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First-principles investigation of oxygen diffusion in compressively strained high-density silicon oxide T. AKIYAMA, Dept. of Physics Engineering, Mie Univ., H. KAGESHIMA, M. UEMATSU, NTT Basic Research Labs., NTT Corp., T. ITO, Dept. of Physics Engineering, Mie Univ — Oxidation of Si nanostructures is a key process in the fabrication of future Si-nano devices such as single electron transistors. It is well known that the oxidation is strongly affected by the initial structural size and shape, called pattern dependent oxidation. This characteristic can be intuitively understood by the oxidation retardation by the oxidation-induced strain: The diffusion of oxygen in the oxide is suppressed by the strained high-density oxide region generated in the nanostructures. However, the understanding of this phenomenon on atomic scale still remains unknown. In this work, we investigate microscopic mechanisms of oxygen diffusion in the strained high-density α-quartz based on first-principles total-energy calculations. The calculations show that both incorporation of O_2 molecules into the oxide and its migration are significant factors of oxygen diffusion in the high-density α-quartz. The calculated activation energy increases by 1.2 eV with a 10% increase of density, indicating that the diffusion of oxygen can be suppressed by the high-density region.

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