Recently, one of the critical issues in the etching processes of the nanoscale devices is to achieve ultra-high aspect ratio contact (UHARC) profile without anomalous behaviors such as sidewall bowing, and twisting profile. To achieve this goal, the fluorocarbon plasmas with major advantage of the sidewall passivation have been used commonly with numerous additives to obtain the ideal etch profiles. However, they still suffer from formidable challenges such as tight limits of sidewall bowing and controlling the randomly distorted features in nanoscale etching profile. Furthermore, the absence of the available plasma simulation tools has made it difficult to develop revolutionary technologies to overcome these process limitations, including novel plasma chemistries, and plasma sources.

As an effort to address these issues, we performed a fluorocarbon surface kinetic modeling based on the experimental plasma diagnostic data for silicon dioxide etching process under inductively coupled C4F6/Ar/O2 plasmas. For this work, the SiO2 etch rates were investigated with bulk plasma diagnostics tools such as Langmuir probe, cutoff probe and Quadruple Mass Spectrometer (QMS). The surface chemistries of the etched samples were measured by X-ray Photoelectron Spectrometer. To measure plasma parameters, the self-cleaned RF Langmuir probe was used for polymer deposition environment on the probe tip and double-checked by the cutoff probe which was known to be a precise plasma diagnostic tool for the electron density measurement. In addition, neutral and ion fluxes from bulk plasma were monitored with appearance methods using QMS signal. Based on these experimental data, we proposed a phenomenological, and realistic two-layer surface reaction model of SiO2 etch process under the overlying polymer passivation layer, considering material balance of deposition and etching through steady-state fluorocarbon layer. The predicted surface reaction modeling results showed good agreement with the experimental data.
With the above studies of plasma surface reaction, we have developed a 3D topography simulator using the multi-layer level set algorithm and new memory saving technique, which is suitable in 3D UHARC etch simulation. Ballistic transports of neutral and ion species inside feature profile was considered by deterministic and Monte Carlo methods, respectively. In case of ultra-high aspect ratio contact hole etching, it is already well-known that the huge computational burden is required for realistic consideration of these ballistic transports. To address this issue, the related computational codes were efficiently parallelized for GPU (Graphic Processing Unit) computing, so that the total computation time could be improved more than few hundred times compared to the serial version. Finally, the 3D topography simulator was integrated with ballistic transport module and etch reaction model. Realistic etch-profile simulations with consideration of the sidewall polymer passivation layer were demonstrated.

**Keywords:** GPU, feature profile simulation, plasma etch