The influence of surface currents on pattern-dependent charging and notching

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Surface charge dissipation on insulator surfaces can reduce local charging potentials thereby preventing ion trajectory deflection at the bottom of trenches that leads to lateral sidewall etching (notching). We perform detailed Monte Carlo simulations of pattern-dependent charging during etching in high-density plasma systems with the maximum sustainable surface electric field as a parameter. Significant notching occurs for a threshold electric field as low as 0.5 MV/cm or 50 V/μm, which is reasonable for the surface of good insulators. The results support pattern-dependent charging as the leading cause of notching and suggest that the problem will disappear as trench widths are reduced. © 1998 American Institute of Physics. [S0021-8979(98)04614-3]

I. INTRODUCTION

Pattern-dependent charging is a serious problem in high-density plasma (HDP) etching of gate electrodes and metal interconnect lines because it can cause apparent sidewall irregularities (notching, bowing, etc.) and latent gate oxide degradation. Since the latter form of damage is feared to impede progress toward smaller critical dimensions, the interest in plasma-induced charging during etching has skyrocketed in the past few years as inferred by the large number of publications on charging damage. Pattern-dependent charging originates in the directionality difference between ions and electrons as they cross the plasma sheath and, subsequently, interact with mixed conducting and insulating microstructures.

The prevailing cause of the notching effect is believed to be the charging of the exposed SiO2 surface at the bottom of cleared trenches between gate electrodes, which can lead to ion trajectory bending and lateral sidewall etching. When SiO2 surface charging is reduced, e.g., by decreasing the thickness of the gate oxide so that electron tunneling becomes important, notching is eliminated. Surface charging could also be reduced by surface conduction. In our original paper on the notching effect, surface currents were neglected; it was realized then and pointed out that this assumption may have led to an overestimation of the surface potentials and could cast doubt on the proposed notching mechanisms. Although the calculated maximum surface electric fields (3–5 MV/cm) did not exceed the threshold for breakdown of bulk SiO2 (~10 MV/cm), they appear to be adequate for field emission of electrons at the triple junction (the interface where the polysilicon electrode, oxide, and vacuum are in close proximity) which could directly neutralize the positive charge accumulated on the oxide in the vicinity of the polysilicon sidewall foot. Electron emission at the triple junction has been suggested as the first step for surface breakdown (flashover) of insulators, which is known to occur for electric fields much lower than bulk breakdown, especially in the presence of surface adsorbates or photon (UV, x-ray) irradiation. While surface flashover may be an extreme case, surface currents could also flow by subsurface conduction, where electrons are injected and propagate in a conduction band of the insulator. With the exception of slow charge leakage (when surface charging is unstable), such mechanisms for surface charge dissipation are typically controlled by an electric field threshold, denoted here by , which determines the maximum charging potential that can form on the surface of an insulator. Irrespective of the surface conduction mechanism, , becomes the crucial parameter that controls the ion dynamics in the trench. Thus, the fate of notching mechanisms based on ion deflection depends on how readily surface currents can reduce charging potentials at the trench bottom.

Although there is overwhelming evidence in the literature to link pattern-dependent charging with notching, surface currents could diminish the importance of charging effects thereby lending credibility to other (nonelectrostatic) mechanisms to explain notching. For example, Flamm proposed that notching is caused by background Cl atoms that spontaneously etch the polysilicon at the bottom, where the protective sidewall blocking layer is removed by oxygen, liberated from the exposed SiO2 by ion bombardment. Based on the observation that in beam experiments notching was enhanced by mechanically stressing the polysilicon lines, Chang and Sawin corroborated the idea of spontaneous etching of polysilicon by providing an explanation for the larger etch rate near the polysilicon-oxide interface, where residual tensile stress is most pronounced. Evidence of such mechanical effects, combined with concern over the large potentials calculated in the absence of surface currents, led these researchers to the conclusion that “stress at the polysilicon-oxide interface is a major factor in the formation of the notch [while] the deflection of ions by feature charging is not sufficient to account for notching.” Thus, techniques that reduce the residual stress in the polysilicon film,
such as annealing or varying the polysilicon deposition conditions, could offer new approaches to preventing notching. Although mechanical effects may be contributing to notch enhancement, they could not be a ‘‘major factor’’ as they fail to explain the fundamental asymmetry of notching; the notch appears typically only on the inner side of the edge line. In fact, none of the dependencies of notching on feature aspect ratio, mask material and thickness, electron temperature, bias voltage and frequency, and plasma power pulsing could be explained by stress at the polysilicon-oxide interface.

