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Kinetic Monte Carlo Simulation for Atomic Oxygen Recombination on Silica Surface[1] SEIJI SHIOZAKI, YUKINORI SAKIYAMA, SHU TAKAGI, YOICHIRO MATSUMOTO, The University of Tokyo — Many studies have been reported about the catalytic recombination of N and O atoms on SiO_2 surface, which is quite important for the reentry of a space vehicle. But, the reaction mechanism is not fully understood. Hence, in this study, we construct a catalytic reaction model using the *ab initio* calculations and the Monte Carlo calculations in order to reveal the reaction mechanism. As the first step of this study, the Kinetic Monte Carlo (KMC) calculation was performed, in which the adsorption of incident atoms, the surface diffusion, and the thermal desorption events can be considered. Here, the two different reaction processes were taken into account. One was the Langmuir-Hinshelwood (L-H) mechanisms, which corresponds to the reaction between two adsorbed species, and the other was the Eley-Rideal (E-R) mechanisms, which corresponds to the reaction between gaseous atoms and the adsorbed atom. The recombination efficiency of O atoms on a SiO_2 surface was calculated and compared with the results in literatures. Agreement between the KMC result and experimental data was good and the contributions of E-R and L-H mechanism were discussed.

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