Simulation and Prediction of Aspect Ratio Dependent Phenomena during SiO_2 and Si Feature Etching in Fluorocarbon Plasmas

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Abstract

A simulator to calculate etching rates in SiO_2 and Si features in fluorocarbon plasmas has been developed. This simulator links the gas (plasma) phase composition with the etching rate inside features and it is used for predicting aspect ratio dependent phenomena during SiO_2 and Si feature etching.

1 Introduction

Etching of SiO_2 and silicon containing low k dielectrics is a very critical process step in microelectronics fabrication. SiO_2 and Si etching is also extremely important for optoelectronics and microsystem fabrication and is performed in fluorocarbon plasmas. It is useful to understand and predict the etching phenomena in order to confront the problems during an etching process

Phenomena such as Reactive Ion Etching lag [1] (i.e. etching rate reduction in narrower trenches and holes, *RIE lag*), *etch stop* [1], and *inverse RIE lag* [2], are usually observed during SiO_2 and Si feature etching and can cause several problems; both RIE lag and inverse RIE lag lead to different etched depths, and overetching is needed, which could result in the damage of the underlying layer. The above-mentioned phenomena have been observed to depend on the Aspect Ratio (AR) of the feature (depth/width of the feature) rather than the absolute feature size and are included in the general term Aspect Ratio Dependent Etching (ARDE). The desirable elimination of RIE lag and inverse RIE lag is denoted by the term Aspect Ratio Independent Etching (ARIE); i.e. etching rate constancy as etching time increases and consequently as AR increases.

A model to calculate etching rates in SiO_2 and Si features in fluorocarbon plasmas has been developed. The model includes a) a surface model [3] for open area etching of SiO_2 and Si, b) a flux calculator [4], which calculates local fluxes on each elementary surface of the feature being etched, and c) a coupling of the two models (a) and (b) to calculate the local etching rate inside features. Based on this model the effect of gas phase composition on ARDE and ARIE is simulated and investigation of processes' window can be done.

2 The surface model

An adsorption-type model [3] accounting for etching and deposition in fluorocarbon plasmas during Si and SiO_2 open area etching is used to describe the surface physical and chemical processes. In this phenomenological model, fluorine atoms (F), fluorocarbon radicals (CF_x), and polymer (produced on the surface) are considered bonded to surface atoms. The basic equations of the model are F, CF_x, and polymer site balances and the model coefficients have been calculated by fits [3] to beam experiments' results. The independent variables are a) the ratios of neutral species (F, CF_x) fluxes to ion flux, b) ion energy, and c) ion composition. If absolute value of etching rate is to be calculated, ion flux value is needed. Besides etching yield (Si atoms/ion) and rate, effective sticking coefficients, S_E, of the neutral species are also outputs of the surface model. S_E of a species represents [5] the net loss ($S_E>0$) or creation ($S_E<0$) of this species during surface reactions.

3 The flux calculator

The flux calculator [4] is used for the calculation of ion and neutral flux on each elementary surface of a structure. It takes into account shadowing of ion and neutral flux and re-emission of neutral flux in features. Charging effects are not considered, but are simulated by an increased ion angular spread. The total flux of a species i (ion or neutral) at an elementary surface s of a feature (trench with infinite length or hole with cylindrical symmetry) is given by the equation

$$j_i(s)=j_{direct,i}(s)+\int_{\text{feature profile}} g_i(s,s')[1-S_{E,i}(j_1,j_2,\ldots,j_N)]j_i(s')ds', \qquad (1)$$

where $g_i(s, s')$ is a function which depends on the re-emission mechanism of the species i and the geometry of the structure being etched. $j_{direct,i}$ is the flux of the neutral species i coming directly from the plasma and expresses the effect of shadowing on the flux. The integral of Eq. 1 stands for the flux coming at s from all other elementary surfaces s' by re-emission.

The calculation of local fluxes and local etching rates *requires a coupling* [4] *of the surface model with the flux calculator*. The key point of the coupling algorithm is the simultaneous calculation of a) $S_{E,i}$ by the surface model [5] and b) total flux for every species by a system of N integral equations such as Eq. 1 (N is the number of species).

4 Results

The proposed model essentially links the gas phase composition with ARDE in SiO_2 and Si trenches. The gas phase composition is defined by the neutral (F atoms, CF_x radicals) and ion fluxes coming from the gas phase of a fluorocarbon plasma and reaching an open area ($j_{F,0}$, $j_{CFx,0}$, and $j_{ION,0}$) and is expressed by the ratios: $R_{F,0}=j_{F,0}/j_{ION,0}$, $R_{CFx,0}=j_{CFx,0}/j_{ION,0}$.

In Fig. 1 *maps of ARDE and ARIE* in SiO_2 and Si trenches are presented. This new approach divides the gas phase composition into regions leading to a specific AR dependent phenomenon. For example, in Fig. 1a, which refers to SiO_2 trench etching, deposition happens in region A, intense RIE lag and etch stop in C, RIE lag with no etch stop in B, inverse RIE lag in D, and ARIE up to a specific AR in E. A similar division of gas phase composition has been done in Fig. 1b for Si trench etching.

