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Conductance considerations in the reactive ion etching of high aspect ratio features

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Very simple vacuum conductance arguments indicate that in the reactive ion etching of high aspect ratio features, the conductance is adequate to allow etch products to flow out of the feature without building up a pressure which would allow gas phase collisions to become important. On the other hand, the conductance can be expected to limit the flow of the reactive species to the bottom of the feature where the etching is taking place, thus creating the possibility of an etch rate dependence on the aspect ratio of the etched feature.

The reactive ion etching of features with large aspect ratios is becoming more and more important in various areas of microelectronics processing.[1–8] The aspect ratio is simply the depth/diameter for a hole or the depth/width for a trench. The etching of these high aspect ratio features poses very stringent requirements on the etch process and various phenomena not normally observed in the etching of low aspect ratio features become very important. The most significant of these is the effect of slightly nonparallel incident ion trajectories caused by ion-neutral collisions in the sheath. These slightly diverging trajectories give rise to a bowing or barrelling[5,9,10] in the shape of the etched feature as is illustrated in Fig. 1. This is not to be confused with the well known undercutting of the mask [see Fig. 1 (middle)] often observed in reactive ion etching in which dimensional control is lost at the mask level. Figure 1 also illustrates another effect seen in the etching of high aspect ratio features which is enhanced lateral etching caused by ions scattered from the mask edge.[2,10,11]

The role of the feature conductance in the etching process is not as clear as the influence of ion trajectories. There are several examples of the etch rate of a high aspect ratio feature decreasing with the etch depth, or more generally, with the aspect ratio.[2,12,13] Whereas the possible role of feature conductance has been mentioned in this regard,[10–12] this etch rate dependence on aspect ratio has usually been attributed to nonparallel incident ion trajectories.[2,6,7,13] It is our opinion that the role of feature conductance should be considered more seriously than it has been and that is the objective of this letter.

The flow of gas into or out of the feature causes a pressure gradient between the top and the bottom which could, in turn, lead to different etch rates at these two locations. This is analogous to the flow of gas through tubes in vacuum systems. It is important to recall in this context that molecular flow conditions will always prevail in the small holes or trenches which are encountered in pattern transfer in microelectronic processing since the mean free path for gas phase collisions at the pressures used in reactive ion etching is much longer than the micrometer size features. Therefore, ideas developed in vacuum physics, which indicate that the gas flow is equal to pressure differential times a constant (the conductance), can be used to understand the present situation.

There are two ways in which the small conductance of a high aspect ratio feature might influence the etching process. The first way is to impede the flow of the gaseous etch product from the bottom to the top of the feature. This would influence the etch process only if the pressure increase at the bottom of the feature is great enough so that gas phase collisions become significant and interfere with the flow of incident ions and neutral etching species. This is very unlikely as can be demonstrated with a very simple estimate. The conductance of a short tube or trench is given by

$$C = 3.64AK(T/M_p)^{1/2},$$

where C is the conductance in ℓ/s, A is the cross-sectional area of feature in cm^2, and $K(z/d)$ is the probability that a randomly directed molecule incident on one end of a tube (or slot) will exit the other end. T is the temperature (kelvin) and M_p is the molecular weight of the etch product.

Tables of K for various aspect ratio tubes and slots can be found in standard texts on vacuum technology.[14,15] The pressure increase resulting from an etch rate of R μm/min at the bottom of a high aspect ratio feature is given by

$$\Delta P = 2.86\times 10^{-5}[nR\rho(M_pT)^{1/2}/KM_s],$$

where ΔP is in Torr, ρ is the density of the etched material ($\mathrm{g\,cm^{-3}}$), M_s is the molecular weight of the etched material, and n is the number of moles of gaseous etch product evolved in the etching of one mole of substrate material. If we consider Si etching at 1 μm/min in a cylindrical hole with a depth/diameter ratio of 10 ($K = 0.11$), then $P \cong 4$ mTorr. This is at least three orders of magnitude below the pressure at which gas phase collisions in these very small features become important.

The second way in which the conductance of the etched feature might influence the etching process is by limiting the flux of the etching species arriving at the bottom of the feature where the etching is taking place. In order to obtain an estimate for the magnitude of this effect, it is necessary to make some assumptions about the nature of the interaction of the etching species with the sidewalls of the etched feature. For simplicity it will be assumed that there is no etching of the sidewalls (reaction probability $S = 0$) and that the species are reflected diffusely. This is the standard assumption made in the calculation of conductances. The reaction probability on the bottom surface S will be a parameter.

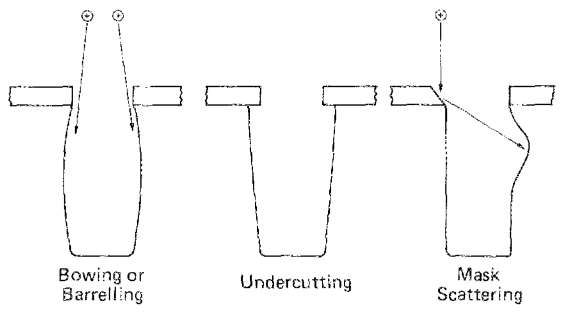

FIG. 1. Illustration of the problems encountered in the reactive ion etching of high aspect ratio features.

