Plasma chemistry of $SiH_4/N_2/O_2$ and $SiH_4/N_2O/Ar$ mixtures for deposition of silicon based film in RF-CCPs

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Abstract: Based on a two-dimensional fluid model, we investigate the plasma chemistry of $SiH_4/N_2/O_2$ and $SiH_4/N_2O/Ar$ in a RF CCP reactor. Our research focus is put on gas phase precursors for silicon based thin film deposition. In $SiH_4/N_2/O_2$ plasma, it is found that SiH_3O, SiH_2O,O and NO may be the most important gas phase precursors. In $SiH_4/N_2O/Ar$ plasma, possible gas phase precursors include radicals of SiH_3, SiH_3O, O and SiO. In addition, the effect of dust particles on silane discharge has also been investigated.

Keywords: capacitively coupled plasma; fluid simulation; dusty plasmas

Silicon oxide, silicon nitride, or silicon oxynitride thin films, which have been widely used in semiconductor devices or integrated circuits, are often deposited in radio-frequency (RF) capacitively coupled plasmas (CCPs) sustained in the mixture gases of SiH_4/N_2O, $SiH_4/N_2/NH_3$ and SiH_4/O_2. In general, inert gases, such as Ar or He, are added into these mixture gases to improve the discharge performance. For silicon based thin film deposition, it is generally considered to be difficult to analyze gas chemical precursors, due to hundreds of chemical reactions involved and uncertain chemical reaction coefficients in the mixure gas. In this work, by using a two-dimensional fluid model, we made some efforts on analyzing the plasma chemistry of $SiH_4/N_2/O_2$ and $SiH_4/N_2O/Ar$ discharges in a RF CCP reactor.

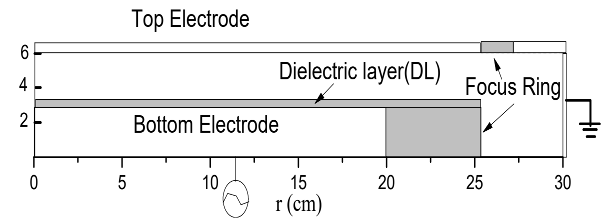

Fig.1. Schematic diagram of the cylindrical CCP reactor taken into consideration in $SiH_4/N_2/O_2$ discharge

We show the CCP reactor considered in the simulation in Fig. 1. The lower electrode, which is about 20 cm in radius and surrounded by a focus ring, is powered by 13.56 MHz RF source. The top electrode is grounded metal and also surrounded by a focus ring. Other surfaces in this chamber are grounded metal. A dielectric layer of 3 mm thick is placed on the lower electrode and the focus ring. The electrode gap is 3 cm. In this CCP reactor, a parameterization study on $SiH_4/N_2/O_2$ plasma will help us identify the likely gas phase deposition precursors.

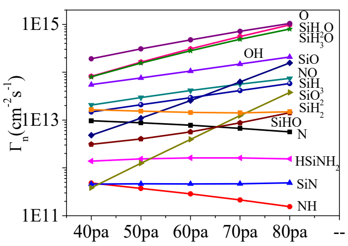

Fig. 2 Fluxes of the neutral particles on the powered electrode as a function of pressure in the mixture gas of $SiH_4/N_2/O_2$. The discharge condition is as follows: 13.56 MHz, 70 V power supply.

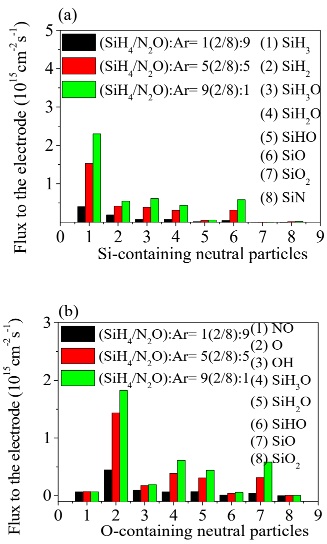

Fig. 3 Fluxes of the neutral particles containing Si (a) and O (b) on the powered electrode with different Ar fraction in the mixture gas of $SiH_4/N_2O/Ar$. The discharge condition is as follow: 13.56 MHz, 70 V power supply and 40 Pa pressure

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From Fig. 2, it is clear that SiH_3O and SiH_2O are the most abundant radicals in the plasma no matter how the pressure changes. And their fluxes increase rapidly with the increasing pressure. Moreover, it is observed that when the pressure increases to 80 Pa, SiO_2 and SiO cannot be ignored. However, the fluxes of SiN and $HSiNH_2$ are much lower than that of SiH_3 and keep almost constant. For O-containing neutral particles, the most abundant radical is O. For N-containing neutral particles, it is obvious that the most important nitrogen-containing particles are N and NO, whose evolution trends are just the opposite as the pressure increases. In sum, the above data suggests that SiH_3O, SiH_2O, O, N and NO may act as the main precursors, rather than SiN and $HSiNH_2$, etc.