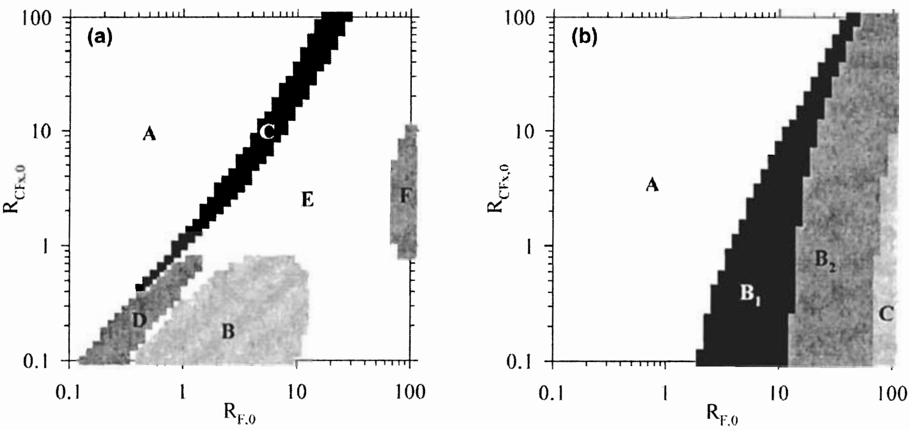

Fig. 1. a) Effect of gas phase composition (i.e. ratios $R_{F,0}$, $R_{CFx,0}$) on SiO_2 trench etching: Region *A*: deposition; *B*: regular RIE lag with no etch stop; *C*: intense RIE lag and etch stop; *D*: inverse RIE lag; *E*: ARIE (less than 5% decrease in etching rate) up to AR=3 to 7 depending on the distance from deposition region. The further from deposition region the higher the AR for which ARIE is observed. *F*: ARIE up to AR=7. A slight inverse RIE lag can be observed for some compositions. **b)** The same as (a) for Si trench etching. Region *A*: deposition. B_1: intense RIE lag and etch stop. B_2: RIE lag. Larger trench AR is needed to observe etch stop. *C*: Mild RIE lag, and ARIE up to AR=3 to 4 for high $R_{F,0}$ and low $R_{CFx,0}$. Ion energy is 100eV, ion composition is 10% CF_3^+, 85% CF_2^+, 5% CF^+.

In Fig. 2a etching or deposition is predicted in SiO_2 trenches: the contours of zero etching rate at SiO_2 trench bottom as a function of gas phase composition are shown for different AR values. Each curve represents a boundary between deposition (left side) and etching (right side). *Knowing the gas phase composition and the trench AR, one can predict what will happen at the bottom of the trench: etching or deposition.*

The proposed model can be used for a preliminary investigation of processes' window satisfying demands on ARIE, etching rate magnitude, and etching rate selectivity. Fig. 2b refers to a process window during etching of SiO_2 trenches over a Si layer have to be etched. In the black region of Fig. 2b etching rate is greater than 240 nm/min, etching rate selectivity (SiO_2/Si) greater than 10, and etching rate deviation from the open area value less than 5%.

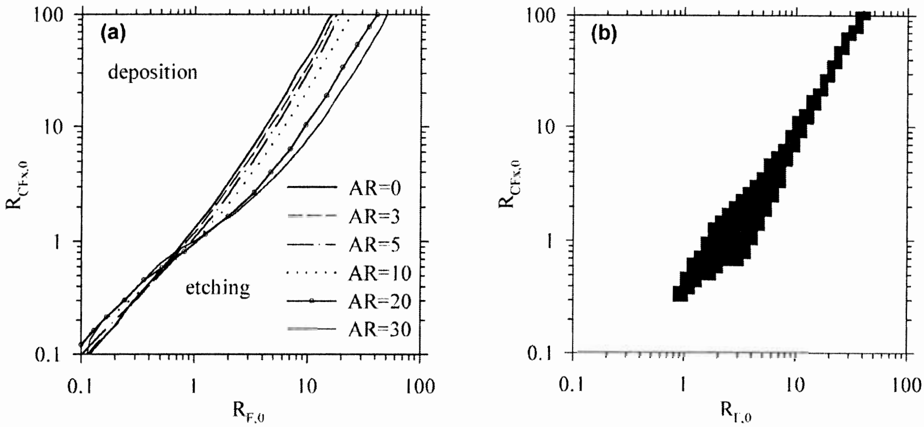

Fig. 2. a) Contours of zero etching rate at a SiO_2 trench bottom as a function of gas phase composition for different trench AR. Each curve represents a boundary between deposition (left side) and etching (right side). **b)** Range of gas phase compositions of an etching process of SiO_2 trenches on a Si layer. The trenches AR lies in the range of AR=1 to 3 during etching. In black region etching rate is greater 240 nm/min (ion flux is 17 mA/cm^2), etching rate selectivity (SiO_2/Si) is greater than 10, and etching rate deviation from the respective open area value is less than 5%. Ion energy and composition are the same as in Fig. 1.

5 Conclusions

Aspect ratio dependent phenomena during SiO_2 and Si feature etching in fluorocarbon plasmas are predicted and preliminary investigation of processes' window can be achieved by a simulator for feature etching that couples a surface model for open area etching with a calculator of fluxes inside features.

References

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