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Reactive molecular dynamics study of very initial dry oxidation of Si(001)

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Very initial stage of oxidation process of Si (001) surface at room temperature (300 K) and high temperature (1200 K) was investigated using large scale molecular dynamics simulation. Reactive force field potential [1] was used for the simulation owing to its ability to handle charge variation as well as breaking and forming of bonds associated with the oxidation reaction. The results show that oxygen molecules adsorb dissociatively or otherwise leave the silicon surface. Initial position and orientation of oxygen molecule above the surface play important role in determining final state and time needed to dissociate. At 300 K, continuous transformation of ion Si^{+} (or suboxide Si2O) to $Si2^{+}$ (SiO), $Si3^{+}$ (Si2O3) and finally to $Si4^{+}$ (SiO2) clearly observed. High temperature silicon surface provide heat energy that enable oxygen atom to penetrate into deeper silicon surface. The heat energy also retards adsorption process. As a result, transformation of ion Si^{+} is impeded at 1200 K.

Reference

1. J. Phys. Chem. A, Vol. 105, No. 41, 2001

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