Study of Plasma-Surface Kinetics
And Feature Profile Simulation of
Poly-Silicon Etching in Cl_2/HBr Plasma

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Abstract

This work characterized the Cl_2/HBr ion-enhanced plasma-surface interactions with poly-silicon as a function of the gas composition, ion energy, ion incident angle and other important process parameters. A realistic inductively coupled plasma beam apparatus capable of generating ions and neutrals representative of a real commercial etcher was constructed and utilized to simulate accurately a high density plasma environment. Etching rate of poly-silicon, the oxygen effect and loading effect are quantified to better describe the etching of patterned poly-silicon in fabricating the gate electrode of a transistor in the VLSI manufacturing process. The kinetics model derived from these measurements are incorporated into a Monte Carlo based feature provile simulator, and profile evolution has been simulated under various processing conditions.

The realistic plasma beam was used to measure the etching yields of poly-silicon with Cl_2/HBr chemistry at different ion energies. The etching yields were found to scale linearly with $\left(\sqrt{E_{ion}}-\sqrt{E_{th}}\right)$, where the threshold energies, E_{th}, are 10 eV for both Cl_2 and HBr. The etching yields at different neutral-to-ion flux ratio were measured and the sticking coefficients are derived for reactive neutrals for Cl_2 and HBr. The sticking coefficient for the HBr system is lower probably due to the relatively larger size of the bromine atom compared with chlorine and its relatively lower chemical reactivity. The etching yields for mixed Cl_2+HBr plasma at different compositions were also measured. The etching yield by the HBr plasma beam is similar to the Cl_2 plasma beam, although the etching rate by the HBr plasma is about 40% lower due to the lower ion flux. The angular dependence of etching yield by both Cl_2 and HBr strongly suggests the mechanism of ion enhanced chemical etching. With Cl_2 plasma beam, the etching yield almost keeps constant until the off-normal ion incident angle increased to 45°, while with the HBr plasma beam, the etching yield starts dropping even with small off-normal angle. The etching yield by Cl_2+HBr plasma at different compositions exhibits a similar trend as pure HBr. The difference of angular dependent etching yield between Cl_2 and HBr might contribute to the difference of feature profile evolution in these two chemistries, i.e., more anisotropic etching in HBr plasma, as suggested by Monte Carlo feature profile evolution simulation.

The XPS peak for Cl(2*p*), Br(3*d*), and Si(2*p*) are integrated to quantify the relative concentration of different species on the sample surface after exposure to the plasma beam. The Cl coverage after etching with a pure Cl_2 plasma beam is about 1.4 times higher than the Br coverage after etching with a pure HBr plasma beam. The lower Br coverage is likely due to site blocking by coadsorbed H and adjacent adsorption site blocking by the larger Br atom. The Si(2*p*) was deconvoluted to differentiate Si(bulk), SiCl, $SiCl_2$ and $SiCl_3$. About 70% of the chlorine adsorbed onto the surface is in the form of di-and tri-chlorine. Similar results are observed for bromine. An inversion method was used to extract the depth profile from the angular resolved XPS measurement. The halogenation layer is about 15 – 25 Å thick, and the concentration of halogen decays exponentially as depth increases.

The effect of oxygen addition on the etching rate of poly-silicon was also studied. The etching rate has a different sensitivity to the oxygen addition with different surface composition. When the surface is chlorine rich, the etching rate is not sensitive to a small amount of oxygen added. When the surface is oxygen rich, the etching rate is more sensitive to oxygen addition. This explains why in a commercial etcher, adding a small amount of oxygen, does not much change the poly-silicon etching rate, but the silicon oxide etching rate decreases significantly; therefore the etching selectivity can be improved.

The loading effect was studied by adding $SiCl_4$ into the feed gas to simulate the effect of etching product buildup in a real commercial etcher. The etching yield by the Cl_2 plasma beam is significantly reduced by the $SiCl_4$ addition due to the deposition of Si-containing species. The etching yield decreases drastsically due to the ion enhanced deposition of Si-containing species, as the concentration of $SiCl_4$ is low. As the active sites created by ion bombardment are filled with $SiCl_x$, further reduction of etching yield is due to the chemisorbtion on nonactive sites, which is much slower than ion-enhanced deposition but more temperature sensitive. A kinetics model has been developed to account for the effect of both ion-enhanced deposition and chemisorbtion on nonactive sites mechanism. The model represents the experimental data quantitatively well.

Feature profile evolution of poly-silicon gate etching under different conditions were obtained by Monte Carlo simulation and compared with experimental measurements. The neutral-to-ion ratio was found to result in the variation of surface chlorination, which could influence the feature profile evolution. Different ion energy would result in different ion directionality and the surface chlorination, thus influence the feature profile as well. Other facts, such as the mask, angle, are also found to have some effects on the feature profile by our simulation, which agree with experimental results. The feature profile simulator was also used to simulate the dual damascene process, specifically the oxide fencing formation. The effect of various factors, including the via shape, etching selectivity, and etching chemistry was studied by the simulation and compared with experimental resuls from literature.

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