Abstract Submitted
for the DFD14 Meeting of
The American Physical Society

Molecular dynamics simulation of oxygen flows in graphene nanochannels HARUKA YASUOKA, RYO TAKAHAMA, MASAYUKI KANEDA, KAZUHIKO SUGA, Osaka Prefecture Univ — MD simulations are performed to investigate the flow characteristics of oxygen flows in graphene nanochannels. For comparison, flows of argon molecules which have relatively similar values of mass and diameter are also simulated. The L-J potential is used for the fluid-fluid interaction and the wall-fluid interaction. For the bond of the carbon molecules for the channel walls, the Brenner potential is used. For all the cases, the normalized number density, pressure and temperature are set as $\rho = 0.2$, P = 0.4 T = 2.0, Two channel height cases H = 20σ and H = 50σ, where σ is the argon molecule diameter, are considered. In those conditions, Knudsen numbers are estimated to be about 0.056 and 0.023. In both channel height cases, it is found that the oxygen flow rates are larger than those of the argon flows even though acceleration acting on fluid molecules is constant. This is because the wall-fluid interaction between oxygen and carbon molecules is weaker than that of argon flow cases. It is found that the normalized velocity profiles are indifferent of the fluid molecules. Therefore, it can be said that the diatomic molecular structure of the fluid molecules does not have significant effects on the flow characteristics in the graphene nanochannels.

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Date submitted: 01 Aug 2014 Electronic form version 1.4