DEPOSITION PROFILE SIMULATION USING THE MONTE CARLO METHOD

Masato Ikegawa and Junichi Kobayashi

Mechanical Engineering Research Laboratory, Hitachi Ltd.
502, Kandatsu-machi, Tsuchiura-shi, Ibaraki-ken, 300 JAPAN

1 INTRODUCTION

Process simulators such as SAMPLE[1], SUPREM[2], 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 collisions[4].

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 P_{sr} (or sticking coefficient S_f) and the others are reflected diffusely with probability $(1-P_{sr})$(or $(1-S_f)$). 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 model[1].

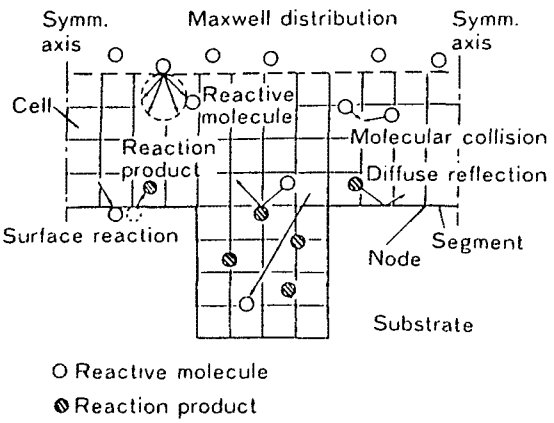

Fig.1 Calculation model[11]

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 μm in width and in depth for Knudsen numbers Kn= ∞, 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.

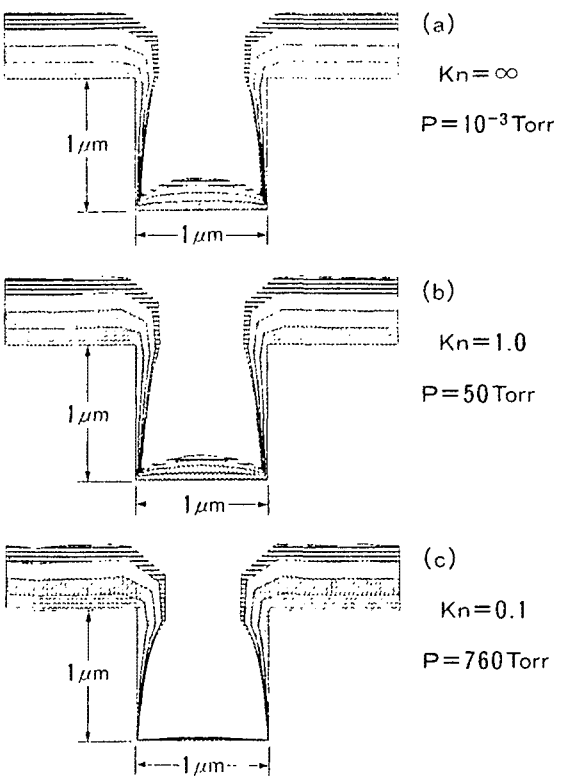

Fig.2 Simulated time evolution of surface contours for CVD -- the effect of the Knudsen number Kn (P_{sr}=1.0)[11)]

REFERENCES

1. Q.R. Neureuther, et al., IEEE Trans. on Electron Devices, Vol.ED-27, No.8, p1449 (1980).
2. D.A. Antoniadis, et al., IEEE Trans. on Electron Devices, Vol.ED-26, No.4, p490 (1979).
3. M. Ikegawa and J. Kobayashi, Proc. of the 7th Symp. on Plasma Processing, Electrochemical Society, p378(1988).
4. G.A. Bird, Molecular Gas Dynamics, Oxford Univ. Press (1976).
5. P.A. Redhead, et al., The Physical Basis of Ultrahigh Vacuum, Chapman and Hall Ltd, London (1968).
6. S.M. Sze, Ed., VLSI Technology, McGrow-Hill International Book Company, p78(1983).
7. J.P. M. Schmitt, J. Non-Cryst. Solids 59/60, p652 (1983).
8. C.C. Tsai, J. Appl. Phys. 59 (8), p2998 (1986).
9. K. Watanabe and H. Komiyama, Proc. of the 21th Autumn Meeting, the Society of Chemical Engineers, Japan, P760(1988), (in Japanese).
10. M. Ikegawa and J. Kobayashi, ibid, P759(1988), (in Japanese).
11. M. Ikegawa and J. Kobayashi, Proc. of the International Aerospace Symposium, Nagoya, Japan, edited by T. Fujiwara, (1989)(in press).