A Feature Scale Model for Trench Capacitor Etch Rate and Profile

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Abstract

To support the optimization of aspect ratio and profile of DRAM trench capacitors we have developed two feature scale models of different complexity. A compact model calculates the etch rate for a given trench geometry by solving an integral equation for the neutral and ion transport inside the trench. This approach yields a quantitative prediction of the variation in etch rate for different trench profiles. An additional high level model calculates both the etch rate and the trench profile as a function of process parameters. This is achieved by using a level set front propagation, Monte Carlo particle transport, and chemical reaction rates. The results of both models are in good agreement with each other as well as with experimental data for several technology nodes. With our high level model it is now possible for the first time to simulate the feature evolution during deep trench etching of advanced DRAM generations.

Introduction

Maintaining a constant capacitance per memory cell is crucial for DRAM scaling. To achieve this objective high-k node dielectrics and HSG surface enhancement [1] are helpful. However, it is still mandatory to achieve high aspect ratios and optimized trench profiles. For viable scaling scenarios below 100nm it is therefore useful to have a realistic model describing the etch rate, its dependence on trench profile, and the mechanisms for generating specific profiles. The overall goal is to achieve the optimum aspect ratio and trench shape with respect to capacitance and cost for each technology generation.

Topography model for high aspect ratio

The accurate calculation of an etch front in extreme geometries is a major challenge for topography simulation. In fact currently *no* simulator is available commercially or academically which is capable of simulating the etching of a deep trench capacitor with aspect ratios of more than 50. Therefore we have developed a 2D/2D-axisymmetric code which is capable of very high aspect ratios as well as essentially arbitrary particle transport and chemical kinetics. The level set front propagation module achieves high accuracy and efficiency by using a narrow band discretization and a fast marching algorithm [2]. The local velocity is calculated on the extracted front segments from the particle fluxes and is extended to the level set grid nodes with a properly weighted interpolation. To illustrate the viability of this approach figure 1 shows a front subject to a perfectly collimated particle beam etching with unit probability. As can be seen even at an aspect ratio of 100 no numerical artifacts are introduced by the level set front propagation.

Feature scale model for etch rate and profile control

The physical fluxes at the front are calculated using ballistic transport from user-defined particle sources. This Monte Carlo approach is well suited for general angular and energetic particle distributions, for example from a plasma sheath model [3]. A novel scheme allows the consistent calculation of thermally and kinetically activated surface reactions of arbitrary order as a function of sampled flux and surface coverages. Fluxes may be used for several level set time steps before they have to be recalculated. For each flux calculation typically 10^7 Monte Carlo particles are sampled.

Conventional silicon etching is based on a $HBr/O_2/NF_3$ plasma generated in a capacitively coupled Merie plasma reactor [4]. The surface chemistry model used for the below simulations is based on the assumption of ion assisted etch of amorphized and subsequently halidized silicon. Profile control is mainly due to the deposition of a thin, continuously growing SiO_2 like passivation layer along the sidewall (see figure 2). The specific surface reactions implemented in our high level trench etch model are:

Ion$^+$ + #Si(b)	**=> Ion$^+$ + #Si*(s)**	amorphization of c-Si
Si*(s)	**=> Si(b)**	recrystallization of a-Si*
Br + Si*(s)	**=> Br(s) + Si*(s)**	Br halidization
Ion$^+$ + #4Br(s) + #Si(b)	**=> Ion + #SiBr$_4$**	Br etch
O	**=> O(s)**	passivation by O
Ion+ + #O(s)	**=> Ion + #O**	resputtering of O(s)

with particle fluxes provided by the plasma sheath model, etch yields and reflective distributions from molecular dynamics [5], and reactive sticking coefficients calibrated to measurements. This model yields a variety of trench profiles as a function of process conditions, namely oxygen flux and surface temperature. For example, figure 3 shows trenches "etched" with (a) optimum, (b) excessive, and (c) variable oxygen flux under otherwise fixed conditions. Depending on the required accuracy the computation time for one trench etch is approximately 15/*n* hours on a *n*-CPU cluster.

The simulated etch rates are consistent with the halidization of the trench bottom by Br with a high reactive sticking coefficient and only moderate energy dissipation of the ions inside the trench. A careful investigation of the simulation results indicates that the etch rate of a deep trench is limited by the neutral precursor transport.