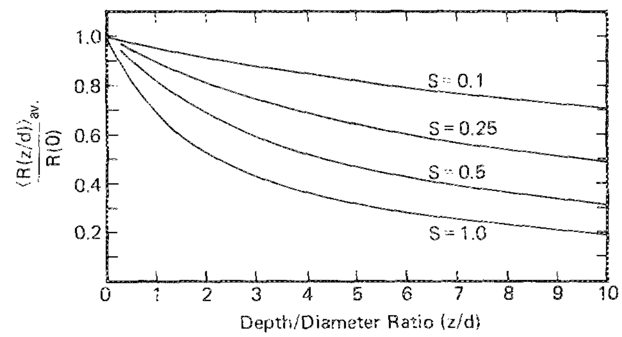

FIG. 3. Same as Fig. 2 except the etch rate is the average etch rate.

There is very little data on the magnitude of S even for the extensively studied gas-solid systems F-Si and Cl-Si. There are measurements of the reaction probability for F atoms on Si at saturation coverages of fluorine[16] but the quantity needed in reactive ion etching is the reaction probability at much reduced fluorine coverages. It is well established that the energetic ion bombardment which is essential for anisotropic etching reduces the steady-state halogen coverage by ion-assisted product formation (i.e., chemical sputtering). Thus, the reaction probability applicable in this discussion is probably somewhat less than the reaction probability for the etching species on an atomically clean surface but will usually be much larger than the reaction probability on a surface fully covered with chemisorbed etching species.

There are several ways to calculate the flux of species at the bottom of a closed hole ν_b, relative to the flux incident at the top end of the hole ν_t. Of course if there is no consumption at the bottom surface (i.e., etching), these fluxes will be identical. Possibly the most conceptually direct approach is to use conservation of gas flow and write an expression for the gas fluxes into and out of the closed feature and equate the difference to the etching reaction. This is done below:

$$\nu_t - (1-K)\nu_t - K(1-S)\nu_b = S\nu_b .$$

The first term in this expression is just the randomly directed incident flux, the second term represents the fraction of the incident flux which is reflected back out of the feature without reaching the bottom surface, the third term represents the species which reach the bottom surface but do not react and eventually escape through the open end, and the term on the right side of the equation represents the species consumed by etching the bottom surface. Since the etch rates will be proportional to the fluxes of etching species, the ratio of the etch rate at the bottom of a feature of depth z and diameter d, $R(z/d)$, to the etch rate at the top of the feature $R(0)$ will be

$$\frac{R(z/d)}{R(0)} \equiv \frac{\nu_b}{\nu_t} = \frac{K}{K+S-KS} .$$

This function is plotted versus the aspect ratio for circular holes in Fig. 2 for several values of the reaction probability S. It is important to point out that the Rs are the instantaneous etch rates and in order to facilitate comparisons with experimental data, the average etch rates have been calculated and are shown in Fig. 3. These data should be compared with experimental etch rates determined from the total etch depth divided by the etching time. The strong dependence of this function on the essentially unknown reaction probability makes it very difficult to establish conclusively the importance of this conductance effect. However, it is difficult to understand why the conductance would not play a role in determining the etch rate at the bottom of a high aspect ratio feature unless the reaction probability S is very small. A small reaction probability would be expected if the ratio of the flux of neutral etching species to the flux of energetic ions is very large or if the ion energies are very low (i.e., relatively high-pressure operation).

Note in Fig. 3 that the etch rate is influenced by this conductance effect even for low aspect ratio features (i.e., $z/d<1$). This may well be the reason for the often-observed etch rate dependence on feature size where small features etch more slowly than large ones (the so-called pattern factor).

An interesting situation can be anticipated if the incident neutral flux is highly collimated so that there are no neutral-sidewall collisions for the incoming species. The unreacted species will be diffusely scattered from the bottom surface and a fraction of these will be returned to the bottom surface after colliding with the sidewall. Thus, the flux of etching species incident on the bottom surface will be larger than the flux incident on the top surface and therefore the etch rate should increase with increasing feature depth in

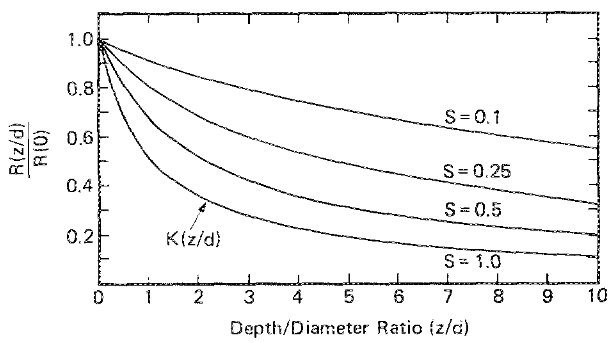

FIG. 2. Effect of the feature conductance on the instantaneous etch rate as a function of the feature aspect ratio for circular holes. The parameter S is the reaction probability of the etching species with the bottom surface of the feature. It has been assumed that the etching species are scattered diffusely from the sidewall and do not react with it.

this special case. Whereas the conductance effect for randomly arriving etching species decreases as the reaction probability S decreases (i.e., see Figs. 2 and 3), the conductance effect for highly collimated etching species increases with decreasing reaction probability with the ratio $R(z/d)/R(0)$ approaching $1/K$ as S approaches zero.

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