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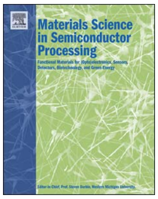

Transport phenomena in a slim vertical atmospheric pressure chemical vapor deposition reactor utilizing natural convection

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ABSTRACT

The gas flow, heat and species transport in a slim vertical silicon chemical vapor deposition reactor for Minimal Fab were evaluated by a numerical analysis. The influences of the inlet gas flow condition on the gas flow direction and the gas phase temperature in the reactor were studied. When the gas flow rate was minimized, natural convection transports the precursor of trichlorosilane gas to the wafer surface. Because the wafer rotation, even very slow at 4 rpm, adjusted the gas flow to shrink the hot region height above the wafer, the gas phase reaction was moderated for preparing the specular surface of the epitaxial film.

1. Introduction

The widely accepted trend for future semiconductor manufacturing is to increase the wafer diameter by shrinking the design rule [1,2]. The large diameter wafer, such as the 450-mm-diameter wafer, will effectively produce a huge amount of low cost electronic devices. However, the initial investment for preparing the equipment will be significantly higher than those for the ordinary diameter wafers. Additionally, because most of the current electronic devices are customized for many types of applications, each production amount becomes rather small. Currently, mass production is often not necessary; the production amount of the electronic devices is flexible, from several to higher than several million chips.

For meeting such situations, the future electronic device manufacturing system should be very flexible and cost effective, while achieving the reasonable consumption of materials and energy. The new practical choice is Minimal Fab [3,4], which employs a quick process using a half inch (12.5 mm) diameter wafer and small instruments. The Minimal Fab is expected to expand the capability and the flexibility of device production, by adding the small diameter wafer to the existed large diameter wafers.

For achieving the Minimal Fab, the silicon chemical vapor deposition (CVD) reactor has been developed [5,6] using the trichlorosilane-hydrogen system, by designing the thermal balance, the film formation process and the reactor cleaning process. For further development, the transport phenomena for the silicon film deposition in the Minimal CVD reactor should be studied and understood for very different conditions. The Minimal Fab, accepting the concept of minimum materials and energy consumption, prefers to the CVD conditions pursuing significantly low gas flow rate.

In this study, the transport phenomena in the Minimal CVD reactor were studied using numerical calculations for the heat, gas flow and chemical reaction. Particularly, the influences of the inlet gas velocity on the gas flow direction and the gas phase temperature were evaluated. Additionally, the role and effect of wafer rotation for arranging the gas flow was evaluated, when the natural convection [7–11] was chosen for the atmospheric pressure CVD condition.

2. Numerical calculation

Fig. 1 shows the geometry of the Minimal CVD reactor. This reactor consists of a half-inch silicon wafer (12.5-mm diameter and 0.25-mm thick), a transparent quartz tube, a wafer holder made of quartz, gas inlets, three halogen lamps, and three reflectors. The inner diameter of the quartz tube is 24 mm. The wafer holder diameter is 19 mm. The gas inlet is divided into two zones, such as the inner inlet and the outer inlet. Two inlets can finely adjust the gas velocity and the gas concentration individually for the inside and the outside region of the substrate, similar to the ordinary reactor. [12] The inner inlet diameter is 7 mm. The distance between the wafer and the low end of the inner inlet is 56 mm. The infrared light emitted from the halogen lamps is concentrated on the wafer surface for heating it. The wall of the quartz

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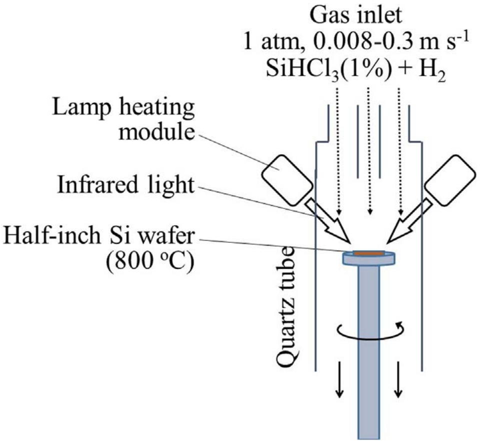

Fig. 1. Chemical vapor deposition reactor for Minimal Fab.

tube is cooled by flowing air, part of which is supplied by an air pump [6]. Because the quartz wall near the wafer is heated by the hot wafer and the body of the three reflectors, which are directly heated by the halogen lamps set inside the reflector [6], the quartz wall between the reflector body and the wafer is assumed to have a temperature near 500 °C.