Compact model for etch rate

To facilitate the discussion of scaling scenarios we have developed a analytical model for the etched depth **L(t)** as a function of process duration **t** and *a given trench geometry*. This model is based on an integral equation for the neutral and ion transport and is consistent with the above complex model (see figure 4). The key parameter describing the trench profile with variable diameter **D(L)** is the generalized aspect ratio **A(L)** as a function of depth **L**:

$$A(L) = \int_0^L dx / D(x) \qquad (1)$$

The etch rate **E(L)** at the trench bottom is a product of the local halogen concentration **c(L)** and the ion assisted reactive sticking coefficient **s(L)**:

$$E(L) = s(L)\, c(L) \qquad (2)$$

s itself depends on aspect ratio and profile and describes the ion energy dissipation and ion intensity variation:

$$s(L) = s_0\, f(A) \left(D(0)/D(L)\right)^2 \qquad (3)$$

with $\mathbf{s_0}$ the planar reactive sticking coefficient, **f(A)** the transport loss and the last term a scaling factor for non-cylindical trenches.

The etchant concentration **c(L)** at the trench bottom is related to **c(0)** at the trench opening via a conductance term:

$$Lag_{Knudsen}(s, A) = \frac{1}{1 + s\,A/2} \qquad (4)$$

Finally the etchant concentration at the trench opening **c(0)** depends on the concentration in the chamber via a loading term $\mathbf{Lag}_{Boundary}$ and is calculated from trench open area **α**, gas flow velocity **v**, and partial pressure **p** with functional parameters using fluid flow simulation:

$$c(0) = c(chamber)\, Lag_{Boundary}(v, p, \alpha) \qquad (5)$$

To account for selectivity dependence on the etch rate of silicon and BSG mask, the etch model for the oxide hard mask also assumes a redeposition on the mask which is proportional to the amount of etched silicon.

Calibration with data

Trenches of several generations with different ground rules have been etched into silicon using an oxide hard mask [1]. The dependence of aspect ratio on time was measured by series of partial etch experiments and compared to results of the 140nm generation. Note that the only free parameters in the compact model are $\mathbf{s_0}$ and **f(A)**. These are calibrated only *once* for all generations. The comparison of the experimentally obtained etch rates and the compact model is shown in figure 5.

In another series of experiments, bottle shaped profiles were generated by widening the trench below a depth of 1.5μ by suitable adjustment of the RIE-process conditions. The measured as well as the calculated etch rates for several bottled trenches are shown in figure 6. As can be seen the etch rate dependence on profile is readily accounted for by the compact model. Note that while the etch rate decreases with bottle diameter (CD), the amount of redeposited material increases and in turn improves the selectivity of the mask (see figure 7).

Optimization

Using the calibrated compact etch model the optimum trench profile can be identified taking different objectives like cost and capacitance into account. Figure 8 for example shows the etch depth of the investigated class of RIE bottles for constant and maximum etch times. These simulations indicate that for constant etch time a slightly tapered trench yields the maximum etch depth. On the other side the maximum etch depth for a certain consumption of the oxide hard mask is reached for trenches with a pronounced bottle.

Conclusion

We have developed a feature scale model for the etch rates and profiles of deep trench capacitors both as a compact model and a high level model. A comparison with experimental data has shown that the model describes the etch rates and trench profiles quantitatively. This enables us to find optimal trench capacitor with respect to the profile, the etch time, and the process costs. Both from feature scale simulation as well as from etch data it is concluded that there is no limit for the etch rate of deep trenches in the next DRAM generations.

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References

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(2) J.Sethian, „Level Set Methods“, Cambridge University Press, 1996
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(5) M.Kratzer, MRS Symp. Proc. 677, AA 5.6., 2001

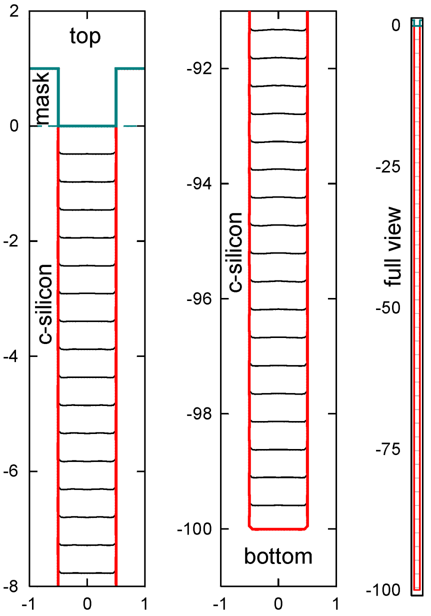

Figure 1: Front moving under an ideally collimated, etching particle beam. Even at an aspect ratio of 100 no numerical artifacts are introduced by the level set front propagation. The left and middle figures show 8% of the upper and lower part of the trench; the full view is given in the right figure.

