

Abstract Submitted
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Surface Catalysis Modeling of Air-SiO₂ Systems Under Hypersonic Conditions Using ReaxFF MD Simulation PAUL NORMAN, TOM SCHWARTZENTRUBER, University of Minnesota, IOANA COZMUTA, NASA Ames — The high-speed entry of a blunt body into Earth's atmosphere brings about the dissociation of diatomic nitrogen and oxygen molecules via the shockwave formed in front of the body. Through surface catalysis, these dissociated atoms can recombine on the heat shield of the body, increasing its overall heating. The goal of this project is to study surface catalysis on amorphous silicon-dioxide (SiO₂), a significant component in the reusable thermal protection system used on the Space Shuttle. Specifically, our objective is to determine the rates of recombination of monatomic N and O for the range of temperatures and pressures experienced by a heat shield during Earth re-entry. Additionally, we aim to determine the rates of specific reaction mechanisms on a SiO₂ surface, including adsorption, desorption, surface diffusion, and various recombination processes. This is accomplished by performing large reactive molecular dynamics simulations using the ReaxFF force field, which naturally allows bond formation/breaking to occur during the course of a molecular dynamics simulation. Several methods for speeding up the equilibration and collection of rates for low-pressure gas-surface systems (typical of re-entry conditions) where events become infrequent will also be discussed.

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