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Large Scale Simulations of Plasma Facing Component Boronization AADITYA RAU, Johns Hopkins University, SIERRA JUBIN, Princeton Plasma Physics Lab, OMESH DWIVEDI, Drexel University, IGOR KAGANOVICH, Princeton Plasma Physics Lab — Boronization of fusion reactor walls has emerged as a crucial technique in improving the performance of fusion devices and remains a topic requiring further understanding. Previous studies in this area have either made assumptions about the structure of the reactor wall, such as randomized atom placement, or have been limited by simulation size. Thus, in this study, classical molecular dynamics was used to simulate a large oxygenated graphite structure undergoing boronization and deuterium bombardment, starting from an ideal graphite crystal. Simulations show the boronization process to occur in phases. First, a layer of boron adheres to the graphite surface. After continued bombardment, the top layers of the graphite fragment and form an amorphous mixture of carbon, oxygen, and boron that rests upon the remaining graphite layers. This behavior may help explain the deuterium retention and sputtering behavior previously cataloged in both simulations and experiments.

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