Abstract Submitted
for the DFD17 Meeting of
The American Physical Society

Confinement effects on liquid oxygen flows in carbon nanotubes: A MD simulation study KAZUHIKO SUGA[1], RINTARO MORITANI[2], YUKI MORI[3], MASAYUKI KANEDA[4], Osaka Prefecture Univ — Molecular dynamics simulations are performed to investigate the liquid flow mechanism of diatomic molecules in armchair carbon nanotubes (CNTs). Oxygen molecules are considered as the fluid inside armchair (n,n) (n=6-20) CNTs at a temperature of 133[K] and a bulk density of 1680[kg/m^3] for the liquid state. The velocity profiles and slip lengths are discussed considering the radial distributions of the fluid density by the finite difference-based velocity fitting method. It is shown that as the diameter of the CNT increases, the slip length and the flow rate enhancement generally become smaller while irregular tendencies (discontinuity points) are observed in the distribution profiles. Between the (7,7) and (8,8) CNTs, a steep drop can be seen in the profiles. Between the (9,9) and (11,11) CNTs, and between the (12,12) and (14,14) CNTs transitional profiles are observed. It is confirmed that those phenomena are caused by an instability of the fluid molecule cluster due to the discontinuous confinement of the CNTs.

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Date submitted: 27 Jul 2017 Electronic form version 1.4