H2/N2 가스를 이용한 CCP 플라즈마 모델링

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Modeling of CCP plasma with H2/N2 gas

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Abstract - The resistance-capacitance (RC) delay of signals through interconnection materials becomes a big hurdle for high speed operation of semiconductors which contain multilayer interconnection layers. In order to reduce the RC delay, low-k materials will be used for inter-metal dielectric (IMD) materials. We have developed self-consistent simulation tool that includes neutral-species transport model, based on the relaxation continuum (RCT) model. We present the parametric study of the modeling results of a two-frequency capacitively coupled plasma (2f-CCP) with N_2/H_2 gas mixture that is known as promising one for organic low-k materials etching. We include the neutral transport model as well as plasma one in the calculation. The plasma and neutrals are calculated self-consistently by iterating the simulation of both species till a spatiotemporal steady state profile could be obtained.

1. Introduction

As ultra large-scale integrated (ULSI) device dimensions continue to decrease and several interconnection layers are used, RC delay, crosstalk noise and power dissipation of the interconnection materials become a bottleneck to increase device speed [1, 2]. The promising method proposed so far is using Cu for interconnection material to reduce resistance and using low-k materials for a substitute of SiO_2 to reduce capacitance [2]. There are many candidates for the low-k inter-metal dielectric (IMD) that have their own specific characteristics [3]. Therefore new etching conditions and process must be developed to match the material properties.

There have been many efforts to establish the etching technology for the low-k materials with different gas plasma [2, 4-7]. Nowadays N_2/H_2 or NH_3 plasma is considered to be the promising candidate for the etching of organic low-k materials [5-8]. These gas compositions have advantages than the O_2 based gas composition because the etching profile is more controllable and post-process damage that affects the dielectric constant change is low. N_2/H_2 gas is more appropriate than NH_3 for practical application because it is non-toxic, easy to process, and permits independent control over the partial pressure of each of the individual gas [8]. There have been many research results about N_2, H_2, and N_2/H_2 plasmas. But numerical investigation of N_2/H_2 plasma for low pressure CCP system has not been executed so far. We have developed a self-consistent modeling tool for plasma and neutrals in 2f-CCP with N_2/H_2 as a first step for the research of low-k materials etching process. In this paper, we present the modeling results of a two-frequency capacitively coupled plasma (2f-CCP) based on relaxation continuum (RCT) model [9] with N_2/H_2 gas mixture. The plasma and neutrals are simulated self-consistently by considering the reactions and transport of both species and simple surface reactions for NH_x molecules

2. Results and Discussion

2.1 Modeling of CCP device

As a continuum model for plasma, RCT model has been developed and applied for the etching process modeling [9]. We have used RCT model for the development of simulation tool for N_2/H_2 plasma in 2f-CCP. The model equations and results obtained by the model are in the reference. Based on the RCT model, we have included the neutral species transport model for the self-consistent calculation of plasma and neutrals in the system. The charged particles used in the simulation are electron, N_2^+, H^+, H_2^+, H_3^+, H^-. The neutral species are H, N, $N(^2D)$, and $N(^2P)$ atoms, $N_2(A)$, $N_2(B)$, $N_2(C)$, $N_2(a)$, $N_2(a')$, NH, NH_2, and NH_3 molecules. Vibrational states of $N_2(1 \leq v \leq 8)$ and H_2 $(1 \leq v \leq 14)$ ground states are also included in the modeling to investigate the effects of these species. Neutral species are followed by the reaction diffusion model. The Neumann boundary condition is applied to the plasma species for all boundaries. In the case of neutral species, thermal-flux loss toward boundaries is used with reflection coefficient, R, $R = 1-p$, p is sticking probability. A simple surface reaction and reflection of N and H atoms are included in the calculation. As it is difficult to obtain exact surface reaction data for the N_2/H_2 gas mixture, we assume the same surface reaction rates for considered surface reactions of N, H, and NH_x species.

The simulation geometry is shown in Fig. 1 and external conditions are shown in table 1. We have adopted cylindrical system with two electrodes that are driven by independent two frequencies. The upper electrode is used to generate high density plasma and the lower electrode to obtain high energy ion flux toward substrate (functional separation). We have confirmed the functional separation of the 2f-CCP by simulation and experiment [9].

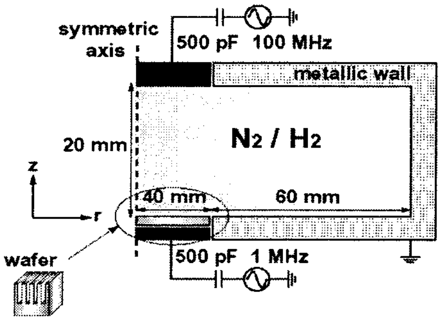

Figure 1. Simulation domain of 2f-CCP with N_2/H_2 gas

Table 1. Simulation Conditions

Gas Pressure	50mTorr
Gas Composition	N_2 (50%)/H_2 (50%)
Drive Frequency	100MHz
Drive Voltage	300V ~ 500V
Bias Frequency	13.56MHz
Bias Voltage	400V ~ 1000V

2.2 Simulation Results

Figure 2 is peak-densities of plasma species and Fig. 3 is that of neutrals. The numbers in the circle indicate the simulation sequence of the modeling. At the sequence 1, the plasma profiles are calculated by RCT model based on appropriate initial densities of plasma and neutrals until the periodic steady state. As the plasma profiles reach periodic steady state after 30 ms that is ion saturation time scale, the neutral transport model is started under the obtained plasma profiles (sequence 2). As shown in the figure, neutrals reach the steady state within msec order. After the density saturation of neutrals, the plasma part is recalculated with the obtained spatio-temporal neutrals density as new initial condition. This process is repeated till the periodic steady state of species densities are obtained.