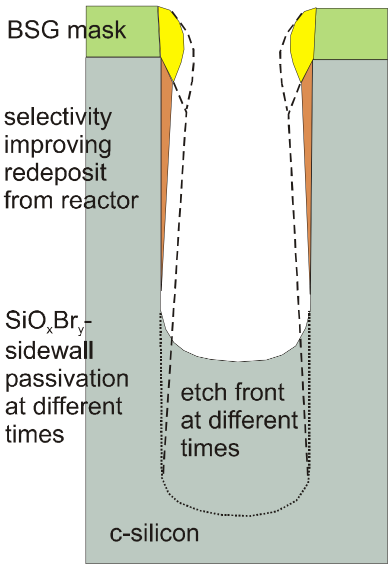

Figure 2: Schematic picture of the silicon etch mechanism: profile control is mainly due to SiO_xBr_y sidewall passivation. Selectivity improvement is due to redeposit of etch product.

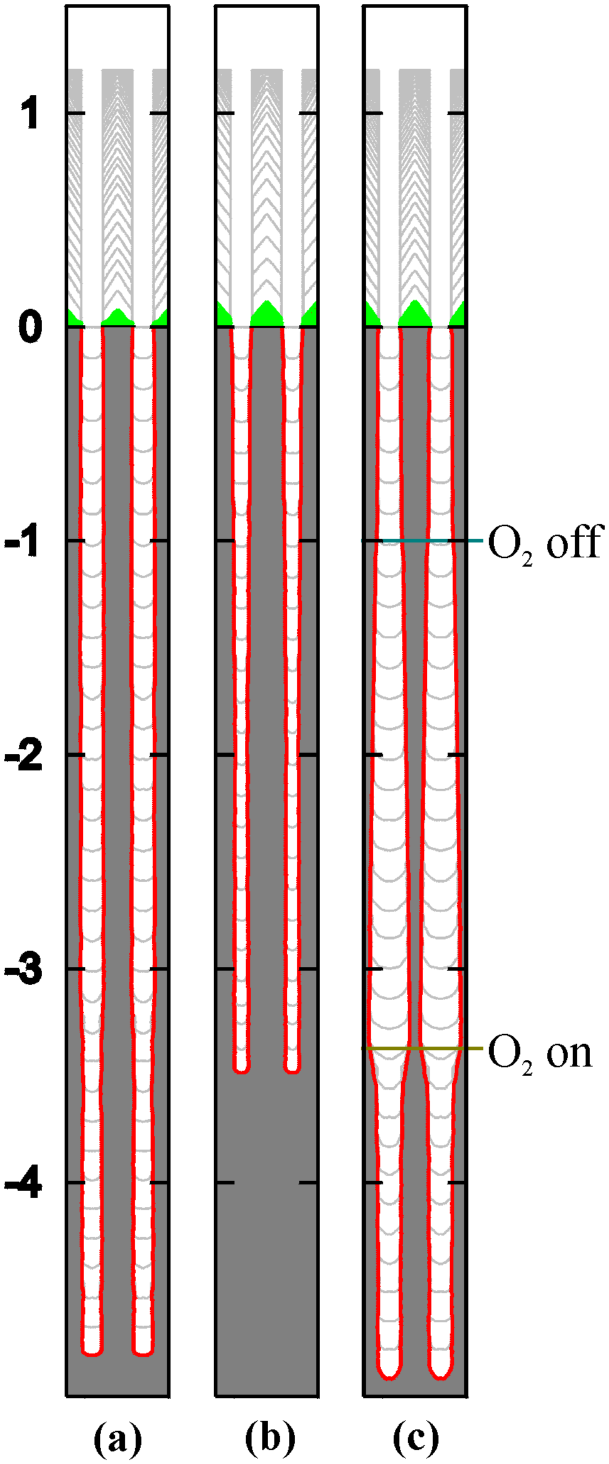

Figure 3: deep trenches "etched" with (a) optimum oxygen flux leading to a nearly straight trench profile, (b) excessive oxygen flux leading to a tapered profile, and (c) variable oxygen flux under otherwise fixed conditions leading to a partially bottled profile.

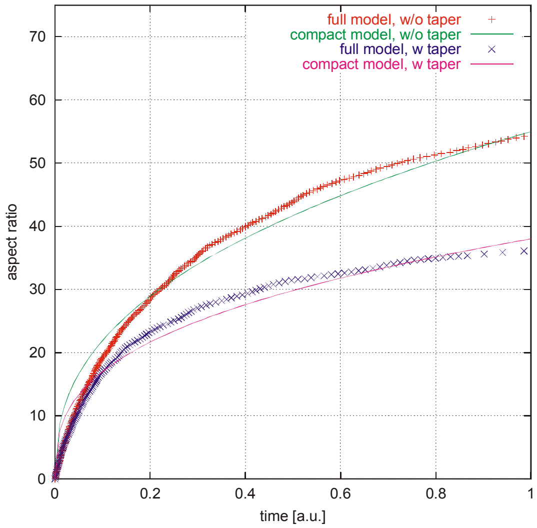

Figure 4: Comparison of the full and compact etch models for an untapered and a tapered trench.

