Molecular dynamics study for a novel AFM application

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Water at interfaces has generated, and continues to generate, significant research interest especially at nanoscale dimensions where unexpected physical phenomena may appear. The study of interfacial water has potential impact in many different fields ranging from geology, nanotribology, microfluidics, lab-on-a-chip and molecular engineering. Experimental studies have elucidated several features about structural and dynamic properties of water in contact with various hydrophobic and hydrophilic systems. In this study we employed molecular dynamic simulations in the canonical ensemble to study the effects of a capped carbon nanotube (CNT) at the solid-water interfacial region. Different types of carbon nanotubes were used to mimic an AFM tip in contact with the surface and study the perturbation in the structure and dynamics of interfacial water. The water-water interactions were modeled using the SPC/E model, the solid substrates (graphite and SiO2) were treated as rigid and the CNT was modeled with a Tersoff potential. Density profiles, surface density distributions, radial distribution functions, and diffusion coefficients of water were calculated in addition to the forces acting on the CNT to study the effect of the AFM at the interfacial region. This study has the potential to aid developing a novel AFM-based instrument to sample water density profiles at solid-liquid interfaces.