The crucial role of surface currents on pattern-dependent charging is the subject of the present paper. We will systematically investigate the effect of the threshold, $E_s$, for surface charge dissipation at the SiO$_2$ surface on charging potentials and notching. We shall demonstrate that reducing $E_s$ results in lower surface potentials at the trench bottom which, however, are still sufficient to cause ion deflection and notching. Notches, similar to those simulated for the case with no surface conduction, can form for voltage gradients as low as 0.5 MV/cm or 50 V/$\mu$m, a reasonable value for the surface of good insulators.

II. SIMULATION DETAILS

When surface currents are not important, the charging distribution in the trench does not change significantly during notch formation and evolution. As a result, one need only focus on the notch area and deal with the charging of the newly exposed SiO$_2$ surface as the notch apex advances. This approach reduces the computational complexity and was followed in our previous work. When surface currents are permitted to flow (subject to a threshold surface electric field), the potential distribution along the bottom surface is modified as the sidewall of the edge line (at low equipotential) retreats. The potential boundary condition along the bottom surface ($V_{b}$) changes, thus requiring that the Laplace equation, $\nabla^2 V = 0$, is solved in the whole domain between the features, including the area of the evolving notch. Now, both ion and electron trajectories must be followed to calculate the continuously evolving charging distribution. Fortunately, the time scale for reaching steady-state charging is still orders of magnitude faster than that for profile evolution, which allows decoupling of the two calculations for sufficiently small time steps. As before, the profile is advanced in a pseudo-steady-state manner: A charging distribution is calculated for a given position of the notch and then is used to deflect ions that reach the sidewall until the notch apex is advanced by one cell in the computational domain. Charge accumulation by both ions and electrons at the exposed surfaces must be monitored during etching, so that new potential boundary conditions can be calculated at the end of each etching step. Surface currents are allowed to flow when the potential gradient along the surface exceeds the threshold electric field. Then a fractional charge, proportional to the potential gradient across neighboring cells, is allowed to flow in the direction of the gradient, modifying the potentials of both cells. The proportionality constant must be sufficiently small to prevent potential oscillations. This procedure is repeated for all cells along the SiO$_2$ surface until there are no potential gradients exceeding $E_s$. The charge flow to the polysilicon lines may modify their potentials and, therefore, it also must be accounted for.

A schematic of the microstructure geometry modeled is shown in Fig. 1. The microstructure and plasma parameters, and the computational domain employed in our paper on the notching effect are taken to be identical for the present study. The only difference consists in using the refined mesh of square cells ($200 \times 200$ cells/$\mu$m$^2$) for both the charging and etch profile evolution calculations. Surface currents are allowed to flow along the SiO$_2$ surface at the bottom of trenches and open areas, subject to a threshold for surface charge dissipation, which will be varied from 0.2 to 2.0 MV/cm. The polysilicon surfaces are taken to be perfect conductors. The photoresist (mask) is presumed to be a perfect insulator; thus, no surface currents will be allowed to flow during plasma exposure. Since potential gradients along the mask sidewalls are typically less than 0.5 MV/cm, this assumption is very reasonable. The oxide thickness is assumed to be >100 nm; thus, we emphasize cases of severe notching, where tunneling currents are too small to play a role in notch reduction.

