DEPOSITION PROFILE SIMULATION USING THE MONTE CARLO METHOD
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1 INTRODUCTION

Process simulators such as SAMPLE1), SUPREM2), etc. for semiconductor manufacturing have much contributed to develop new VLSI devices. Now more accurate simulator for deposition profile is becoming increasingly important with the ULSI technology because of much smaller dimension of trench and hole on the substrate.3)

Gas flow around a trench or a hole of 1μm in width must be analyzed as a rarefied gas flow using the Boltzmann equation because Knudsen number Kn (=λ/B) is larger than 0.01, where λ is mean free path, and B is characteristic dimension (=1μm).

This paper demonstrates the deposition profile simulations on a small trench in the sputter deposition, plasma CVD, low pressure CVD, and atmospheric pressure CVD using Direct Simulation Monte Carlo method (DSMC) with molecular collision, sticking coefficient and surface reaction probability.

2 OUTLINE OF NUMERICAL METHOD

The DSMC method is one of the numerical methods to solve the Boltzmann equation, in which the positions and the speeds of tens of thousands of molecules are calculated with their flights and molecular collisions4).

The calculation model around the trench of 1 μm in width formed on the substrate is shown in Fig. 1. Reactive molecules come down to the flow field from the upper flow region in the Maxwell velocity distribution. Some reactive molecules reaching the substrate become part of the film according to surface reaction probability Pr (or sticking coefficient Sr) and the others are reflected diffusely with probability (1-Psr)(or (1-Sr)). When surface reaction occurs on the film surface, the reaction product is emitted in the flow field. Molecular collisions are calculated in each cell by their collision probabilities. The algorithm of film growth is called a string model5).

3 RESULTS OF SIMULATION

3.1 Sputter deposition, Plasma CVD, and Low pressure CVD

These processes are accurately simulated with the free molecular flow and the appropriate sticking coefficients. The flows around the trench in
these processes are free molecular because the Knudsen numbers are much larger than 10.

In the case of Al sputter deposition, the sticking coefficient of an Al atom on substrate can be estimated to be close to 1.0 according to the data in surface science \(^5\(^6\)). And the simulation results with sticking coefficient 1.0 show good coincidence with the experimental results\(^3\).

In the case of Plasma CVD for amorphous silicon, J.P.M. Schmitt's experimental results \(P_{sr}\)^7 is close to 0.7. And the simulation result with \(P_{sr}=0.7\) shows good agreement with C.C. Tsai's\(^8\) experimental result\(^3\).

In the case of LPCVD, Watanabe and Komiyama obtained \(P_{sr}=0.2\) in the case of SiO\(_2\) film\(^9\). The results of step-coverage in their experiment and our calculation with \(P_{sr}=0.2\) agree well.

3.2 Atmospheric Pressure CVD

The deposition simulation results on the trench of 1 \(\mu\)m in width and in depth for Knudsen numbers \(Kn=\infty\), 1.0, and 0.1 with the surface reaction probability \(P_{sr}=1.0\) are shown in Fig. 2. The film thickness on the bottom of the trench decreases with the decrease in Knudsen number or with the increase in pressure. This is because the reactive molecules are sometimes rejected from entering the trench by collision with the reaction product in the case of smaller Knudsen numbers\(^10\)^11.

The simulation result with \(P_{sr}=0.1\) is close to the experimental results of PSG (phosphosilicate glass) film by APCVD\(^3\). But the value of \(P_{sr}\) for APCVD is not known and is difficult to measure. And more intensive researches on its measurement are strongly required.

REFERENCES