Low dimensional molecular dynamics of water inside a carbon nanotube JUNICHIRO SHIOMI, The University of Tokyo, YUAN LIN, GUSTAV AMBERG, Royal Institute of Technology (KTH), SHIGEO MARUYAMA, The University of Tokyo — While carbon nanotubes (CNTs) have attracted a number of researches as the key building blocks for nanotechnology, they have also caught attentions as ideal materials that realize quasi-one-dimensional channel environment, a key system in bioscience. Such materials stimulate studies in fluid dynamics under low dimensional confinement, which is restricted and departs significantly from that in three-dimension. The current study serves to explore such atomic scale dynamics by performing a series of molecular dynamics (MD) simulations on water confined in a CNT with a diameter of the order of 1 nm. The MD simulations have successfully probed the phase transition of a water cluster confined in a CNT to an ice-nanotube with anomalous diameter dependence. It has also been applied to investigate the possibility of transporting water through a CNT by a temperature gradient. In this study, we particularly highlight the dielectric properties of water confined inside a CNT. The confinement gives rise to strongly anisotropic dielectric relaxation, where the relaxation becomes faster and slower in the cross-sectional and axial directions, respectively. The diameter dependences of the dielectric properties are discussed in connection with water dynamics and structures in quasi-one-dimension.

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Date submitted: 03 Aug 2008

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