

## Initial oxidation process on vicinal Si(001) surface: ReaxFF based on molecular dynamics simulation

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Si oxidation is a key process in developing silicon devices, such as highly integrated metal-oxide-semiconductor (MOS) transistors and antireflection-coating (ARC) on solar cell substrate. Many experimental and theoretical studies have been carried out for elucidating oxidation processes and adsorption structure using ab initio total energy and electronic structure calculations. However, the initial oxidation processes at step edge on vicinal Si surface have not been studied using the ReaxFF reactive force field.

In this work, structural change, charge distribution of oxidized Si throughout the depth from Si surface were observed during oxidation processes on vicinal Si(001) surface inclined by 10.5 ° of miscut angle toward [100]. Adsorption energies of step edge and flat terrace were calculated to compare the oxidation reaction at step edge and flat terrace on Si surface.

**Keywords:** silicon vicinal oxidation molecular dynamics reactive force field