

Abstract Submitted
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**Atomic Force Microscopy Simulation in Aqueous Environment
by RISM Theory** MASANORI HARADA, MASARU TSUKADA, Waseda University — Many theoretical simulations of atomic force microscopy (AFM) have been performed so far to clarify the underlying physics in experimental AFM images which were difficult to understand intuitively. Most of the simulations use the models consisting of only tip and sample atoms and successfully reproduce experimental AFM images obtained in vacuo. However, those models are not suitable to simulate the AFM experiments performed in liquid or gaseous environments. Reference Interaction Site Model (RISM) is used in our simulation to incorporate liquid effect. This method is based on statistical mechanics and has the advantage of low computational cost over all-atom molecular dynamical simulations. To investigate the efficiency of the method, we simulated the force-distance curves and 2D force maps in constant height mode for a few simple models. The overall methodology is referred to the studies of Koga et al.[1], specially for the AFM-RISM interface. [1] K. Koga and X. C. Zeng, Phys. Rev. B 60, 14328 (1999).

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