New simulation method for profile feature evolution of high aspect ratio trenches in Si under SF₆/O₂ plasma mixture

G. Marcos¹,², A. Rhallabi¹, P. Ranson²

¹ Laboratoire des Plasmas et des Couches Minces, IMN, UMR 6502, CNRS-Univ. Nantes, 2 rue de la Houssinière, BP 32 229, 44 322 Nantes Cedex 3, France. E-mail: gmarcos@ireste.fr; Tel: 02 40 68 32 03; Fax: 02 40 68 30 66
² GREMI-CNRS-Université d’Orléans, UMR 6606, 14 rue d’Issoudun, BP 6744, 45 067 Orléans Cedex 2, France

Abstract

A better understanding of the plasma-surface interactions is needed to perform the etching processes. In this article, we present the results of a Monte-Carlo method describing the temporal evolution of the etched silicon substrate by SF₆/O₂ plasma mixture. Actually, atomic oxygen is not included. An ion transport model based on Monte Carlo techniques is coupled with this etched surface model. The role of certain parameters (like F-atom flux or mask geometry) is allowed and interpreted by a series of simulations for which the stop criterion is depth (the concept of time is not introduced yet). Our results show that undercut is produced by spontaneous chemical etching, while the ion reflexion on the lateral slopped surface of the mask can explain partly the bowing formation during the etching process.

1 Introduction

Nowadays, etching processes must follow the continually renewed requirements of microelectronic technologies. Plasma etching has taken the place of wet processes, because it allows reach a better anisotropic rate. Challenges in connection in particular with emergence of microelectro mechanical systems (MEMS), concern in fast obtaining in silicon substrate (etch rate of a few µm/min on average) very deep trenches (≈ 100 µm) with high aspect ratio (≈ 20) for the fabrication of supply power components. An high density low plasma pressure (HDL) plasma reactor is good adapted to reach these aims. It permits actually, contrary to standard reactive ion etching (RIE) equipment, to control independently ion energy and ion density which is at least one order of magnitude higher than in RIE.

Gas phase used is a mixture of SF₆/O₂. In fact, while fluorine based chemistries are generally used to achieve high etch rates for deep etching, atomic oxygen creates by sticking a passivation layer on the sidewalls to protect them and maintaining thus high anisotropy. A cryogenic method by a drop in

Fig 1: Experimental profile. On right, we can distinguish undercut and bowing.
the chuck temperature (≈ 100 °C) of an ICP Alcatel reactor, reduces significantly chemical spontaneous etching which is an isotropic process modifying seriously general anisotropy of trench profiles.

The results obtained in our laboratory are very encouraging. Fig 1 shows an example of an experimental trench profile. The deep is about 40 µm for 2 µm wide. Although general aspect is strongly anisotropic, a zoom of the upper part lets appear two defects. Note undercut formation which is a lateral overetch takes place just under the mask and increases trench aperture. More in depth, we can also see the bowing [1], an other lateral overetch whose consequences are very dramatic for post etching steps (a void appears during the trench refilling). These two defects so damage geometrical characteristics of trenches and it is necessary to understand their formation processes to minimize their effects. This research implies a detailed study of plasma-surface interactions mechanisms.

In this article, we shall present numerical simulations of profile evolution of silicon surfaces subject to HDLP etching. To advance the surface, we developed a two dimensional etching model based on Monte-Carlo techniques. Unlike others methods, this removes adjustments or certain profiles smoothing (particularly where surfaces have breaking slopes), which can dissipate or suppress physical and geometrical phenomena. A piece of information is in this way lost and final topography can be modified. After a brief description of our model, we will show some results according to specified parameters.

II The 2D etching model

II.1 Introduction: Plasma kinetic

The adopted model does not consist in developing a general etching one, including a kinetic model and a part for surface layer displacement. Plasma mixture (SF₆/O₂) being complex from the kinetic point of view [2] [3] [4], we will use data concerning it by in-situ plasma measurements. A series of experimental actions are in hand: measurements by Langmuir probe, analyses by optical and mass spectroscopy. These studies will allow characterize respective radicals and ions fluxes, densities, temperatures, etc...(cf in this conference the communication of F.Grangeon et al and M.Boufnichel et al). These data will be also introduced in our etching model.

