Simulation of defect formation and sputtering of Si(100) surface under low-energy oxygen bombardment using a reactive force field

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The interaction of oxygen atoms with surfaces is of interest for a series of issues and applications. They include the formation of oxides, the interaction of oxygen atoms and ions with surfaces in plasma surface treatments or the bombardment of surfaces with oxygen atoms for sputtering and nanopatterning. For silicon, the formation of the native oxide layer as well as irradiation-induced damage and sputtering has major importance. In previous studies [1-2], results on single impacts of oxygen atoms on amorphous and Si(100) surfaces have been presented. It was shown that the sputtering of Si atoms and clusters largely depends on the damage in the target, i.e. more sputtering and formation of larger Si and SiO clusters was observed for the amorphous target.

In this presentation, we will study the interaction of low-energy oxygen atoms with a silicon surface by Molecular Dynamics (MD) simulations using the reactive force field developed by John Kieffer at the University of Michigan [3-5]. We will show results on continuous 250eV oxygen bombardment of a Si(100) surface and compare them to the aforementioned results. Amorphization, oxide formation and sputter mechanisms are studied with respect to oxygen fluence. Defects are monitored as function of time after a given oxygen impact.

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