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# Oxidation structures at vicinal Si(001) surfaces: A first-principles study

Jin Nam Yeo and Byung Deok Yu

Department of Physics, University of Seoul, Seoul 130-743

Oxidation of silicon surfaces has attracted much attention as one of the most important processes in Si technology. For better function of Si microelectronics, an understanding of initial oxidation processes on Si surfaces is required. In this work, we studied the adsorption of a single oxygen atom at single-layer steps of Si(001) using first-principles total-energy calculations based on density-functional theory (DFT). In the calculations a (1,1,19) vicinal surface was used. On each terrace, the orientation of surface Si dimers is different, leading to the formation of alternate single-layer  $S_A$  and  $S_B$  steps. Our total energy calculations showed that a single oxygen atom is preferentially incorporated into sites at the  $S_B$  step edges. We also calculated the electronic properties of the oxidation structures proposed here. Our result of the preferential oxidation at the  $S_B$  step is in good agreement with experimental observation that the  $S_B$  step edge acts as sink for the oxidation of Si. The computations were performed at the UoSPCC-II facility at the Seoul Parallel Computation Center of University of Seoul. We gratefully acknowledge support from the MOCIE of Korea through the National Research Program for the 0.1 Terabit Non-Volatile Memory Development.