II.2 Definition of the target

First step is the characterization of the target submitted to etching plasma. It is defined by a substrate and a mask above which we must specify physical and geometrical parameters. The method consists in a two dimensional discretization. Each cell has the same size which

![Grid and etch processes: Undercut vs F-atom chemistry result while sputtering takes place essentially at the bottom of trench.](image)

Fig 2: Grid and etch processes; Undercut vs F-atoms chemistry result while sputtering takes place essentially at the bottom of trench.
really defines a number of sites inside. In this manner, this matrix study gives at any moment a specific photography of physical state of surface. Figure 2 shows an example. We can distinguish the left mask side, mask aperture and the substrate. With time, this grid will be more complex, in relation with new sites appearance.

II. 3 Plasma radicals

The main reactive species in the gas phase plasma are fluorine and oxygen radicals. They are competing to react with silicon atoms. The firsts, whose are provided by SF6 dissociation, form SiF4, an etching volatile product. Atomic oxygen sticks on silicon to create SiO2 which passivates the sidewalls.

In our preliminary model, results presented here concern only F atom chemistry. Role of oxygen is in progress and will be probably showed for the congress. In Fig 2, we have taken an inventory of typical etching mechanisms. F atom flux is represented by solid black pointers. Their flux is supposed to be isotropic. Placed randomly above the target, its displacement is realized in straight lines because we assume that no collisions occur in the trench. Interaction with the mask is defined only actually by random reflexion. With Si substrate, the impact study is realized with a probabilistic manner: random reflexion or sticking on corresponding SiF_{4-y} site. This sticking is a chemisorption that produces a new Si-F bond: SiF_{4-y} + F \rightarrow SiF_{y+1}. The final step of this process is SiF_{y} formation, a volatile etching product.

II. 4 Plasma ions

In our experimental conditions, recent measurements by a Langmuir probe showed an ions flux of about 10^{5} cm^{-2} s^{-1}, that corresponds to less than 3% of total fluxes. Ions incident energy and angle are determined by a transport model in the sheath [7]. This model is based on Monte Carlo techniques and takes account sheath characteristics that are controlled by pressure, bias tension voltage and injected power in the reactor. We show in Fig 3 an example of distributions function obtained for a 22 mTorr pressure (V_{DC} = 30 V and V_{p} = 15V). This layer is for energies (expressed in eV on x-axis) well recognized saddle horse in shape with two peaks (for E = 45eV and E = 60 eV). The angular part exhibits a narrow distribution with a majority of normal incidence ions (there is no significant population above 3\(^\circ\)).

For mask and substrate, two mechanisms are treated: specular reflexion and preferential sputtering [5]. In the future, some calculations with the TRIM (TRansport of Ions in the Matter) software will allow determine precisely post-reflexion ions distributions. In this

![Figure 3: Example of ions distribution function for a 22 mTorr pressure](image)

![Figure 4: Simulation of a trench profile obtained with a pressure of 22 mTorr](image)
first model, the sputtering yield is not sensitive to the angle of incidence of ions [6], but we
take into account a linear variation with ions energy. Fig 4 shows one simulated 3.5 μm deep
trench profile obtained for a 22 mTorr pressure. The mask thickness is 1 μm, for an aperture
of 0.5 μm and sides slope of 9°. The imposed F-atom flux is of 30% of the total flux and there
is no correspondence with pressure.

II. 5 Surface displacement
In the model, etching is symbolized by a cellular transition between a full state to an
empty state. So, etched surface displacement is realized by sites disappearance, produced by
spontaneous chemical etching or preferential sputtering.

III Results and discussion

We have studied final trench topography by varying independently four relevant
plasma surface interactions parameters: ions distributions, F-atom reflexion rate, proportion of
F-atom flux and mask geometry. The simulations were stopped when the trench depths
attained a fixed value (2 or 4 μm for example). So, actually no time evolution can be deduced
from these trench profiles.

