PREDICTIVE MODEL EXTRACTION FROM COMMERCIAL SCALE POLY-SILICON LPCVD REACTOR

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In this work we investigated the poly-silicon CVD using commercial scale LPCVD reactor. The deposition rate profiles in the axial direction of the reactor and within the 6inch silicon wafer were experimentally and theoretically examined. The comparison of actual growth behavior with the elementary reaction analysis revealed the chemical species that control the CVD uniformity. Thus we could extract the predictive model of silane-based poly-silicon CVD system for the first time in a manufacturing scale reactor.

We used longitudinal type CVD reactor of 6inch manufacturing scale. Sample wafers were charged with a spacing of 4.1mm in horizontal manner and the 100% silane and 0.8% phosphine gases with nitrogen carrier gas were introduced from the bottom of the reactor. The result on a monitor wafer is shown in figure 1 on the condition of 550℃, 100Pa and wafer spacing 4.1mm as a relative thickness distribution along an axis compared with the thickness at the wafer center.

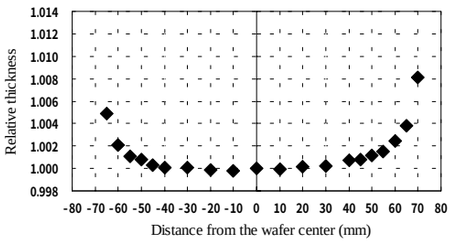

Fig.1 Relative thickness profile of poly-silicon film

To analyze the experimental result, we derived the basic equation of the CVD system from the mass balance relation, which can be described as follows,

$$\frac{d^2C}{dr^2}+\frac{1}{r}\cdot\frac{dC}{dr}-\left(\frac{\phi}{R}\right)^2 C=0,\phi=R\sqrt{\frac{2k_s}{wD}}=R\sqrt{\frac{v_a}{2wD}}\sqrt{\eta} \quad [1]$$

where $C(r)$ is a reactive gas concentration at a distance r from the wafer center, R is the radius of wafer and ϕ is a constant in relation with the sticking probability η of the gas species with a thermal velocity v_a and diffusion constant D. By use of this solution the thickness of poly-silicon thin film is expressed as follows,

$$t(r)\propto\eta_0 C_0+\sum_i \beta_i\eta_i C_i \quad [2]$$

where subscript *0* stands for silane and *i* for precursors.

In equation [2], we optimized β and η to fit calculated curve with the measured thickness data as shown in figure 2. The fitting of calculated curve with the measured data is excellent. From this simulation, three kinds of gas species with different sticking probabilities were found to contribute the poly-silicon deposition. They are silane with the sticking probability 1×10^{-6}, and two kinds of radical species with 5×10^{-2} and 7×10^{-4}, respectively. The wafer-edge concentration of two kinds of precursors are 4×10^{-7} and 3×10^{-6} relative to the concentration of silane gas, respectively.

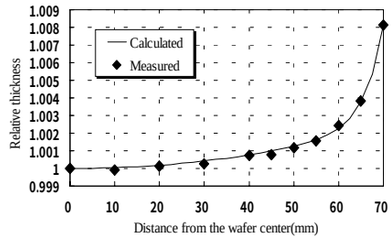

Fig.2 Simulation analysis of experimental profile

Thickness profiles on other 5 monitor wafers were analyzed similarly and wafer-edge concentrations at all positions were derived, which are summarized in figure 3.

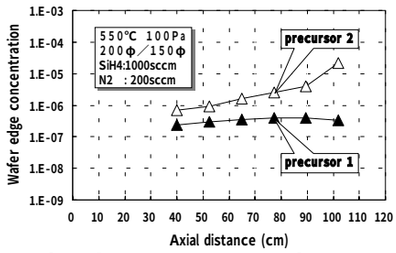

Fig.3 Wafer-edge concentrations of precursors 1 and 2

Figure 4 compares the elementary reaction analysis (1) results executed using OvenD in CHEMKIN 3.7 with the wafer-edge concentrations derived from the fitting of calculated curves indicated as precursor 1 and 2.

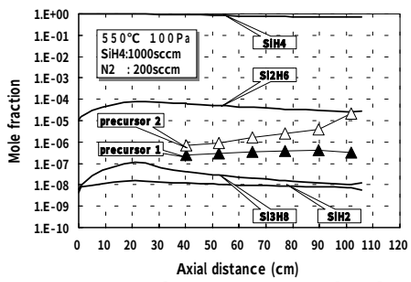

Fig.4 Comparison of main precursors by elementary reaction analysis with the wafer-edge concentrations

From this figure precursor 1 with a large sticking probability 5×10^{-2} is most probable to be SiH_2, because the sticking probability of Si_3H_8 is about 3 orders below the one of precursor 1. Precursor 2 with a moderate sticking probability 7×10^{-4} is considered to be Si_2H_6.

According to the above analyses, poly-silicon deposition mechanism can be explicated to be as follows in commercial scale of CVD reactor for the first time. The basis deposition of poly-silicon film is due to the surface reaction of the material gas silane, and the profile is almost flat because of its extremely low sticking probability, 1×10^{-6}. While the generation rate of precursors from the material gas silane are very low, the extraordinary deposition around the peripheral region of wafers is explained by the large sticking probabilities, such as 5×10^{-2} for SiH_2 and 7×10^{-4} for Si_2H_6.

To validate the reaction kinetics of silane, the temperature dependence of sticking probability and the gas-phase decomposition rate of silane were investigated with the temperature and wafer-spacing dependences of the deposition rate at the wafer center, respectively.

1. P. Ho et al., J. Phys. Chem. **98**, 10138 (1994)