Bridging technology between molecular dynamic simulation and density function theory for plasma etching process

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The plasma technology has attracted a great deal of attention as the next-generation semiconductor fabrication process strongly depends on it. Recently, the nanoscale fabrication process requires the basic knowledge of atomic scale phenomena in terms of surface damage and detailed surface kinetics. However, current computational technologies are difficult to simulate all the concerned regime of semiconductor materials. In this work, we demonstrated that the semiconductor fabrication process can be investigated reasonably with coupling strategies between molecular dynamic (MD) simulation and density functional theory (DFT). We used MD simulation based on reactive empirical bond order (REBO) for plasma etch process. The surface structures taken by the MD simulation results were separated to be an input of DFT simulation so that the stable atomic structure could be obtained. Finally, this approach could be verified with experimental data of the XPS taken from the plasma etched substrate. For this work, the detailed plasma conditions such as plasma-generated species were monitored by cut-off probe a quadrupole mass spectrometer (QMS).