III. RESULTS

The steady-state charging potential distribution in the edge trench reveals the perturbation in the local ion dynamics occurring as a result of surface charging. Gradients on this potential surface are a measure of the electric field that influences ion motion. Figure 2 compares the charging potential distributions for decreasing values of $E_s$ along the bottom SiO$_2$ surface. The plots describe results for a perfectly etched trench, before notching commences; the equipotential of the edge line is also shown as a flat surface to the right, for $X$-axis values between 0.0 and 0.5 $\mu$m (as defined in Fig. 1). We remind the reader that in the absence of surface currents, the potential distribution in the trench was asymmetric, with a pronounced peak (of about 58 V for the same conditions) near the sidewall foot of the edge line. Such distributions also occur for $E_s > 3$ MV/cm. However, a threshold of 2.0 MV/cm already allows surface currents to reduce considerably the maximum potential at the SiO$_2$ surface, as shown in Fig. 2(a). Notice, though, that the potential surface further away from the trench bottom is tilted toward
the edge line; thus, ions traversing the trench region are still subjected to a transverse electric field in the same direction. As before, the asymmetry results from the lower potential of the edge line, maintained by the greater electron irradiation of the outer sidewall. The potential gradient is large enough to impart sufficient energy to the deflected ions so that they can etch the sidewall and begin forming the notch. Remarkably, there is also a potential gradient toward the neighboring line which, however, is too small to result in ion energies sufficient for etching the sidewall.

Decreasing $E_s$ to 1.0 MV/cm eliminates the potential peak by the sidewall and shifts the broad peak of the distribution toward the center of the trench [Fig. 2(b)]. Note that the overall shape of the potential surface remains unchanged; the potential gradient toward the edge line is still larger than toward the neighboring line. When $E_s=0.5$ MV/cm, the intertrench potential distribution assumes a pyramidal shape, shown in Fig. 2(c), with a peak that no longer appears in the vicinity of the notch but rather closer to the neighboring line. The peak value is considerably reduced from that for $E_s=2.0$ or 1.0 MV/cm. A further decrease in $E_s$ shifts the peak even closer to the sidewall of the neighboring line; for $E_s=0.2$ MV/cm the potential distribution becomes planar with a slope of exactly 0.2 MV/cm toward the edge line [Fig. 2(d)]. These observations suggest that notching will decrease as surface charge dissipation becomes more and more facile.

It is instructive to continue at this point with the potential distributions after significant overetching; discussion of the corresponding notch profiles is postponed to the next paragraph. Overetching time is extremely difficult to compute in the absence of specific information about the surface condition at the sidewall. The horizontal etch rate must be measured experimentally to calibrate the simulation; in the absence of such measurements, we let the profile evolve by launching an arbitrary number of ions, which will be held constant for all cases discussed below. Figure 3 compares the modified charging potential distributions after a fixed overetching time, and must be viewed in conjunction with Fig. 2. For $E_s=2.0$ MV/cm (or larger), charging of the bottom surface has increased significantly. As Fig. 3(a) illustrates, the potential distribution becomes highly structured and asymmetric, reminiscent to that calculated when surface

**FIG. 2.** Three-dimensional charging potential distributions in the edge trench, including the edge polysilicon line, at the onset of overetching. Results are shown as a function of the threshold for surface charge dissipation ($E_s$): (a) 2.0, (b) 1.0, (c) 0.5, and (d) 0.2 MV/cm. The axes are defined in Fig. 1.
currents were neglected. Remarkably, the potential peak (55 V) appears in the notch region, that is, under the polysilicon line. Note that the ion deflection mechanism that slows down ions in the direction normal to the wafer and accelerates them in the parallel direction is still operational. Decreasing $E_{\text{s}}$ to 1.0 MV/cm [Fig. 3(b)], lowers the potential maximum (to 32 V), as expected; the peak now appears just outside the notch region. The potential distribution is still asymmetric about the trench centerline. Lower values of $E_{\text{s}}$ (i.e., 0.5 and 0.2 MV/cm) result in distributions that differ only slightly from those observed at the onset of overetching, as would be expected for very little or no notching at all.