III. 1 Ions distribution
Using the sheath model described above, we calculated ions function distributions. We
display in fig 5 two examples of ion distribution for pressures at 7.5 and 45 mTorr
respectively (VDC = 30V and Vp = 15V). In two cases, most of ions have an angular incidence

\[ \text{Fig 5: Two ion distribution functions for 7.5 mTorr (left) and 45 mTorr (right). Solid line: } \theta_{in} = 1°; \text{ Solid line with circles: } \theta_{in} = 2°; \text{ Dotted line: } \theta_{in} = 3°. \]

\[ \text{Fig 6: Simulations results for the two pressures above (a: 7.5 mTorr; b: 45 mTorr). On right-hand side, trench topography is more bowed.} \]
below three degrees. For the second one, the distribution is less anisotropic because of the increase of the ion-neutral collision processes. Fig 6 shows two simulations realized with these distributions and the following parameters: fluorine atom flux/ ion flux = 30% of the total flux, F-atom reflexion rate = 70%, mask sides slope = 9° and depth = 3 μm. Even for the higher pressure, final trench profile is still anisotropic, although topography is a quiet deformed.

III. 2 F-atom reflexion rate

In order to show the effect of F-atom reflexion rate, we display two trench profiles for 2 μm deep, 0.5 μm mask aperture and for ion distribution corresponding to a pressure of 22 mTorr. The simulations (Fig 7.1 and 7.2) have been realized with F-atom reflexion rate of 70% and 30% respectively. The results show that this rate on the trench sidewalls is a very important parameter for anisotropy. When it decreases, undercut increases and the trench topography becomes more bowed in the upper part. That is explained by an enhance in sticking coefficient which produces more significant fluorine cover on sidewalls just below the mask. Spontaneous chemical etching is also more important there.

III. 3 Proportion of F-atom flux

Figures 7.2 and 7.3 show trench profiles for 2 μm deep and 0.5 μm mask aperture. Angular and energetic distribution functions of ions correspond to a pressure of 22 mTorr. The proportion of F-atom flux is respectively 70% for the left simulation and 30% for the right one. F-atom reflexion rate are the same (30%). The results indicate that anisotropy is strongly dependent on the ion to neutral flux ratio. It decreases for the first profile where undercut caused by the isotropic neutral flux is more pronounced.

III. 4 Mask geometry

In figure 8, we display the topographic profile evolution for a trench between two different aspect ratio (3 and 7), for 22 mTorr of pressure and 70% of ion to neutral flux ratio. The first profile is strongly anisotropic, even if a weak undercut appears. The sidewalls are
sloped of 88 degrees (it is a “positive profile”). For an higher aspect ratio, we can cut the second profile in three distinct zones. Firstly, we see the α-zone (see Fig 8), where spontaneous etching, which is the dominant mechanism, creates undercut. On the opposite side, at the bottom of the trench (the β-zone), topography remains anisotropic: in this area,

![Diagram](image)

Fig 8: Two trench simulations versus aspect ratio (3 and 7). An overetch at 1.5 μm deep on average appears (γ-zone).

![Diagram](image)

Fig 9: Studies for searching overetch formation. On left-hand side, the mask has vertical sides while we stopped ions reflection at right.

sputtering mechanism controls the etching processes. Round about 1.5 μm deep, appears a γ-zone where a second lateral etching occurs. This overetch extends on a little less than 1 μm, as its aspect is rather similar among that of the bowing introduced previously, it is necessary to determine its mechanisms of formation.

In figure 9, two simulations have been realized. We introduced the same parameters as previously, but with two modifications: we imposed a mask with vertical sidewalls for the first, while we suppressed ions reflection for the second one. For these two cases, the lateral etching at 1.5 μm is suppressed. So, we can explain the formation of the bowing phenomenon by a lateral sputtering caused by reflected ions from the mask side slopes.

IV Conclusion and perspectives

We have described and illustrated our preliminary etching model. The results permit to show implications of certain parameters in plasma etching processing: angular and energy ion distribution, F-atom reflexion rate, proportion of F-atom flux and mask geometry. We will quantify these different effects to determine their respective role in the final trench topography.

Experiments and surface analyses are in hand to obtain kinetic parameters and surface data. For the simulations displayed in this paper, we have introduced them as input parameters.

Improvements of the model to simulate the etching profiles with a good accuracy are necessary. First, let recall that in this first stage, we took only account of the fluorine flow, while experimental studies show that atomic oxygen is really a key parameter for the passivation layer formation by creation of Si-O bounds. We have to determine for this study the competition of sites occupation (SiF₃₋ₓ/Oₓ) by fluorine and oxygen.

We will add also etched species redeposition, because they play a role in passivation layer formation process. Sputtering yield will be adjusted and we will determine consequences of mask erosion on the final trench profiles.