Single Wafer Atomic Layer Deposition Reactor Design

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Abstract: Atomic layer deposition (ALD) is a very attractive ultra-thin film deposition technique. With the feature size of IC industry continues going down, ALD has received more and more attentions for its accurate sub-nanometer thickness control as well as superior uniformity and conformality. The further development of ALD technology emphasizes on both process and equipment innovations. A single-wafer bottom-heated reactor is constructed successfully, and the Al_2O_3 is deposited with ~2% uniformity across a 4-inch wafer. Furthermore, the gas delivery system and heating devices are studied by the combination of ANSYS simulation and experiments. These parameters that influence the uniformity and conformality of deposited films have been further optimized to obtain better performance. As a result, a new reactor with showerhead gas delivery and radiation heating system is designed.
Key words: ALD, Reactor design, Gas delivery, Heating system, FEM, ANSYS simulation

1. Introduction

The concept of atomic layer deposition (ALD) was proposed by Dr. Suntola in the 1970s[1]. It was applied in thin film electroluminescence (TFEL)[2] flat displays and photonics[3] in the early time. Since 1990s, with the need of smaller semiconductor devices[4] and the development of integrated circuits[5], ALD has received more and more attentions for its accurate sub-nanometer thickness control as well as superior uniformity and conformal coating. As a consequence, this technique has been applied in relevant industries [6, 7].

ALD is a thin film deposition technique where the pulsed precursors are introduced alternately into a reactor and react with the substrate to form a monolayer[8]. Between the two precursor pulses, the inert gas is applied to purge the reactor[9]. A typical ALD full cycle consists four steps[10] : 1) The precursor A gets into the reactor and adsorbed (both physically and chemically) on the substrate; 2) The inert gas purges the surplus precursor A and by-products out of the reactor; 3) The precursor B is introduced into the reactor and reacts with ligands of precursor A on the substrate, and a monolayer of film is formed; 4) The inert gas purges surplus precursor B and by-products out of the reactor, and the surface gets ready for next cycle. With the control of ALD cycles, we can obtain layer-by-layer film growth. As a consequence, ALD has advantages in uniformity and conformality[10] compared with other thin film techniques, such as physical vapor deposition (PVD) or chemical vapor deposition (CVD).

One important parameter for ALD deposition is the process temperature. The optimal temperature range (T_1~T_2) is called ALD window[11]. Below the temperature T_1, it may encounter condensation, activated adsorption or reaction. While above T_2, it tends to have thermal decomposition or thermal desorption. Therefore, it is vital to design a proper heating system to maintain the substrate's temperature in the ALD window.

Additionally, it is essential to design the optimal ways of gas delivery of precursors which influences the pressure distribution and thus affects the uniformity and conformality of films.

2. The 1st Reactor Design

A bottom-heated single wafer ALD reactor is successfully constructed, the finite element method (FEM) simulation and deposition experiment results will be discussed in this chapter.

2.1 reactor structure

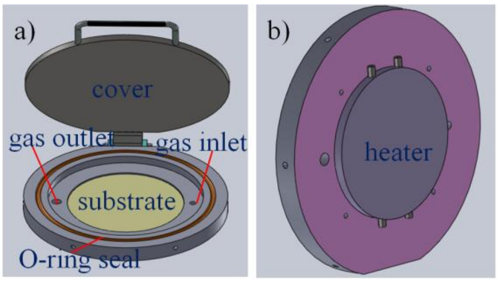

Fig. 1 a) the axonometric graph of chamber; b) the bottom graph of chamber

As shown in Fig. 1a), the reactor has a gas inlet and outlet which is welded to a 1/4 inch tube made of 316L stainless steel[12] and a KF flange respectively. The sample stage is designed to hold a substrate with the maximum diameter of 4 inch. On the bottom of chamber, a heater (as shown in Fig. 1b)) with two heating pipes made of cast iron, is placed to heat the substrate.

2.2 ANSYS simulations

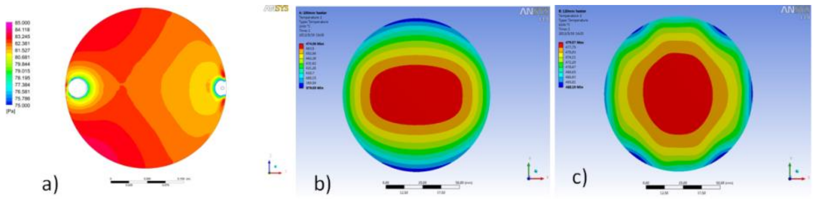

Fig. 2 a) pressure distribution; b) temperature distribution (two heating pipes with the range of 379~474℃); c) temperature distribution (four heating pipes with the range of 463~479℃)

A conjugate heat transfer analysis is conducted by ANSYS CFX. A steady state simulation is proposed with N_2 ideal gas[13]. The pressure and temperature distributions are presented in Fig. 2a) and 2b), respectively. Fig. 2a) shows the pressure distribution of gas inlet and outlet varies significantly, while the pressure distribution of substrate is relatively uniform. The reason is that the gas tends to gather near the line drawn from single inlet to outlet, but the less gas is distributed far from the line. In Fig. 2b), the chamber is heated by a cast iron with two heating pipes where is the area of heat concentration, thus the distribution is non-uniform with temperature decreases from the center to the edge. Yet the temperature is well-distributed if four heating pipes used as Fig. 2c) shows. As a result, the heating system could be optimized to achieve more uniform temperature distribution if several parallel heating pipes are applied, while optimizing the gas delivery system becomes an important problem to solve for the next step.