Profile evolution is performed by considering the same mechanisms and procedures, described in detail in our original paper on notching. Etching of the neighboring sidewall is not simulated to decrease the computational cost; the inward tapering, seen when surface currents were neglected, becomes considerably smaller when $E_{\text{s}}$ is decreased, thus reducing its influence on charging potentials. Sequential notches were neglected. Remarkably, the potential peak (55 V) appears in the notch region, that is, under the polysilicon line. Note that the ion deflection mechanism that slows down ions in the direction normal to the wafer and accelerates them in the parallel direction is still operational. Decreasing $E_{\text{s}}$ to 1.0 MV/cm [Fig. 3(b)], lowers the potential maximum (to 32 V), as expected; the peak now appears just outside the notch region. The potential distribution is still asymmetric about the trench centerline. Lower values of $E_{\text{s}}$ (i.e., 0.5 and 0.2 MV/cm) result in distributions that differ only slightly from those observed at the onset of overetching, as would be expected for very little or no notching at all.

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The simulated profiles are consistent with the initial (Fig. 2) and final (Fig. 3) potential distributions in the trench.
for each case of $\bar{E}_s$. However, it is instructive to consider in Fig. 5 the time evolution of the potential distribution along the bottom SiO$_2$ surface, in conjunction with the profile sequences shown in each panel of Fig. 4. The initial potential distribution, before notching starts, is also shown. Figure 5(a) corresponds to $\bar{E}_s=2.0$ MV/cm and illustrates how the peak in the potential distribution by the sidewall foot increases significantly with time and shifts under the polysilicon as the notch evolves. Note that the potential drops linearly from the peak location to the notch boundary with the SiO$_2$ surface. Moreover, for all cases considered, the potential gradient defined by the straight lines is exactly equal to 2.0 MV/cm, that is, the location of the potential peak shifts in unison with the notch apex. The behavior is identical for $\bar{E}_s=1.0$ MV/cm [Fig. 5(b)] although the charging potential does not increase as much. The straight lines connecting the potential peak to the notch boundary with the SiO$_2$ surface have a slope of exactly 1.0 MV/cm. The situation is repeated for $\bar{E}_s=0.5$ MV/cm [Fig. 5(c)], although the potential peak remains in the vicinity of the trench centerline. Note that the slope of the lines connecting the potential peak to polysilicon/SiO$_2$ interface of both the edge line and the neighboring line is fixed at 0.5 MV/cm. Finally, the lines merge together for $\bar{E}_s=0.2$ MV/cm [Fig. 5(d)], as expected from the lack of notching. The potential gradient from the neighboring line to the edge line is now exactly equal to 0.2 MV/cm.

**IV. DISCUSSION AND IMPLICATIONS**

We have argued elsewhere that surface currents along the surface of SiO$_2$ must exist, as a result of the ability to
etch deep trenches in field oxide. Then, the threshold \( E_s \) for surface charge dissipation on the insulator surface becomes a crucial parameter for pattern-dependent charging. For established mechanisms of charge dissipation, the magnitude of \( E_s \) depends strongly on the insulator material (dielectric constant, band gap, secondary electron impact energy, etc.), the length of surface between electrodes, the surface roughness, the surface temperature, the chemical nature and density of the adsorbed gas on the surface, and the illumination of the surface by photons. To the best of our knowledge, no measurements of \( E_s \) have been reported for thermal- or chemical-vapor-deposited SiO\(_2\) exposed to chlorine plasmas. There is, however, a vast literature on surface flashover of quartz and various grades of Pyrex\textsuperscript{TM}, used in vacuum feedthrough applications, where the adsorbed gas is usually water or air. A typical value of the flashover field for such glasses is \( \approx 0.5 \) MV/cm, as discussed by Blaise and Gressus.\textsuperscript{9} Such low electric fields are measured for insulator surface lengths between electrodes of at least a few millimeters. It is extremely important to report the surface length, because of a well-known nonlinear dependence of the flashover voltage on surface length. The relationship, developed theoretically by Pillai and Hackam\textsuperscript{15} for the prevailing mechanism of surface flashover (surface discharging in a layer of desorbed gas from the insulator surface),\textsuperscript{8} predicts that the surface electric field required to cause flashover depends on the length of the insulator to a power law of \( \approx 0.5 \). The inverse square-root dependence has been validated experimentally for many insulator materials to “give a correct description of the decrease in dielectric strength of the surface with increasing insulator length.”\textsuperscript{15} When applied to thinner insulators, the relationship suggests that larger surface electric fields are required for surface flashover. For example, Pillai and Hackam\textsuperscript{15} reported a flashover voltage of 40 kV for a 2-mm-thick quartz disk, corresponding to 0.2 MV/cm; using the aforementioned relationship, a flashover field of \( \approx 9 \) MV/cm is predicted for a (quartz) surface length of 1 \( \mu \)m under the same measurement conditions. This value approaches the bulk breakdown of good quality oxide,\textsuperscript{7} which suggests that the relationship may not be extrapolated to insulator lengths in the micron regime. Although the region of applicability was not discussed,\textsuperscript{15} we can think of no physical reason why it should not apply to lengths in the vicinity of 100 \( \mu \)m, yielding fields of about 1 MV/cm. The point of this discussion is that significantly larger electric fields could be supported along the surface of SiO\(_2\) at the bottom of narrow trenches (micron regime) than those reported for typical feedthrough applications (millimeter regime).

