

FORMATION MECHANISM OF LOCAL THICKNESS PROFILE OF SILICON EPITAXIAL FILM

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1. Introduction

The local thickness profile of a silicon epitaxial film [1] formed using the horizontal single-wafer epitaxial reactor in a trichlorosilane-hydrogen system at atmospheric pressure is evaluated using numerical calculations based on the transport and epitaxy model [2], taking into account the details of the entire gas inlet geometry.

2. Theoretical model

Figure 1 shows the geometry of the horizontal cold wall single-wafer reactor evaluated in this study for silicon epitaxial film growth having a 200-mm-diameter silicon substrate (1400K) which is held horizontally and rotates at 20 rpm and the multi-inlet with three sections, left (L), center (C) and right (R). A gas mixture of trichlorosilane and hydrogen is used for the silicon epitaxial growth at atmospheric pressure.

The transport and epitaxy model [2] used in this study consists of theoretical equations for the transport phenomena and the surface reactions to form the silicon epitaxial film. In order to evaluate the film growth rate in the reactor, the mass, momentum, energy and chemical species transport equations are solved and linked with the surface chemical reactions, taking into account the ideal gas law, using the CFD software package, Fluent version 5.5 (Fluent, Inc.).

The key processes for the silicon epitaxial film growth are represented by the chemisorption of trichlorosilane to form the intermediate species at the substrate surface and its decomposition by hydrogen gas. The mole growth rate of silicon epitaxial film, V , is described as follows:

$$V = k_{ad} k_r [\text{SiHCl}_3] [\text{H}_2] / (k_{ad} [\text{SiHCl}_3] + k_r [\text{H}_2]),$$

$[i]$ is the mole concentration of species i at the silicon substrate surface, k_{ad} is the chemisorption rate constant, and k_r is the decomposition rate constant.

3. Results and discussion

The calculated silicon epitaxial film thickness profiles are shown in Fig. 2. The calculated silicon epitaxial film thickness profile has three valleys, which agrees with the empirically known characteristics [1] for the industrially used horizontal cold wall single-wafer epitaxial reactor having the multi-inlet, consisting of three inlet plates, a stair and three adjustable inlet sections.

The mechanism to form the characteristic local distribution of the epitaxial film thickness is considered to be the following four steps:

- (1) The plate of the multi-inlet generates the region with a small gas velocity around itself.
- (2) In this slow stream region, the gases are rapidly heated by the hot substrate and susceptor.
- (3) The increased gas temperature induces the gas volume expansion to decrease the trichlorosilane gas

concentration, and the increase in the diffusivity of trichlorosilane gas.

- (4) Because the growth rate increase by the increase in the diffusivity cannot compensate the growth rate decrease due to the decrease in the trichlorosilane gas concentration, the transport rate of trichlorosilane gas to the silicon substrate surface locally decreases with increasing the gas phase temperature in the cold wall reactor.

4. Conclusion

The thickness profile of the silicon epitaxial film formed using the horizontal cold wall single-wafer epitaxial reactor in a trichlorosilane-hydrogen system at atmospheric pressure is evaluated using numerical calculations taking into account the details of the gas inlet geometry. The characteristic thickness profile can be formed by the non-uniform distribution of the gas flow velocity and the gas temperature above the silicon substrate due to the gas inlet.

Acknowledgment

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References

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- 2) H. Habuka et al., *J. Crystal Growth*, **169**, 61 (1996).

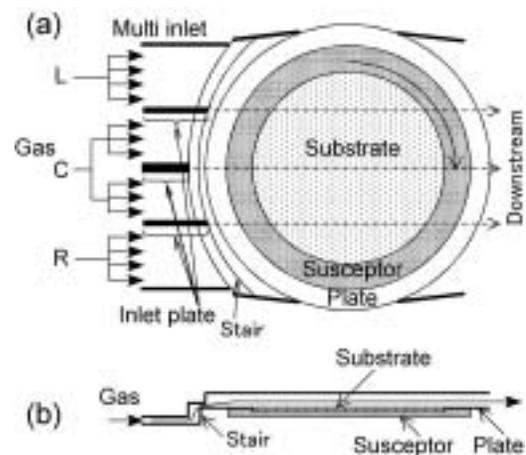


Fig. 1 Horizontal single-wafer reactor. Broken lines with arrows indicate the position of the downstream region corresponding to the inlet plate.

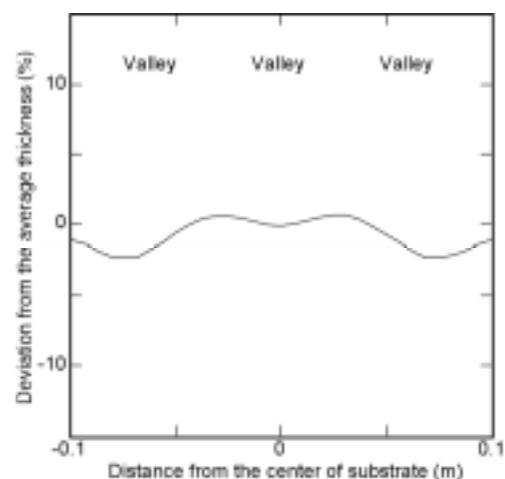


Fig. 2 Calculated silicon epitaxial film thickness profiles using the deviation from the average epitaxial film thickness.