (7)$$

where ε is the emissivity of the radiation, σ_{sb} represents the Stefan-Boltzmann constant, h is the heat transfer coefficient, and T_{c} is the environmental and initial temperature. The symmetric condition used is

$$\frac{\partial T}{\partial r}=0 \text{ at } r=0. \quad (8)$$

The above equations and boundary conditions Eqs. (1)–(8) are used in the model, and an FEM model for simulating the electromagnetic field in the vertical MOCVD reactor is developed. The model includes the following parts: the graphite susceptor, the sapphire substrate which is on the upper surface of the susceptor, the coils, the inner walls of the reactor, the upper flange, the down flange and so on, which are axial-symmetric, as shown in Fig. 1(a). The radius of the winding of the coil r = 3.5 mm, and the coil turn value is 6. The radii of the susceptor and the substrate are 28 mm and 25.4 mm, respectively. A 2D model for analyzing the axial-symmetric electromagnetic field is used. Considering the skin effect, the method of layer-mesh area is employed to ensure 4 to 5 grids within the skin effect layer. The meshing area of the half susceptor is shown in Fig. 1(b). It is assumed that the current in the coil is time-harmonic, and the current density is 2.45×10^7 A/m^2. The current frequency is 30 kHz.

We assume that the initial temperature is 25 °C, and the corresponding electric and thermophysical parameters including electrical conductivity, density, thermal conductivity, specific heat, radiation emissivity of the graphite susceptor and the sapphire substrate, as well as the quartz wall of the reactor chamber, are referred to in Ref. [8]. The effects of the varying temperature on the materials of modules in the reactor are

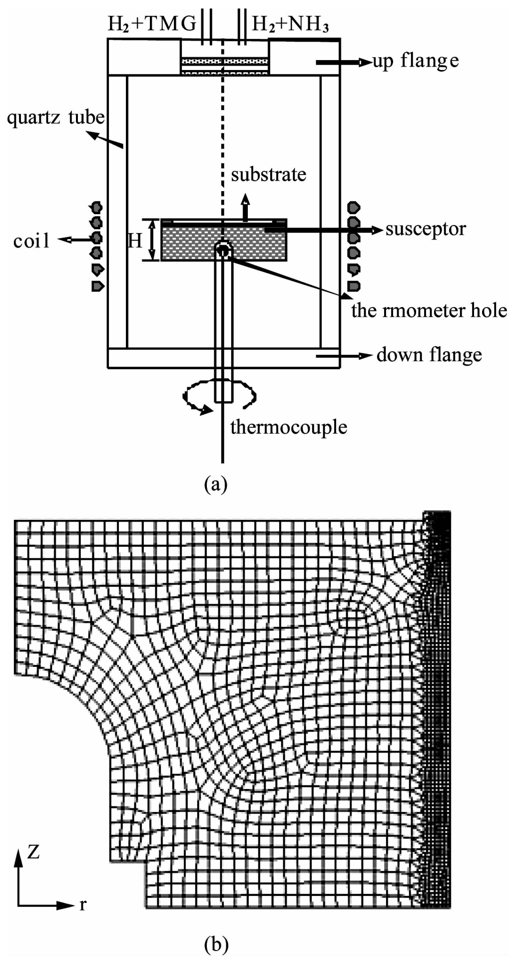

Fig. 1. Axially symmetrical model of (a) induction heat system and (b) FEM mesh of the half susceptor.

also taken into account[9]. The sequential coupling method is performed. After the electromagnetic field has been analyzed, the heat generation rate by induction is used as the thermal source loading. The detailed modeling process is referred to in Ref. [10]. A default value of 10^{-6} for convergence on heat flow is used. The simulation is run on a Pentium IV PC and each run takes 30 to 40 min to reach convergence. Thus, the temperature distributions in the system are finally obtained.

3. Results and discussion

The temperature characteristic of the MOCVD reactor is investigated based on the above model in the following.

