

Atomic Study of Oxidation of Si(001) surface by MD Simulation

Mauludi Ariesto Pamungkas, Byung-Hyun Kim, Minwoong Joe, Kwang-Ryeol Lee

¹한국과학기술연구원 계산과학센터

Very initial stage of oxidation process of Si (001) surface was investigated using large scale molecular dynamics simulation. Reactive force field potential was used for the simulation owing to its ability to handle charge variation associated with the oxidation reaction. To know the detail mechanism of both adsorption and desorption of water molecule (for simulating wet oxidation), oxygen molecule (for dry oxidation) and their atom constituents, interaction of one molecule with Si surface was carefully observed. The simulation is then continued with many water and oxygen molecules to understand the kinetics of oxide growth. The results show that possibilities of desorption and adsorption depend strongly on initial atomic configuration as well as temperature. We observed a tendency that H atoms come relatively into deeper surface or otherwise quickly desorbed away from the silicon surface. On the other hand, most oxygen atoms are bonded with first layer of silicon surface. We also noticed that charge transfer is only occur in nearest neighbor regime which has been pointed out by DFT calculation. Atomic structure of the interface between the oxide and Si substrate was characterized in atomic scale.