カーボンナノチューブ内の水の誘電緩和
Dielectric relaxation of water inside a carbon nanotube

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Abstract : Classical molecular dynamics simulations were performed to identify the dynamic and dielectric properties of water confined inside a single-walled carbon nanotube. 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.

Investigation of water dynamics confined in low dimension holds great importance, being a key issue in bioscience and nanotechnology under aqueous environments. In this course, water confined inside carbon nanotube (Fig. 1) has caught attentions as a representative system where anomalous mass transport and phase transitions takes place owning to the restricted dynamics in low dimension. The confinement effects [1] are also expected to strongly alter the dielectric relaxation of the water, and hence to impact the dielectric properties of the overall system.

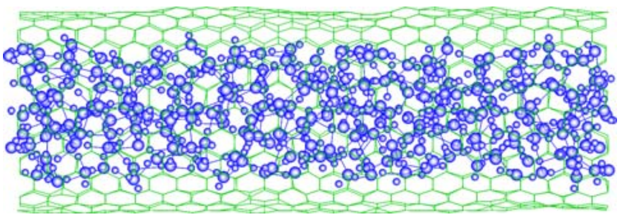

Fig. 1 Water inside a single-walled carbon nanotube.

In this study, we have carried out classical molecular dynamics simulations to characterize the dielectric relaxation of water inside a single-walled carbon nanotube (SWNT). The dynamics of water and SWNTs are modeled by extended single point charged potential (SPC/E) with Ewald treatment and the Brenner potential, respectively. The system allows us to investigate orientational polarization and relaxation of water by recording the dipole correlations. As shown in Fig. 2, the dielectric function of water inside an SWNT appears strongly anisotropic. In the axial direction, the confinement makes the static dielectric constant larger and relaxation slower. On the other hand, in the cross-sectional plane, the permittivity is significantly attenuated due to the confinement. We have further calculated the dependence on the relaxation on the nanotube diameter and water density. The results will be discussed in connection with the dynamical and structural properties of the water in quasi-one-dimension.

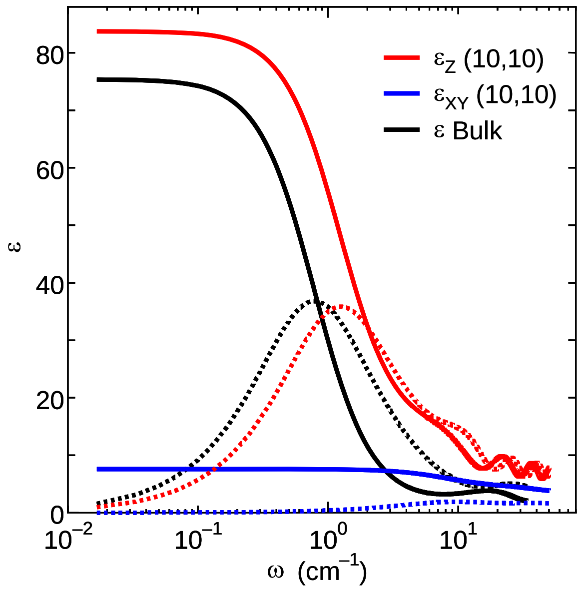

Fig. 2 Anisotropic dielectric relaxation of water inside a (10, 10) single-walled carbon nanotube. Subscripts *Z* and *XY* indicate axial and cross-sectional directions.

[1] J. Marti and M. C. Gordillo, J. Chem. Phys. 114 (2001) 10486.

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