Deposition Efficiency Modeling according to Precursor Flow Rate in ALD Process with Fixed Chamber Pressure

Dong-Ho Shin[1], Seung-Jae Kim[1], Eun-Kyung Hong[1], Oh-Hyuk Kwon[1], Eung-Su Kim[1] and Kyu-Hee Han[1]

Deposition Equipment R&D Team, Mechatronics Research, Samsung Electronics,

Gyeonggi-do, South Korea 18848

1 Modeling

1.1 Supply Model

Since diffusion is the main mechanism of precursor behavior in pattern, the density of precursor on wafer or the exposure time must be increased to achieve good step coverage. The formula for achieving perfect coverage is shown in Eq. (1).[1]

$$P_{precursor}t = S(2\pi mkT)^{\frac{1}{2}}\left(1+\frac{19}{4}a+\frac{3}{2}a^2\right) \tag{1}$$

where $P_{precursor}$[Pa] is the precursor partial pressure, t[s] is the exposure time, S[molecules/m^2] is the saturation coverage of the molecule, m[kg] is the mass of one precursor molecule, k is the Boltzmann constant, T[K] is temperature, and a is the aspect ratio.

In the ALD system, gases such as argon, hydrogen, and nitrogen flow with precursor for the purpose of purging or dilution. Assuming that the gas flowing with precursor is argon, $P_{precursor}$ in Eq. (1) is given by Eq. (2) below.

$$P_{precursor} = \frac{Q_{precursor}}{Q_{precursor}+Q_{Ar}}\,P_{chamber} \tag{2}$$

where $Q_{precursor}$, Q_{Ar} and $P_{chamber}$ represent the flow rate of precursor, the flow rate of argon gas and the pressure of chamber, respectively. Deposition Efficiency (DE) is defined as the ratio of the thickness of deposited film to the volume of the precursor consumed. For discussing DE, the total required amount of the precursor to achieve 100% step coverage (D_{total}) can be defined as Eq. (3).

$$D_{total} = Q_{precursor}t \tag{3}$$

Considering Eqs. (1), (2) and (3), D_{total} is expressed as Eq. (4) as follows:

$$D_{total} = \frac{Q_{precursor}+Q_{Ar}}{P_{chamber}}S(2\pi mkT)^{\frac{1}{2}}\left(1+\frac{19}{4}a+\frac{3}{2}a^2\right) \tag{4}$$

Assuming an ideal fixed pressure control system, the $P_{chamber}$ can be considered constant. $S(2\pi mkT)^{\frac{1}{2}}\left(1+\frac{19}{4}a+\frac{3}{2}a^2\right)$ is also a constant value determined by the given conditions. Therefore, according to Eq. (4), if the $Q_{precursor}$ is reduced, the total amount of precursor required to deposit the same thickness while achieving 100% step coverage is reduced.

A decrease in D_{total} means an increase in the DE of the precursor. The phenomenon of increasing DE of precursor by decreasing $Q_{precursor}$ can be explained in the graph shown in Fig. 1 drawn by Eq. (2). As $Q_{precursor}$ increases, $\triangle P_{precursor}/\triangle Q_{precursor}$ gradually decreases. That is, even if $Q_{precursor}$ is increased, the $P_{precursor}$ transmitted to the wafer surface hardly increases and gradually converges to the $P_{chamber}$. This is because the ratio of precursor discarded to the pump increases in proportion to $Q_{precursor}$ due to fixed pressure control characteristic. In order to enhance DE of the precursor, the precursor must be supplied from the efficient supply region. The decrease of the flow rate results in the higher DE of the precursor.

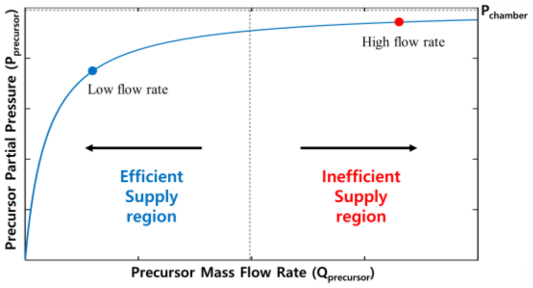

Fig. 1. Precursor partial pressure according to precursor flow rate.

1.2 Simulation

CFD simulation is performed to check how the wafer surface concentration behaves by precursor flow rate. The model in Eq. (4) is verified with conditions in case 1, case 2 and case 3 in Table 1. In order to maintain total usage of precursor, dose time is increased under the condition of lowering the flow rate.

As a result, it is confirmed that the lower the flow rate, the higher the total amount of reaching the wafer surface during dose time as shown in Table 1.

Table 1. Simulation & evaluation conditions and integral value of gas density on wafer during dose time.

Case	Flow rate	Dose time	Total supply	Integral value of gas density on wafer surface [kg*s/m^3]
1	1	1	same	0.0192
2	0.25	4		0.0525
3	0.125	8		0.0887

1.3 Model Verification in Pattern

To verify the model, evaluation is conducted in pattern under the conditions in Table. 1.

As shown in Fig. 2, the DE on the pattern increases as the flow rate is decreased, even though the total amount of precursor supplied is same in 3 cases. That is, as flow rate decreases, the precursor is well transferred to the wafer surface, so it can be seen that the DE inside pattern increases.

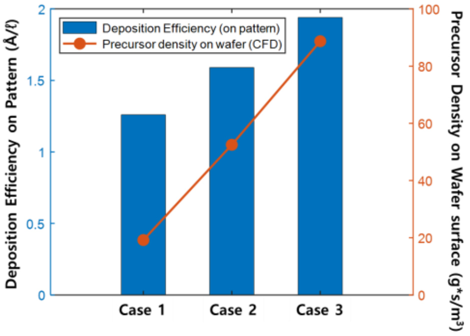

Fig. 2. Comparison of simulation & evaluation results in Table 1 conditions.

References

[1] Roy G. Gordon, and Dennis Hausmann. A kinetic model for step coverage by atomic layer deposition in narrow holes or trenches. *Chem. Vap. Deposition*. 9, No.2 **(2003)**