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Molecular dynamics simulation for dissociative adsorption of SiH4 on Si(100) surface YUKINORI SAKIYAMA, YOSHIHIKO IGA, SHU TAKAGI, YOICHIRO MATSUMOTO, The University of Tokyo — In this presentation, we introduce a new interatomic potential model optimized for the dissociative adsorption of SiH4 on Si(100) surface. We have chosen Tersoff-Murty-Brenner potential form to model Si-H interaction. The parameters were optimized to reproduce the various reaction paths and their activation energies of the dissociative adsorption of SiH4 obtained by the DFT calculations using the nudged elastic band method. The activation energies calculated from the present model successfully reproduced the DFT calculations. With this potential model, the molecular dynamics simulation was conducted to investigate the reaction dynamics and compare with the molecular beam experiments. We found the dissociation probability calculated by the molecular dynamics simulations increased exponentially with the increase of the translational energy of incoming SiH4, which is consistent of experiments.

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