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New Interpretation of Non-contact Atomic Force Microscopy Images of Dihydride Si(001) Surface Based on Simulation AKIRA MASAGO, SATOSHI WATANABE, The University of Tokyo, KATSUNORI TAGAMI, MASARU TSUKADA, Waseda University — Hydride Si(001) surfaces have attracted attention as a substrate of organic semiconductor devices. In non-contact atomic force microscopy (NC-AFM) observation of dihydride Si(001) surface, 1x1 and 2x1 images were observed depending on the preset frequency shift value [1]. For both images, bright spots were assigned to hydrogen atoms. Recently, we have developed a simulator on the basis of the density-functional based tight-binding method, and have simulated NC-AFM image of the dihydride Si(001) surface. As a result, we obtained frequency shift images with the 1x1 and 2x1 periodicities, which agree well with the experiments. Surprisingly, we have found that the bright spots of the 2x1 image do not correspond to hydrogen atoms. Each spot corresponds to the bridge site, where the sum of the attractive forces from two nearby hydrogen atoms becomes large.
[1] S. Morita, Y. Sugawara, Jpn. J. Appl. Phys. Vol. 41 (2002) pp. 4857.

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