Identification of BCl_x Fragments on Si(100) Surfaces During APAM Processing Through a Combined STM/DFT Approach

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Atomic precision advanced manufacturing (APAM) techniques leverage a scanning tunneling microscope (STM) to generate dangling bond sites on a hydrogen/halogen terminated Si(100) surfaces, where a reactive dopant molecule (BCl_3, PH_3, etc.) can selectively absorb and dissociate into molecular fragments. After thermal annealing, the dopant atom will be incorporated into the underlying surface, providing a route to achieving single dopant atom placement with atomic precision. To improve the success rate of single dopant atom incorporation however[1,2], deeper understanding of the molecular dissociation pathway and which molecular fragments are present before incorporation is critical. However, establishing a relationship between features observed in STM with density functional theory (DFT) predicted dissociation fragments remains a challenging prospect due to the number of potential configurations available to the molecular fragments. Here, we discuss our work in using DFT simulated STM images as a guide for identifying BCl_x ($x = 0, 1, 2, 3$) decomposition fragments on sub-monolayer BCl_3 dosed Si(100) surfaces. We expect to apply both the identified BCl_x fragments STM images as well as simulated STM images as training and test data sets for the development of convolutional neural networks, which will be able to automatically identify fragments in an STM image.

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