Numerical Simulation of Organic Low-κ Etching in H₂/N₂ Plasma

Takashi Yagisawa¹ and Toshiaki Makabe¹

¹Department of Electronics and Electrical Engineering, Keio University,
3-14-1, Hiyoshi, Kohoku-ku, Yokohama 223-8522, Japan.
Phone: +81-45-563-1141 E-mail: yagisawa@mkbe.elec.keio.ac.jp

1. Introduction
As the size of ULSI continuously shrinks toward 20 nm and multi-layer interconnect with more than 12 layers is applied, RC (resistance-capacitance) signal delay should be made smaller to meet the demand for higher performance of signal transmission. The dielectric constant (κ) of interlayer dielectric (ILD) can be reduced by lowering electric polarizability of the material. Alternatively introducing porous nano-holes within the material to reduce its density decreases the κ value. Increasing porosity is considered as a promising candidate for obtaining low-κ ILD, though it may bring up new serious problems in its processing. Materials with low dielectric constant tend to possess poor mechanical strength and adhesiveness to the wire. In addition, low-κ dielectric has low heat conductance and low resistance against heat, which makes it difficult to go through the post annealing in back-end processes.

Currently, H₂/N₂ plasma is developed as the most suitable tool for the etching of organic low-κ material. The etching profile is determined under the balance among isotropic etching by reactive H radical, physical sputtering by energetic ions and surface protection by the deposition of N radical [1]. In order to achieve the optimal profile, detailed understanding of these elements throughout the whole plasma etcher is strongly required. We have carried out a series of numerical simulation consisting of the design of plasma reactor, prediction of velocity distribution of reactive species, such as positive ions, neutral radicals H and N, and the etching profile of organic low-κ materials.

In the present study, we will first estimate the density of reactive species, such as H, N and NHₙ radicals, generated mainly via direct dissociation from parent gas molecules in two-frequency capacitively coupled plasma (2f-CCP) in the admixture of H₂/N₂. Furthermore, the effect of dissociation degree on the etching profile of organic low-κ material will be discussed as a function of the mixture ratio of feed gas molecules, H₂ and N₂.

2. Simulation model
The 2f-CCP reactor, having geometry similar to that used for SiO₂ etching, considered in this study is shown in Fig. 1. The reactor is cylindrical with respect to the vertical axis and has two electrodes; the upper electrode driven by a very high frequency of 100 MHz at the amplitude of 300 V is responsible for the production of high density plasma, while the lower electrode driven by 1 MHz at 700 V is for the precise control of energy distribution of ions incident on a wafer to be etched. In the 2f-CCP in H₂/N₂ at the gas pressure of 50 mTorr, we consider 6 charged species: electron, N₂⁺, H⁺, H₂⁺, H₁⁻, and H and 12 neutral species: N, H, N(D), N(P), N₂(A'Σ_u⁺), N₂(B'Π_g), N₂(C'Π_g), N₂(a'Π_g), N₂(a'Σ_u⁻) and NHₙ (n = 1, 2, 3), in addition to the vibrational states of feed gas molecules: N₂(v = 1 ~ 8) and H₂(v = 1 ~ 14). In H₂/N₂ plasma, the atomic radicals H, N and NHₙ have important roles for organic low-κ etching. Therefore, we mainly focus on the behavior of these radicals, especially on the flux at the wafer surface.

As shown in Fig. 2, the surface of the organic low-κ film exposed to H₂/N₂ plasma can be modeled by two-layer structure consisting of a top CN-polymer layer and underlying low-κ material. The effective etching rate on the surface ER_eff is expressed in terms of the etching rates of CN-polymer layer ER_CN, low-κ layer ER_low-κ and deposition rate of CN-polymer DR_CN as follows,

\[ ER_{eff} = ER_{CN} + ER_{low-κ} - DR_{CN} \]

The surface evolution is described by level-set equation including the effective etching rate,

\[ \frac{\partial \Phi}{\partial t} - ER_{eff} |\nabla \Phi| = 0 \]

where Φ denotes a level set function, which is essentially a distance between the surface and each grid point. The detail of the numerical procedure on the model is summarized in Ref. [2].

3. Result and Discussion
As is experimentally known, organic low-κ materials have narrow process window for plasma etching. First of all, we have investigated the active ions and radicals coming to the etched surface at different mixture ratio of feed gas molecules. The incident fluxes on the center of the wafer surface as a function of gas mixture ratio, H₂ / (H₂ + N₂) are shown in Fig. 3. The flux of H₂⁺ increases with a fraction of H₂ gas molecules, while N₂⁺ flux is almost the constant. H radical flux has a maximum, 5.0 x 10^{16} cm⁻²s⁻¹, at H₂ (50%), while N radical flux with a maximum of 1.2 x 10^{16} cm⁻²s⁻¹ decreases linearly with a fraction of H₂. The etching characteristics of organic low-κ film can be classified into two resumes, i.e. intensive CN-polymer deposition and etching dominant cases.

The first resume will be remarkable at H₂(25%), where Γ_N ∼ Γ_H and Γ_N₂⁺ < Γ_H₂⁺ are satisfied on the surface. N
and H radicals incident on the surface have isotropic energy distribution, while the ions have a beam-like profile. The excess deposition of N radicals to the sidewall forming the hard CN-polymer contributes to an etching profile with a little bit taper as shown in Fig. 4(a). The second resume appears clearly at H2(75%), where $\Gamma_N \ll \Gamma_H$ and $\Gamma_{N^2+} \sim \Gamma_{H^2+}$ are satisfied, as shown in Fig. 2. The etching profile gives an anti-tapered profile (see Fig. 4(b)), probably due to the sidewall etching carried out chemically by H radicals, and to less passivation of N radicals. The etching rates are 250 nm min$^{-1}$ at H2(25%), and 440 nm min$^{-1}$ at H2(75%), respectively. It is confirmed that N and H radicals have significant influence on the etching characteristics in both resumes. The etching profile and the rates agree reasonably with the experimental results [3].

4. Conclusions
Through a series of our works based on numerical simulation from the gas phase 2D-t plasma design to the surface processing, such as etching and deposition, the etching characteristics of the organic low-k material exposed to the 2f-CCP in H2/N2 have been predicted. The narrow process window for the etching is elucidated from the dominant radical processes either N or H, assisted by high energy ions as a function of mixture ratio of feed gas molecules. In a gas phase, a collisional dissociation of NH3 produced on the reactor wall plays important roles in the behavior of reactive H radical. In addition, it is confirmed that N and H radicals have significant influence on the etching characteristics. The etching profile and the rates reasonably reproduce the experimental results.

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References

Fig. 1: 2f-CCP reactor for organic low-k etching considered in this study

Fig. 2: Surface model for organic low-k etching by H2/N2 plasma

Fig. 3: Fluxes of reactive species incident on the surface as a function of gas mixture ratio, H2 / (H2 + N2).

Fig. 4: Temporal evolution of the etching profile of organic low-k material in 2f-CCP in H2/N2. H2(25%)/N2 (a) and H2(75%)/N2 (b).