3.1. Effect of the relative position between the coils and the middle section of the susceptor on the temperature distributions

In this case, the radius of the coil R= 54.5 mm and the height of the susceptor H= 25.4 mm both remain constant. With different coil turns under the middle section of the susceptor (denoted as n, $6-n$ is the coil turns over the middle section of the susceptor), Figure 2 shows the temperature distributions of the susceptor and substrate, when the system of the reactor reaches a heat equilibrium state. It can be seen that

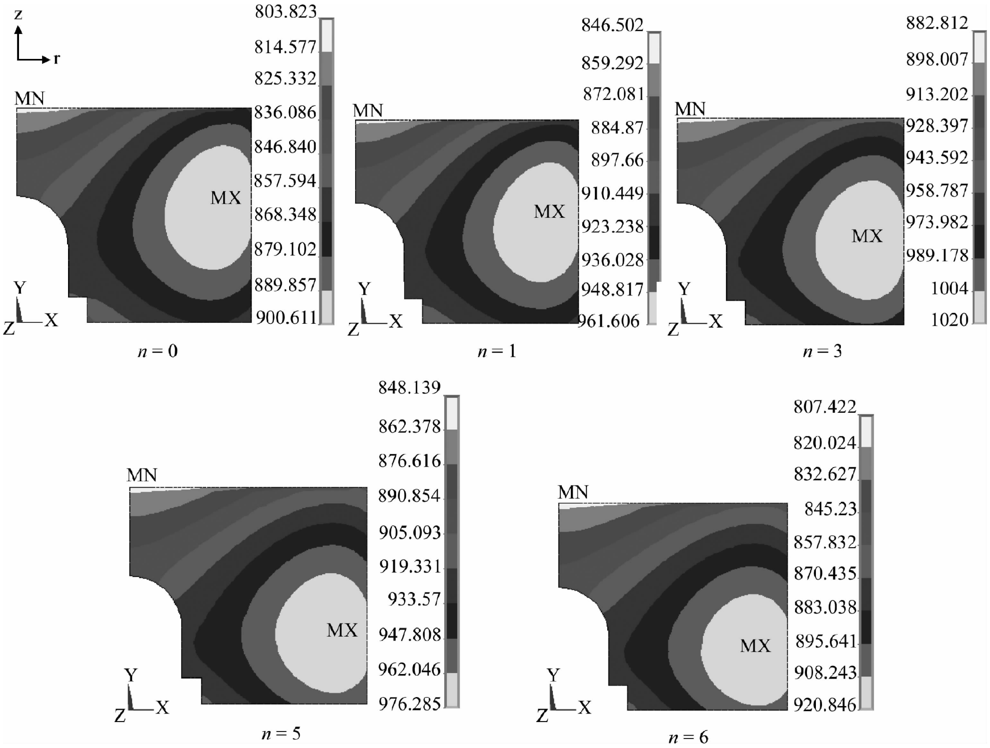

Fig. 2. Coil turns (n) under middle section of susceptor and temperature distributions of susceptor.

