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Combined plasma and molecular dynamics simulations for a better prediction of plasma surface interactions: Cryogenic etching of silicon with fluorine-containing gases STEFAN TINCK, ERIK NEYTS, ANNEMIE BOGAERTS, University of Antwerp, PLASMANT TEAM — A hybrid Monte Carlo-fluid plasma model as well as molecular dynamics (MD) simulations are applied together to obtain detailed information on surface reaction mechanisms during plasma processing. With this modeling setup, results on the surface behavior of fluorine plasma species etching Si wafers at room and cryogenic temperatures will be discussed. When numerically investigating low pressure plasmas used for microelectronics applications, one should always consider wall effects if possible. Especially in low pressure plasmas, where collisions with the reactor walls and wafer are quite probable compared to gas phase collisions, knowing at which rate the plasma species are lost or produced at these surfaces is of utmost importance. Unfortunately, the probabilities of wall reactions such as sticking, reflection, incorporation, etching or sputtering are often not well known. With MD, these surface reaction probabilities can be calculated and applied as input in the plasma simulation. In this modeling setup, surface probabilities as a function of surface temperature, chemical composition and reactor operating conditions are obtained and considered for the overall plasma simulation for a better description of the investigated plasma process.

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