There are other reasons to corroborate larger values of \( E_s \) for the surface of SiO\(_2\) exposed to chlorine plasmas. Donnelly and Layadi\textsuperscript{16} have shown experimentally that, after brief etching of thermal SiO\(_2\) in a Cl\(_2\) plasma at moderate ion energy, a surface layer (\( \approx 1–2 \) nm) forms which contains a significant amount of chlorine. The oxygen concentration in this layer is depleted, indicating that chlorine displaces oxygen to form a silicon oxychloride (SiO\(_x\)Cl\(_{1-x}\)). Although its properties are unknown, the SiO\(_x\)Cl\(_{1-x}\) film could have a lower relative permittivity \( \kappa \) by analogy to fluorinated oxides, which are currently pursued as low-\( \kappa \) dielectrics. There is an inverse relationship between the relative permittivity \( \kappa \) of a material and its flashover voltage,\textsuperscript{8,9} which suggests that the SiO\(_2\)Cl\(_{1-x}\) film may have a higher flashover voltage than does SiO\(_2\). Furthermore, chlorine incorporation is expected to significantly roughen the surface of SiO\(_2\); surface roughening has been known for decades to be an effective way to raise the surface breakdown voltage of smooth insulators.\textsuperscript{17}

Thus far we have not considered the geometric differences between typical surface flashover cases and the particular situation encountered during overetching and notch formation. The potential peak in the vicinity of the polysilicon sidewall, observed in the simulations for \( E_s \approx 1 \) MV/cm, forms because of direct ion bombardment from the plasma. Obviously, positive surface charging pre-exists in the latter situation, while it forms as a result of the secondary electron emission avalanche during flashover.\textsuperscript{8,10} Thus, field emission of electrons from the triple junction could occur directly onto the charged spot; the large charge density would then prevent secondary electrons from being re-emitted. This provides a mechanism for supplying electrons without surface breakdown and suggests that larger surface electric fields may be tolerated in the vicinity of the notch without flashover. Despite the uncertainty in the maximum sustainable potential gradient along the surface of the oxide, the parametric study presented above dispells the notion that large charging potentials are required to induce ion deflection at a scale capable of causing notching. Indeed, even for a potential gradient as low as 0.5 MV/cm or 50 V/\( \mu \)m,\textsuperscript{18} the potential distribution in the trench [Fig. 2(c)] is capable of deflecting and accelerating ions to the sidewall so that deep notches can be formed. This is further demonstrated in Fig. 6, which extends the last profile of Fig. 4(c) in increments of equal overetching times. Of course, larger overetching times are required for smaller values of \( E_s \) to reach a certain notch depth. Note that the notch shape looks very similar to that obtained when surface currents were neglected.