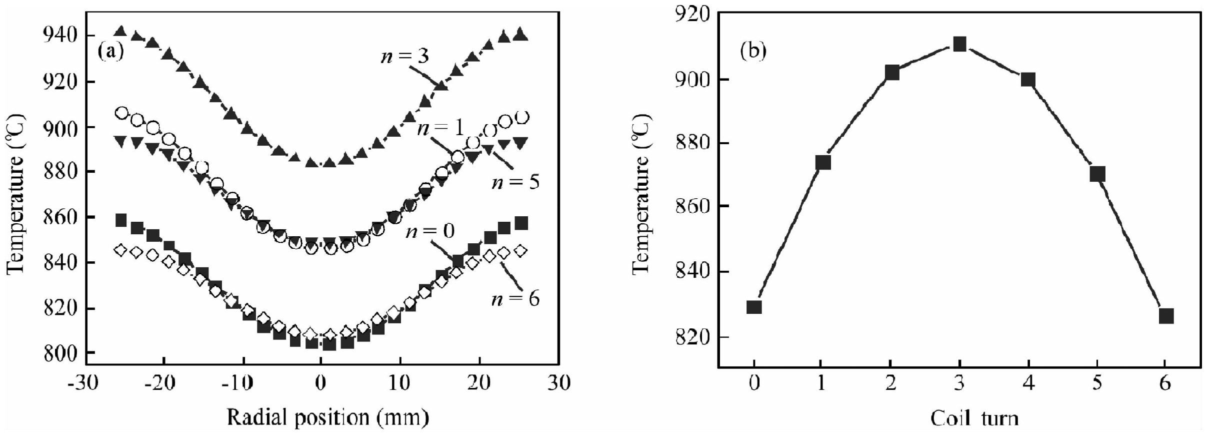

Fig. 3. (a) Temperature distributions of substrate under different turns of the coil in the middle section of the susceptor; (b) Average temperature of different n.

the maximum temperature distribution area moves gradually towards the lower surface of the susceptor with increasing n. Furthermore, the temperature in the susceptor increases at first then decreases with n, and it is highest when $n = 3$.

The radial temperature distributions of the substrate are shown in Fig. 3(a) with different n. Figure 3(b) shows the average temperature of different n. It is observed that the temperature of the substrate increases at first then decreases with increasing n. The temperature of the substrate increases with n when $n < 3$, and its increasing rate decreases gradually, and conversely, it decreases with n when $n > 3$. When $n = 3$, that is to say, when the coil distributes symmetrically about the middle section of the susceptor, the temperature of the substrate reaches its maximum. In addition, it can be seen from Fig. 3(b) that the average temperatures of the substrate are approximately symmetrically distributed. Namely, the average temperature of the substrate when $n = 0$ is approximately equal to that of the substrate when $n = 6$, and the average temperature when $n = 1$ equals that when $n = 5$. Furthermore, their differences are less than 4 °C. This is because the thermometer hole lies under the susceptor, which means that the susceptor figure is not on the symmetry of the middle section of the susceptor. Thus, with the same number of coil turns on or under the middle section of the susceptor, the area on the middle section of the susceptor heated by induction is larger, which makes the temperature of the substrate higher in this case. Whether or not the coils distribute symmetrically with respect to the middle section of the susceptor has a great effect on the temperature of the susceptor and substrate. When the coils distribute symm- etrically about the middle section of the susceptor, namely,when $n = 3$, the average temperature of the substrate is 81.7 °C higher than that when $n = 0$, and 36.6

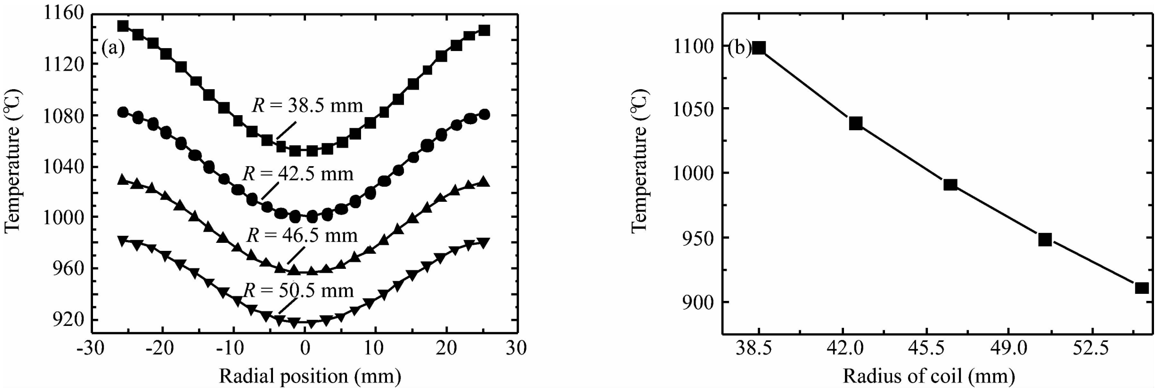

Fig. 4. (a) Temperature distributions of substrate and (b) average temperature under different coil radii.

