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Theoretical simulation of tapping mode AFM in water MASARU TSUKADA, Waseda University, NAOKI WATANABE, Mizuho Inf. & Res. Inst. — For the AFM of bio-molecules as proteins, the measurement in water is essential, since properties of bio-systems in vacuum are different from those in water. We developed a basic simulation method for the tapping mode AFM in water and applied to protein samples. First, the cantilever elastic body oscillation in water very close to the sample is analyzed, by solving the fluid dynamics of water simultaneously by a specially designed finite element method. The calculated resonance curve showed strong nonlinear features, as well as the reduction of resonant frequency and lose of the sharpness of the resonance. This method is useful for designing cantilever shapes. Next, the tapping process of the tip by the sample is simulated by a visco-elastic model of bio-samples obtained coarse graining the atomistic model. Sticking and detaching of the tip to the sample, which causes large disturbance of the cantilever motion, are also analyzed. With including these processes altogether, the frequency shift, dissipating energy, phase delay of the oscillation are obtained and used to calculate tapping mode images of proteins.

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