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Oxidation of step edges on vicinal Si(001) surfaces: A first-principles study

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Formation of silicon dioxide has attracted much attention as one of the most important processes in the technological development of current and future Si devices.[1-3]. Not surprisingly, the initial oxidation process on Si surfaces on an atomic scale is an important issue that must be addressed for better-functioning Si devices. In this work, we have studied possible adsorption structures of a single oxygen atom at single-layer S_A and S_B steps of Si(001) using first-principles total-energy and electronic-structure calculations based on density-functional theory. The total energy calculations in this study showed that a single oxygen atom is preferentially incorporated into sites at the edge of the rebonded S_B step. The obtained binding energies at the S_B step are much higher than those at terraces and at the S_A step. In order to understand the characteristic features of the scanning tunneling microscopy (STM) images observed in experiments, the comparison between the simulated STM images of the clean vicinal Si surface and the corresponding images of the oxygen-reacted structures was also made together with the calculated local densities of states (DOS) of the Si atoms at the S_B step edge. The computations were performed at the UoSPCC-II facility at the Seoul Parallel Computation Center of the University of Seoul. We gratefully acknowledge support from the Korea Research Foundation under Agreement No. KRF-2006-312-C00122.

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