The precursor gas and the carrier gas, trichlorosilane and hydrogen, respectively, are introduced from the gas inlet at the top of the reactor at atmospheric pressure. Trichlorosilane is the popular and important precursor for the silicon epitaxial growth, as well as dichlorosilane and monosilane. They undergo a chemical reaction at the silicon wafer surface to produce the silicon epitaxial film. Particularly, the trichlorosilane is preferred for obtaining a high film growth rate by the atmospheric pressure chemical vapor deposition. The overall reaction and the rate equation following the Eley-Rideal model [13] are as follows:

$$SiHCl_3 + H_2 \rightarrow Si + 3HCl\cdot \tag{1}$$

$$R_{Si} = \frac{k_{ad} k_r [SiHCl_3][H_2]}{k_{ad} [SiHCl_3] + k_r [H_2]}. \tag{2}$$

R_{Si} is the silicon epitaxial growth rate, and $[i]$ is the concentration of species i at the wafer surface. k_{ad} and k_r are the rate constants of the trichlorosilane chemisorption and the silicon production, respectively

For evaluating the gas flow, heat and gas species transport in the reactor, the governing equations of mass, momentum, enthalpy and chemical species following the ideal gas law are numerically evaluated using the software Fluent 15 (Ansys Inc., USA). The wafer temperature is 800 °C. The wafer is rotated at 0 and 4 rpm. The trichlorosilane concentration at the inlet is 1%. The gas velocity at the inlet is 0.008–0.3 m s^{-1}, which was set as the boundary conditions for the calculation. For the experiment, the gas flow rate was adjusted using the mass flow controller. For the atmospheric pressure condition, the gas velocity of 0.008 m s^{-1} corresponded to the gas flow rate per unit area of 160 sccm/cm^2, which was comparable to or larger than that of 30–320 sccm/cm^2 for the epitaxial reactors using various diameter wafers at various pressures. The gas flow rate per unit area will be able to be reduced following the concept using the natural convection, which have a potential to significantly reduce the gas flow by means of the naturally formed gas recirculation. Natural convection is applicable to the atmospheric pressure chemical vapor deposition reactors, although this concept cannot be applied to the reduced pressure reactor [14–17], in which the gravity does not cause natural convection.

Because most of the gas approaches the wafer surface to cause the chemical reaction following the gas direction prepared by the horizontally-placed wafer occupying most of the reactor horizontal cross section in the vertical process tube, the precursor could be effectively consumed. Thus, the total gas consumption could be reduced. The energy consumption simultaneously decreased by the decreasing gas flow rate [5]. The heat transport by the gas flow from the hot wafer is reduced by reducing the gas flow rate, while that by the radiation is maintained. Thus, the natural convection is expected to have a potential to realize a significantly effective reactor.

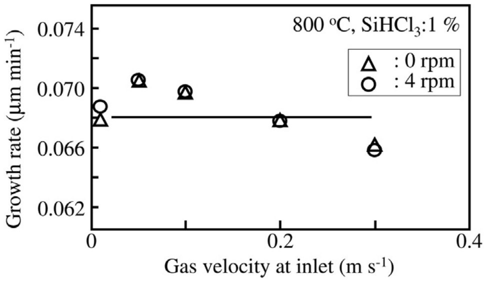

Fig. 2. Epitaxial growth rate, calculated at the wafer rotation rates of 0 rpm (triangle) and 4 rpm (circle) in this study.

3. Results and discussion

3.1. Epitaxial growth rate

Fig. 2 shows the silicon epitaxial growth rate calculated for the trichlorosilane gas concentration of 1%. The epitaxial growth rate is about 0.068 μm min^{-1}. The growth rate stays in the very narrow range between 0.066 and 0.07 μm min^{-1}, while the gas velocity at the inlet significantly changes from 0.008 to 0.3 m s^{-1}. The growth rate at the low temperatures, such as 800 °C, is very often in the reaction limited regime [6]; the rate equation is simplified to the following form depending only on the hydrogen concentration.

$$R_{Si} \cong k_r [H_2]. \tag{3}$$

Because the hydrogen concentration at the wafer surface is typically higher than 95%, the epitaxial growth rate is nearly constant like that shown in Fig. 2.

When the reaction limited regime is produced by the significantly fast wafer rotation [12], the epitaxial growth rate depends on the wafer rotation rate. However, as shown in Fig. 2, the epitaxial growth rates at 0 and 4 rpm are similar. Thus, the slow wafer rotation, 0 – 4 rpm, in this study has a quite small influence on the epitaxial growth rate.

3.2. Gas flow and heat

The gas flow direction and the gas phase temperature in the entire reactor were evaluated. Fig. 3(a), (b) and (c) show the gas velocity vectors at the inlet gas velocities of 0.008, 0.05 and 0.3 m s^{-1}, respectively. Similarly, Fig. 4(a), (b) and (c) show the gas phase temperatures at the inlet gas velocities of 0.008, 0.05 and 0.3 m s^{-1}, respectively.

As shown in Fig. 3(c), the gases introduced from the inlet at the top position quickly flow downward and immediately reach the wafer surface. The gas flow vectors in the center region show that the major stream goes straight to the wafer surface. In the entire reactor, no upward gas motion is observed.

Because such a one-way gas stream can cool the entire reactor, most of the gas phase temperature remains near room temperature, as shown in Fig. 4(c). The cold gases reach the wafer surface; they are very quickly heated to 800 °C that causes the epitaxial growth. In this figure, the gas phase temperature near the bottom of the quartz wall becomes slightly high, because the quartz wall is assumed to be heated by the hot wafer and the hot reflector body.

Figs. 3(b) and 4(b) show the gas flow vectors and the gas phase temperatures at the inlet gas velocity of 0.05 m s^{-1}. The gases introduced from the inlet flow downward. Around mid-height, the natural