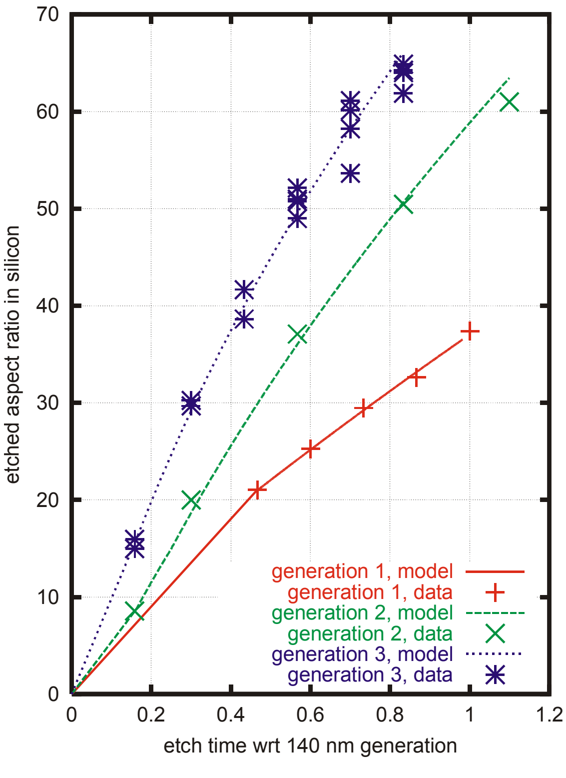

Figure 5: Partial etch data for several technology generations measured in units of etch time wrt. 140nm generation. The data is used for the universal calibration of the compact model. The calibration yields a high reactive sticking coefficient and only moderate energy dissipation of the ions.

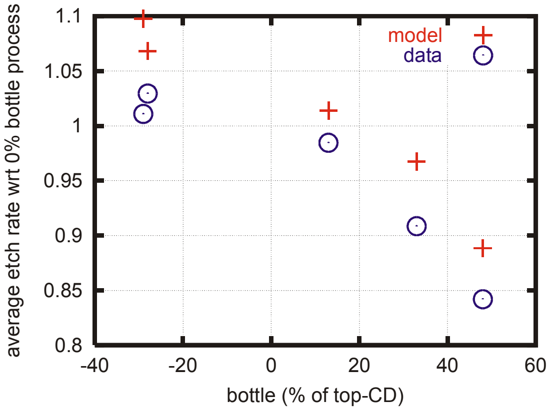

Figure 6: Average etch rates of trenches which are bottled below 1.5µ as a function of widening.

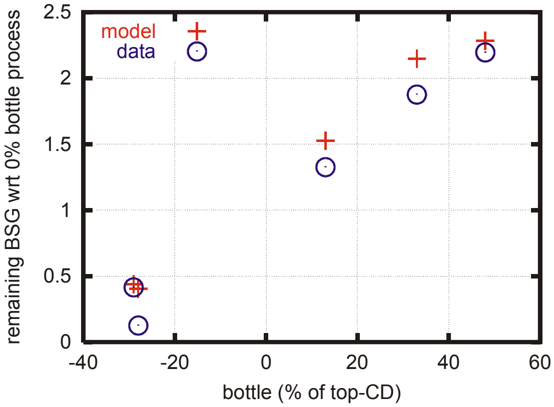

Figure 7: Remaining oxide hard mask after fixed process time is thicker for bottled trenches due to a larger amount of redeposited material. The remaining thickness is measured relative to a reference mask thickness.

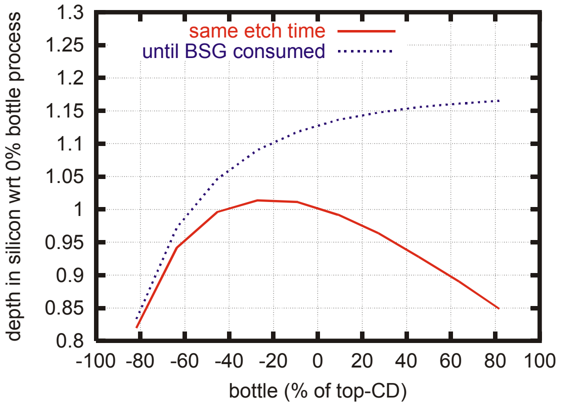

Figure 8: Optimization of bottle shape and AR for a bottle starting at 1.5 mu depth: the maximum depth for a given time is achieved for a slightly tapered trench whereas the maximum capacitance is achieved for a bottle with longer process time.