

Abstract Submitted  
for the MAR06 Meeting of  
The American Physical Society

**Simulation of contact and non-contact AFM images of H-terminated Si(100) surface with a CH<sub>3</sub> impurity** AKIRA MASAGO, SATOSHI WATANABE, Department of Materials Engineering, The University of Tokyo, KATSUNORI TAGAMI, MASARU TSUKADA, Department of Nanoscience and Nanoengineering, Waseda University — Using a density-functional-based tight-binding method, we have investigated whether atomic force microscope (AFM) images with atomic resolution can be obtained for hydrogen-terminated silicon (100) 1x1 surface including a methyl. We have simulated contact mode images of this surface using a silicon tip with and without a hydrogen atom at the apex. For the silicon tip without hydrogen at the apex, we obtained good images with anisotropic spots reflecting the symmetry of a methyl for large tip-sample distance. For the silicon tip with hydrogen at the apex, we found that better images with atomic resolution, showing internal hydrogen and carbon atoms of a methyl, are expected if the forces can be measured precisely. We have also examined non-contact mode images. Although a force line profile of non-contact mode is smoother than one of contact mode, their difference is not so large.

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Date submitted: 15 Jan 2006

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