If surface currents along SiO\(_2\) surfaces during overetching in high-density plasmas are not to be disputed, what is the validity of our published work on the influence of the electron temperature,\textsuperscript{19} aspect ratio,\textsuperscript{20} and other parameters on notching? Although surface currents were previously neglected, the potential gradients obtained never exceeded 5 MV/cm.\textsuperscript{5} The potential distributions were not unlike those for \( E_s \approx 2.0 \) MV/cm presented in this study, with the exception of the distribution at the onset of overetching. Thus, the
mechanisms and trends presented then should still hold, even when surface currents are allowed to flow. The same applies to lower thresholds for surface charge dissipation. Indeed, the effect of the electron temperature and aspect ratio, for example, was to increase the polysilicon equipotentials, which perturb the potential distribution in the trench. Even when surface currents limit the maximum potential gradients on the SiO$_2$ surface, the line potentials will increase with aspect ratio or electron temperature, shifting the potential distribution higher without changing the gradients. Then, the flux of the deflected ions to the sidewall of the edge line will increase accordingly as more incident ions are slowed down, resulting in deeper and broader notches. But how could the trends remain identical, if the potential maximum by the edge trench is so much larger in the absence of surface conduction? The peak potential affects primarily the most energetic of the incident ions; the majority of the ions have significantly lower energies and are deflected before they approach the potential maximum. One could artificially reduce these potentials by more than 50% and still observe substantial notching. We thus stand by our proposed mechanisms and predicted trends of our published work; they should be valid in the presence of surface currents subject to a threshold electric field as low as 0.5 MV/cm.

Since $E_\text{c}$ is a gradient, the value of the maximum potential on the trench bottom surface scales linearly with the trench width. In other words, the surface charging potential at the trench bottom must decrease as the trench becomes narrower, with a concomitant reduction in notching. Then, the sequence of profiles of Figs. 2 and 3 could roughly correspond to the same threshold electric field, say 2.0 MV/cm [Figs. 2(a) and 3(a)] but decreasing trench width to 0.25 μm [Figs. 2(b) and 3(b)], 0.12 μm [Figs. 2(c) and 3(c)], and 0.05 μm [Figs. 2(d) and 3(d)]. Consequently, as critical dimensions are getting smaller and the packing density of devices on a chip increases, notching should decrease continuously until it disappears altogether! The generation of devices where notching is completely eliminated depends on the magnitude of the threshold for surface charge dissipation along the surface of the dielectric material on which the interconnect lines are formed. The latter does not apply to polysilicon gates formed on thin gate oxides because tunneling currents reduce pattern-dependent charging and eliminate notching independent of surface currents.

Our simulation results suggest interesting experiments that could shed additional insight into the role of surface currents along insulators on plasma processing. For example, one could focus on the correlation between oxide doping level and the notch depth. Doping introduces defect states in the band gap of the insulator, changes the bulk dielectric constant, and should also influence surface charge dissipation; one would then expect less notching for more heavily doped oxide. Further, notching could be used to estimate $E_\text{c}$ for various insulators (e.g., SiN, SiOF, etc.) in realistic environments by etching the same polysilicon line-and-space structures formed on the different insulator material and comparing the extent of notching to that for thermal oxide.

V. CONCLUSIONS

Surface currents can play an important role in reducing charging on the surface of insulators at the bottom of trenches during overetching. The maximum electric field that can be sustained along the surface, in conjunction with the equipotentials of the polysilicon (or metal) lines that confine the trench, determine the potential distribution in the trench and the perturbation in the local ion dynamics. Notching can be reduced by decreasing the threshold electric field for surface conduction. The continuous reduction in critical dimensions for larger device packing density is expected to decrease the importance of charging at the bottom of narrower trenches as the same threshold field for surface conduction will produce lower absolute charging potentials, thereby influencing the in-trench ion dynamics to a lesser extent.

The parametric study presented herein suggests that pattern-dependent charging is still the main cause for notching even when surface conduction limits the maximum sustainable surface electric fields to values as low as 0.5 MV/cm or 50 V/μm. Such fields appear to be reasonable for the rough chlorinated oxide surface encountered during overetching of gate electrodes in high-density plasmas. The significance of charging effects in plasma processing warrants an experimental effort to measure thresholds for surface conduction on SiO$_2$ in submicron geometries while exposed to realistic plasmas.

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18. An estimate from etching boro-phospho-silicate glass in a fluorocarbon plasma yielded a threshold of 0.42 MV/cm for charge dissipation along the oxide surfaces; see Ref. 14.