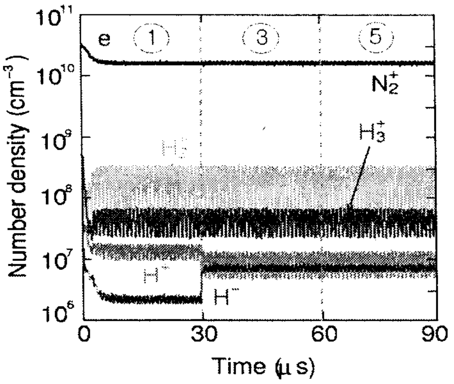

Figure 2. Time trace of plasma peak density

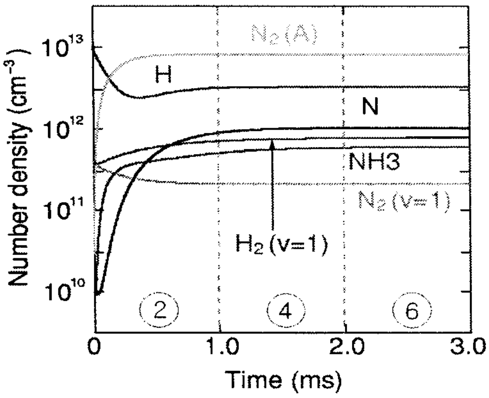

Figure 3. Time trace of neutrals

The time-averaged densities of charged particles at axis are shown in Fig. 4. The main charged particles are electron and by N_2^+ions in the system. The positive and negative ions of hydrogen are one or two orders of magnitude smaller than N_2^+. As shown in the figure, the H_3^+ is the most populated hydrogen ion. The H_2^+ ions are generated in the high field region by ionization and easily converted to H_3^+ ions with the collision of hydrogen parent gas because the threshold energy is very low compared with ionization energy of H_2 molecule. The negative ion density is two orders of magnitude smaller than N_2^+ ion as seen in the figure.

As stated in introduction, H and N atoms are important species for low-k materials etching because they have reactions which result in the passivation layer of side walls and etching of bottom of trench [8]. As a result, the estimation of density and flux near the substrate is important parameter for low-k material etching process. The spatial profile of N atom is shown in Fig. 5. The profile of H atom is similar with the N atoms. The maximum density of hydrogen atom is $3.3*10^{12}$ cm^{-3} and that of nitrogen one is $1.0*10^{12}$ cm^{-3}. The fluxes of H and N atoms are $2.0*10^{16}$ cm^{-3} and $3.8*10^{15}$ cm^{-3} respectively. The molecules of NH_x have been simulated together in the modeling. As the generation of NH_x molecules is second process in the space, the number density decreases with time without including surface reactions. We have included simple surface reaction model and obtained saturated densities of NH_x molecules. As an example, we have shown NH_3 molecules density profile in the system.

3. Conclusions

We have developed a self-consistent modeling tool for plasma and neutrals in 2f-CCP with H_2/N_2 for the research of low-k materials etching process. The simulation results of a 2f-CCP based on RCT model with N_2/H_2 gas mixture were presented. Self-consistent simulation has done by considering the reactions and transport of plasma and neutrals. In the simulation of neutrals, the vibrational states of nitrogen and hydrogen ground state molecules were included, too. The vibrational states have not only interactions with themselves but also with the other neutrals. The vibrational states of hydrogen molecules are the main source of hydrogen negative ions. The trend of vibrational states showed similar with previous results.

We have presented the simulation results of plasma and neutrals. In the mixture of N_2/H_2, the main ion is N_2^+ and hydrogen ions are one or two order of magnitude smaller. The N_2 metastable is a important species because it is a direct or indirect source of N and H atoms, and has many interactions with plasma and the other neutrals. We also obtained the profiles of N and H atoms that are considered to be important species for the etching of low-k materials. The saturated densities of NH_x molecules are obtained by adopting surface reaction model.

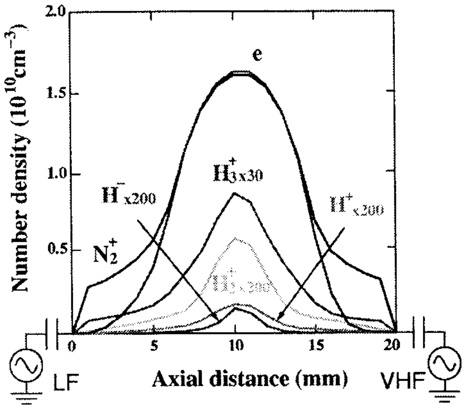

Figure 4. Density of plasma along the axis

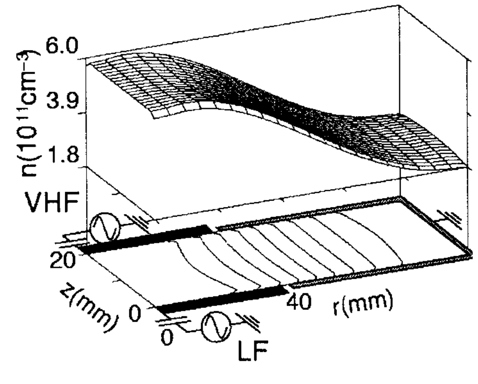

Figure 5. Spatial density profile of N atoı

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