

Abstract Submitted  
for the MAR07 Meeting of  
The American Physical Society

**AFM Simulations of H-terminated Si surfaces** AKIRA MASAGO, SATOSHI WATANABE, The University of Tokyo, KATSUNORI TAGAMI, MASARU TSUKADA, Waseda University — Si currently plays an important role in electronics. In order to search for more powerful and novel devices based on Si, significant attention has been recently focused on the fabrication of hybrid structures using organic molecules on Si surfaces, and a number of investigations have been reported. In such a situation, atomic force microscopy (AFM) and scanning tunneling microscopy (STM) are powerful techniques for observation and manipulation. In particular, since AFM can be used not only for conductors but also semiconductors and insulators, it has been widely used for observations or manipulations of various materials. However, compared to STM, there have been few reports on AFM of organic molecules adsorbed on Si surfaces. We guess that this is due to the difficulty in analyzing the AFM images of such systems. In this situation, simulations are expected to be useful, and our major objective is the development of such simulators. Thus far, we have performed non-contact AFM simulations of bare, hydrogen and methyl-terminated Si surfaces using the density-functional based tight-binding method. Results of these simulations are in good agreement with experiments quantitatively. In the present report, we talk about such Si surfaces including various defect types.

Akira Masago  
The University of Tokyo

Date submitted: 27 Dec 2006

Electronic form version 1.4