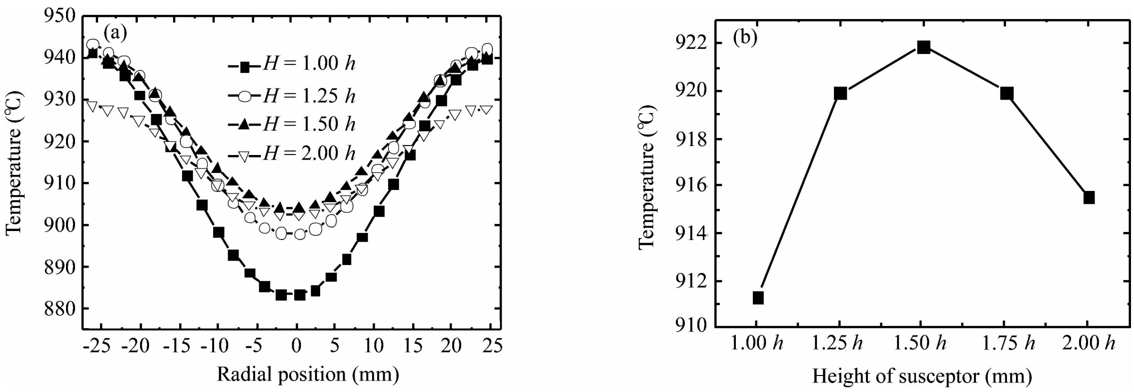

Fig. 5. (a) Temperature distributions of substrate and (b) average temperature under different heights of susceptor.

°C higher than that when $n = 2$. So the coils are to be placed symmetrically about the middle section of the susceptor in practice, which will improve the heat rate.

3.2. Effect of the radius of the coil on the temperature distributions

Under the conditions that the height (H) of the susceptor remains constant at $H = 25.4$ mm, and the coils distribute symmetrically in the middle section of the susceptor, the temperature distributions of the substrate are shown in Fig. 4(a) when the radii of the coils R are 38.5, 42.5, 46.5 and 50.5 mm, respectively. The relationship between the different coil radii and the average temperature of the susceptor is shown in Fig. 4(b). It can be observed that the temperature of the substrate is proportional to the radius of the coils. The average temperature of the substrate decreases as the radius of the coils increases, and its decrease tends to be slow.

3.3. Effect of the height of the susceptor on the temperature distributions

In this case, the radius (R) of the coils remains constant: $R = 54.5$ mm, and the coils distribute symmetrically about the middle section of the susceptor. Figure 5(a) shows the temperature distribution curves of the substrate with different H (1.00h, 1.25h, 1.50h, 2.00h, $h = 25.4$ mm). Figure 5(b) shows the relationship between different heights and the average temperature of the substrate. It can be seen the temperature of the substrate increases at first then decreases with increasing susceptor height. It is highest when $H = 1.5$ h, and the heating efficiency achieves its highest value. The ratio of the height of the susceptor to that of the coils is 3/4. So when the turns and the height of the coils remain constant, the heating efficiency of the susceptor is related to the ratio of the height of the susceptor to that of the coils. When the ratio is approximately 3/4, the heating efficiency reaches its maximum. Thus, the two aspects are to be taken into account when designing the susceptor and the coils. In addition, improvement in the susceptor will cause improvement in the uniformity of the temperature distributions of the substrate, as shown in Fig. 5(a).

4. Conclusion

Using the finite element analysis method (FEM), the effect of the relative position between the coils and the middle section of the susceptor, the radius of the coil, and the height of the susceptor on heating condition has been analyzed. The results show that the temperature of the susceptor and substrate increases at first and then decreases on increasing the coil turns in the middle section of the susceptor, and the heating efficiency reaches its maximum when coils distribute symmetrically in the middle section of the susceptor. The temperature of the susceptor and the substrate is inversely proportional to the radius of the coils; thus, decreasing the radius of the coils appropriately can improve the heating efficiency. The heat rate is related to the ratio of the height of the susceptor to that of the coils, and it reaches its maximum when the ratio is about 3/4. On the other hand, a certain improvement of the temperature distribution uniformity of the substrate can also be obtained.

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