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Hybrid molecular dynamics simulation for plasma induced damage analysis

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In order to enable further device size reduction (also known as Moore's law) and improved power performance, the semiconductor industry is introducing new materials and device structures into the semiconductor fabrication process. Materials now include III-V compounds, germanium, cobalt, ruthenium, hafnium, and others. The device structure in both memory and logic has been evolving from planar to three dimensional (3D). One such device is the FinFET, where the transistor gate is a vertical fin made either of silicon, silicon-germanium or germanium. These changes have brought renewed interests in the structural damages caused by energetic ion bombardment of the fin sidewalls which are exposed to the ion flux from the plasma during the fin-strip off step. Better control of the physical damage of the 3D devices requires a better understanding of the damage formation mechanisms on such new materials and structures. In this study, the damage formation processes by ion bombardment have been simulated for Si and Ge substrate by Quantum Mechanics/Molecular Mechanics (QM/MM) hybrid simulations and compared to the results from the classical molecular dynamics (MD) simulations. In our QM/MM simulations, the highly reactive region in which the structural damage is created is simulated with the Density Functional based Tight Binding (DFTB) method and the region remote from the primary region is simulated using classical MD with the Stillinger-Weber and Moliere potentials. The learn on the fly method is also used to reduce the computational load. Hence our QM/MM simulation is much faster than the full QC-MD simulations and the original QM/MM simulations. The amorphous layers profile simulated with QM/MM have obvious differences in their thickness for silicon and germanium substrate. The profile of damaged structure in the germanium substrate is characterized by a deeper tail than in silicon. These traits are also observed in the results from the mass selected ion beam experiments. This observed damage profile dependence on species and substrate cannot be reproduced using classical MD simulations. While the Moliere potential is convenient to describe the interactions between halogens and other atoms, more accurate interatomic modeling such as DFTB method which takes the molecular orbitals into account should be utilized to make the simulations more realistic. Based on the simulations results, the damage formation scenario will be discussed.