THESIS

STRUCTURE AND DYNAMICS OF WATER CONFINED IN SINGLE-WALLED NANOTUBES: A MOLECULAR DYNAMICS STUDY

NONGNUCH ARTRITH

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Structures and dynamics of water molecules in nanoporous media exhibit interesting characteristics different from their ordinary bulk properties and may lead to potential applications in sophisticated nanofludic devices. In this study, molecular dynamics simulations were performed to investigate water molecules confined in single-walled carbon nanotubes (SWCNTs) and boron nitride nanotubes (SWBNNTs). Water density of 1.00 g cm^{-3} was placed inside the models of (*n*,*n*)-armchair nanotubes with different diameterrs (*n* = 9, 10, 12, 14, 16 and 20) and the simulations were performed in the canonical *NVT* ensemble at 298 K by using the Nosé-Hoover thermostat in DL_POLY program package. The wall-water interactions were varied within reasonable limits by changing the strength of the Lennard-Jones (LJ) parameters. Distribution functions were reported for the water in the tubes in spherical and cylindrical coordinates and the single-molecule dynamics, in particular self-diffusion, were monitored. While this motion was very much slowed down in narrow tubes, in keeping with previous findings (Mashl, R.J. *et al*. 2003 Nano Lett. 3(5):589-592.), bulk-water like self-diffusion coefficients were found in wider tubes. Axial diffusion coefficient increased with increasing tube diameter and reached its bulk value in the widest tubes with diameters of about 24 Å. The convergence was faster for smaller wall-water interactions. An anomaly is, however, found for the SWBNNTs where the convergence was not monotonous.

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Student's signature Thesis Advisor's signature

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LIST OF ABBREVIATIONS

Dz	=	Self-diffusion coefficient (z axis)
BLYP	=	Beck-Lee-Yang-Parr functional
BN	=	Boron nitride
BNNTs	=	Boron nitride nanotubes
CNTs	=	Carbon nanotubes
GlpF	=	Glycerol the crystal structure (F is symbol of native glycerol)
HF	=	Hartree-Fock
Ix	=	Angular momentum x component
Iy	=	Angular momentum y component
Iz	=	Angular momentum z component
LJ	=	Lennard-Jones
MC	=	Monte Carlo
MD	=	Molecular dynamics
MSD	=	Mean square displacement
MWCNT	=	Multi walled carbon nanotube
n(r)	=	Coordination number
NPT	=	Isothermal-Isobaric (NPT) ensemble
NT	=	Nanotubes
NVE	=	Microcanonical ensemble (NVE)
NVT	=	Canonical ensemble (NVT)
PW	=	Plane-Wave
RDF	=	Radial distribution function
SPC	=	Simple point charge
SPC/E	=	Extended simple point charge
STM	=	Temperature scanning tunneling microscope
SWBNNT	=	Single walled boron nitride nanotube
SWCNT	=	Single walled carbon nanotube
TEM	=	Transmission electron microscopy