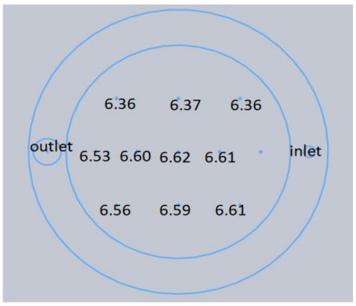

Fig. 3 the thickness of aluminum oxide (6.52±0.11nm)

2.3 growth experiments

Growth experiments are conducted with tri-methyl aluminum (TMA)[14] and water as two precursors to deposit ~5 nm thick aluminum oxide[15] film on Si(100) wafers (*p*-type, 525 μm thickness, resistivity of 1×10^{-3}Ω •cm). Each sample has been performed 50-cycle ALD runs and the growth rate of aluminum oxide is ~1Å /cycle[16]. The thickness map of sample A is shown in Fig. 3 (1.7% uniformity) and all data is shown in Table 1. The result indicates that the film in the line drawn from inlet to outlet is slightly thicker than that far from the line. The experiments are well agreed with the simulation results. Uniformity could be improved with fine process tuning.

Table 1 three samples with the thickness of Al_2O_3 film

	U_1	U_2	U_3	M_1	M_2	M_3	M_4	M_5	D_1	D_2	D_3	Average	Uniformity
A	6.36	6.37	6.36		6.61	6.62	6.60	6.53	6.61	6.59	6.56	6.52±0.11	1.7%
B	6.80	6.84	6.85	6.81	7.30	7.26	6.98	7.09	7.22	7.36	7.20	7.06±0.22	3.1%
C	6.51	6.58	6.68	6.90	6.89	6.97	6.97	7.00	6.86	6.96	7.00	6.85±0.18	2.6%

3. The 2nd Reactor Design

With the inputs from both experiments and simulations, a new reactor with improved gas delivery and heating system will be presented in this chapter. The new reactor has a showerhead structure aiming to improve the uniformity of the pressure distribution, and radiation heating system to achieve better heat distribution.

3.1 reactor structure

Instead of contact heating, the radiation heating system with heating pipes around the reaction chamber is used in this reactor as Fig. 4 shows. The 1st reactor with four heating pipes has comparatively uniform temperature distribution on the substrate. Therefore we believe similar design could be applied for the radiation heating. Additionally, radiation heating is superior for non-flat, bulk, or porous samples.

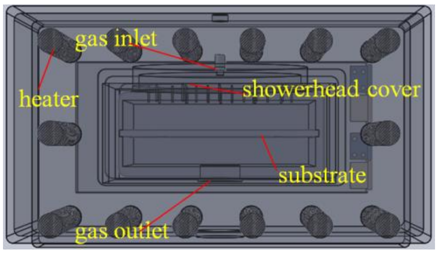

Fig. 4 a series of parallel heating pipes to form radiation heater

On the other hand, the precursors are delivered vertically and the gas inlet that utilized showerhead structure with circular array pinhole distribution (Fig. 5a)) ensures the uniform gas flow distribution on the substrate. Furthermore, the surplus precursors and by-products will be withdrawn from the circular groove near the substrate (Fig. 5b)) to the atmosphere by the system pump.

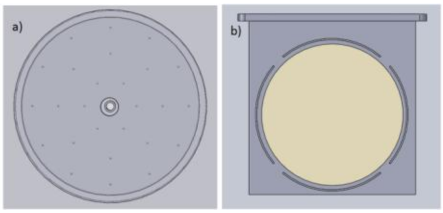

Fig. 5 a) showerhead gas inlet; b) circular groove gas outlet

3.2 ANSYS simulations

The gas flows from the gas inlet to the substrate vertically and the pressure on the substrate is uniformity. However, two distance factors must be considered. One is the distance between the showerhead and the substrate (*h*). With *h* increasing, the pressure is better distributed. Besides that, the volume of reactor should be taken into account. The other distance between the circular groove and the edge of substrate (Δr) presents the same tendency. If Δr is elevated, the pressure is more balanced. Once the value is equal to 20mm, the

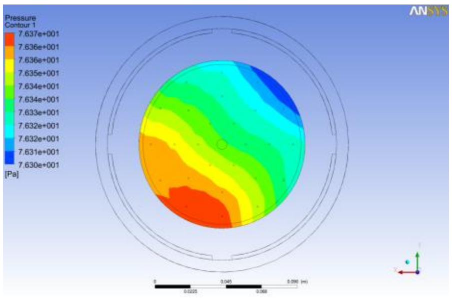

Fig. 6 pressure distribution (h=20mm, Δr=20mm) pressure gets quite uniform. Eventually Δr keeps a constant of 20mm and h varies. Several simulations have been performed and it is concluded that the pressure distribution is considerably uniform when h is equal to 20mm (as Fig. 6 shows). Therefore, the final design is in accordance with these two values.

4. Conclusions

The Al_2O_3 is deposited with ~2% uniformity across a 4-inch single wafer reactor with bottom heating. Subsequently, the ANSYS simulations and experiments for studying this reactor and find the gas delivery and heating system affect the uniformity and conformality of films deposited. Thus a new reactor model that adopted showerhead gas delivery and radiation heating is designed aiming to improve the pressure and temperature distribution. Through the results of simulation, the reactor model shows a reactor with improved performance.

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