Fluid and PIC simulations on electronegative SiH4 and O2 discharges in RF CCPs

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Reactive electronegative mixture gases in radio-frequency capacitively coupled plasmas (RF CCPs) have been widely adopted in etching and deposition processes of semiconductor industry. For plasma enhanced chemical vapor deposition (PECVD), SiH_4/N_2O, $SiH_4/N_2/NH_3$, or SiH_4/H_2 are usually taken as main mixed gases for silicon oxide, silicon nitride, or silicon oxynitride thin film deposition, while for etching, generally, discharges are operated in O2, Cl2, CF4 and SF4. Meanwhile, inert gases, such as Ar or He,are often added in order to improve discharge characteristic.

First, based on a two-dimensional fluid model, we investigate the discharge processes in a RF CCP reactor sustained in $SiH_4/N_2/O_2$ and SiH_4/N_2O/Ar. In $SiH_4/N_2/O_2$ plasma, the possible gas phase precursors for the deposition of Si-based film, such as SiH_3O, SiH_2O, SiO, SiN, $HSiNH_2$,and NH, are examined as a function of pressure, gas mixture and voltage. In SiH_4/N_2O/Ar plasma, apart from the discussion of possible gas phase precursors, we also analyze gas ratio effects on deposition precursors at relatively higher pressure, i.e. 1 and 2 Torr, and discuss the role of the inert gas Ar in the discharge and the effect of vibrational excitation of N_2O and SiH_4 on possible gas phase precursors. Further, important chemical reactions in possible gas phase precursors are also analyzed in detail for precise control of the chemical reaction path by the changing external conditions.

Moreover, by using 1D3V particle-in-cell/Monte Carlo collision model (PIC/MCC) simulation, the effects of secondary electron emission in a capacitive oxygen discharge are studied in our group. We examine the transition of the electron heating mode in this strongly electronegative discharge with the introduction of secondary electrons emitted in the bulk. And also, the striated structure, which is induced by charge separation and opposite oscillation direction for positive and negative ions since decreasing conductivity for lack of electrons, is noticed but becomes enlarged and weakened gradually as the γ heating mode dominates.

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