MOLECULAR DYNAMICS STUDY ON THE FIELD EFFECT ION TRANSPORT DEVICE BASED ON CARBON NANOTUBE

Ho Jung Hwang, Ki Ryang Byun, Won Young Choi, and Jeong Won Kang
Nanoelectronic and Future Technology Laboratory
Department of Electronic Engineering, Chung-Ang University, 221 HukSuk-Dong, DongJak-Ku, Seoul 156-756, Korea

Ion and molecule transports in nanoscale channels have recently received increasing attention [1]. We investigated potassium ion transport through a (5, 5) carbon nanotube by using classical molecular dynamics simulations under applying external force fields. We found controllable potassium ion transport in the (5, 5) carbon nanotube. As the applying external force field increased, the potassium ions rapidly went throw the nanochannel. Under the low external force fields, the thermal fluctuation of the nanochannel affected on the tunneling of the potassium ions, whereas the effects of the thermal fluctuation were negligible under the high external force fields.

Previous works have been shown the possibility of the solid-state field-effect ion-transport devices based on the nanotubes and the encapsulated ions. In this paper, we investigate potassium ion transport through (5, 5) CNT by using classical MD simulations under applying external force fields. We present controllable potassium ion transport in (5, 5) CNT by using the molecular dynamics (MD) simulations.

For carbon–carbon interactions, we used the Tersoff potential function [2] that has been widely applied to carbon systems. For potassium–potassium and potassium–carbon interactions, we employed the force-field-method developed and used for studying the potassium-intercalated fullerenes by Goddard III and co-authors [3].

Figure 1 shows the structure investigated in this work. Figure 2 shows the trajectories of thirteen potassium ions as a function of MD time under the applying external force fields at 300 K, respectively. Figure 3(a) shows the mean position of the 13 potassium ions as a function of the MD time for the MD simulation of 13 potassium ions under 0.02 V/Å. Figure 3(b) shows the distributions of the number of ions along the tube axis as a function of the MD times.

[1] D. Qian, G.J. Wagner, W.K. Liu, M.-F. Yu and R.S. Ruoff, Appl. Mech. Rev. 55 (2002) 495.
[2] J. Tersoff, Phys. Rev. B 38 (1988) 9902.
[3] G. Gao, T. Cagin and W. A. Goddard III, Phys. Rev. Lett. 80 (1998) 5556.

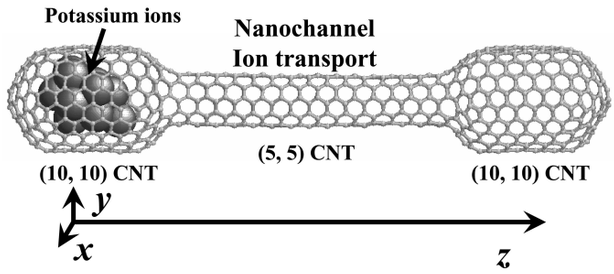

Figure 1. The structure considered in this work. The nanochannel is a (5, 5) CNT that is seamlessly connected with both side cages that are extended C_{240} fullerene. The length of the system along the tube axis (*z*-axis) is 80 Å.

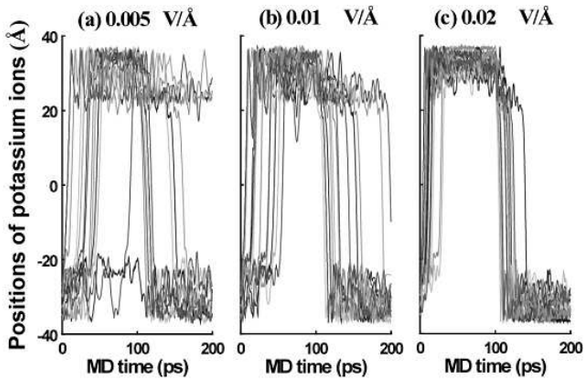

Figure 2. Trajectories of thirteen potassium ions under the applying external force field 0.005 V/Å by using the MD simulations at 300 K.

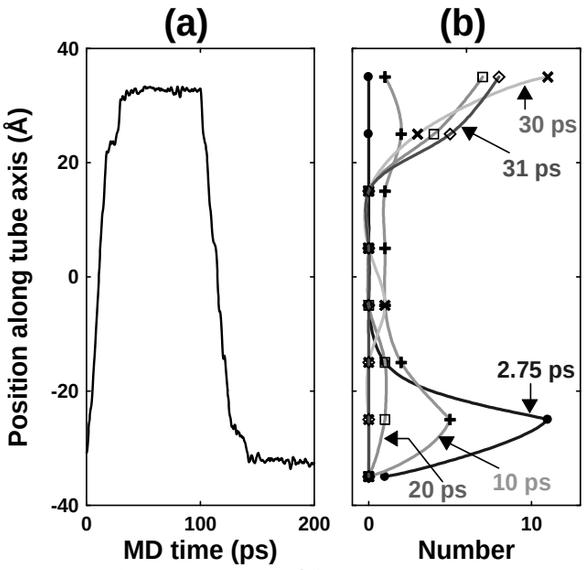

Figure 3. (a) Mean position of the 13 potassium ions as a function of the MD time for the MD simulation of 13 potassium ions under 0.02 V/Å. (b) Distributions of the number of ions along the tube axis as a function of the MD times.