In $SiH_4/N_2O/Ar$ plasma, possible gas phase precursors are also discussed. Fig. 3 shows fluxes of the radicals on the powered electrode. For Si-containing neutral particles at the case of low content of Ar in the mixture gas, the flux of SiH_3 is the largest, followed by SiH_3O or SiO. At the case of high content of Ar, the most abundant radicals are SiH_3 and SiH_2. Similarly, for O-containing neutral particles, it is obvious from Fig. 3(b) that O, SiH_3O and SiO are the most particles.

We also discuss the effect of the inert gas Ar in $SiH_4/N_2O/Ar$ on plasma characteristics, such as ion bombardment energy and plasma radial uniformity under different pressure conditions. We find that an increase in Ar fraction in the mixture gas can increase the ion bombardment energy on the electrode, but deteriorate the radial uniformity of the plasma under the pressure of 266 Pa, as can be seen in Fig. 4.

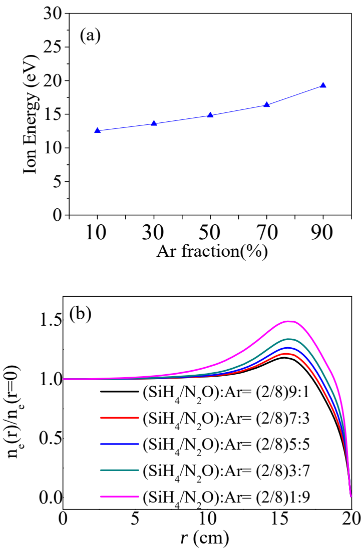

Fig.4. The ion bombardment energy on the electrode as the function of Ar fraction in the mixture gas (a) and the radial distributions of electron density at the center of discharge for different Ar fraction in the mixture gas (b) at the pressure of 266 Pa. Other discharge conditions are same as in Fig. 3

In addition, since dust particles often appear in silane plasmas, a 1D hybrid fluid/MC model has been developed to study the effect of different sizes of dust particle on the plasma properties in silane discharge, especially for the heating mode. The simulations reveal that when the plasma may get little perturbation by dust particles with radius of 1 nm, a hybrid combination of α and local field reversal heating mode is present. However, by increasing the dust particle radius in the plasma, the drift field heating mode is enhanced gradually and dominates the heating mechanism. These changes in the heating modes can be clearly seen in Fig. 5.

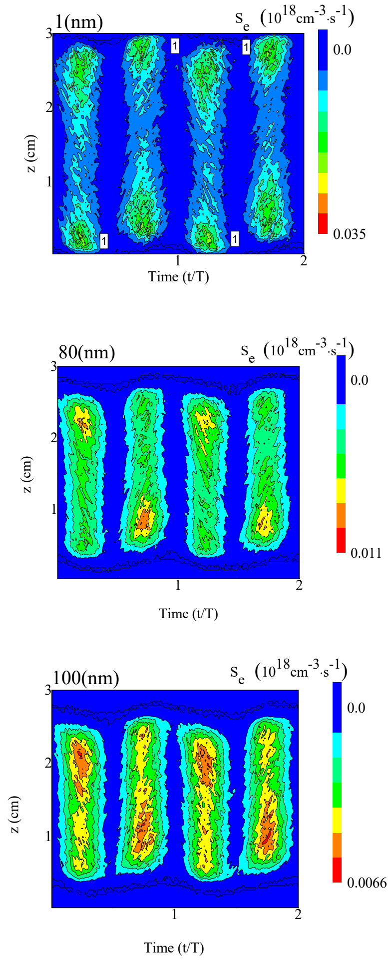

Fig.5. Spatiotemporal plots of electron impact source term during two rf cycles in SiH_4 discharge driven by 50 MHz power supply, for different dust particles radius in the plasma. First row: 1 nm, second row: 80 nm, third row: 100 nm. The reversal electric field heating mode are labeled “1” in the graphs.

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