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Molecular dynamics simulations of blanket and small feature etching in fluorocarbon- and fluorine-containing plasmas

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As device scale-down continues, fundamental understanding of etch mechanisms at very small dimensions (<10 nm) is becoming increasingly important for the development and control of future plasma processing steps. We utilize molecular dynamics (MD) simulations to examine the interactions of representative plasma species from typical fluorocarbon (FC) and F containing etch systems on Si substrates. Our current MD work examines the etching of very small (< 5 nm) features. By using an amorphous C masking layer (or confined beams of the desired dimension with no masking layer), ions (Ar^+, CF_x^+) and radicals (CF_x and F) were used to fabricate trenches and holes in Si substrates. The nature and formation of the feature sidewalls are examined in detail, and the limitations of hole size are explored, including the collapse of the masking layer at very small dimensions (∼2 nm) and the transport of etchants and products into and out of the feature. For the maskless confined beam experiments, etch limitations are primarily transport related as depth increases. In order to maintain pattern transfer fidelity and limit mask collapse, 'pulsed' etching was simulated by alternating bombardment of the surface with CF_x radicals and Ar^+ or Ar^+/F. The chemistries for this scheme were chosen to optimize selectivity between the C mask and the Si substrate. We compare the small feature simulations to our previous MD studies of blanket etching of Si with various FC/F/Ar^+ ratios. These simulations established a clear relationship between FC layer thickness and the Si etch yield at steady-state and showed semi-quantitative agreement with plasma experiments in the literature. We discuss how these effects translate to the Si yields in small feature etching, in relation to the surface compositions along the sidewalls and bottoms of the features.