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Oxygen-deficient defects and hydrogen in irradiated Si/SiO2 systems RENEE VAN GINHOVEN, Sandia National Labs, HAROLD HJALMARSON, Sandia National Labs — Performance of Si/SiO2 devices is degraded by ionizing radiation through the production of interface traps and buildup of trapped charge in the oxide. This process is connected to the presence of hydrogen in the oxide. Exposure to ionizing radiation stimulates release of mobile hydrogen, which can migrate through the oxide to the Si/SiO2 interface and depassivate H-terminated Si-dangling bonds. The resulting interface trap states act as charge recombination centers. Our calculations focus on the interaction of hydrogen with oxygen deficient centers in the oxide. In the bulk oxide, these defects can release hydrogen from Si-H groups, or crack H2 molecules. These active sites may also act as border trap recombination centers when near the interface. Our presentation will describe molecular scale mechanisms for radiation-induced generation of free hydrogen using density functional theory applied to fully periodic models. The oxide is represented by both crystalline and amorphous configurations. Sandia is a multiprogram laboratory operated by the Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy under contract DE-AC04-94AL85000.

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