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Transport diffusion in deformed carbon nanotubes

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Abstract: Using non-equilibrium molecular dynamics and Monte Carlo methods, we have studied the transport diffusion of gas in deformed carbon nanotubes. Perfect carbon nanotube and various deformed carbon nanotubes are modeled as transport channels. It is found that the transport diffusion coefficient of gas does not change in twisted carbon nanotubes, but changes in XY-distortion, Z-distortion and local defect carbon nanotubes comparing with that of the perfect carbon nanotube. Furthermore, the change of transport diffusion coefficient is found to be associated with the deformation factor. The relationship between transport diffusion coefficient and temperature is also discussed in this paper. Our results may contribute to understanding the mechanism of molecular transport in nano-channel.

Keywords: Transport diffusion; Deformed carbon nanotubes; Fick's law; Non-equilibrium dynamics.

1. Introductions

Since the discovery of carbon nanotubes (CNTs) by Sumio Iijima[1], the development of nanotechnology and nanomaterials has taken a brand new step. Being one kind of quasi-one-dimensional nanomaterials, CNTs have aroused abundant attentions due to their distinctive geometrical, electronic, mechanical, optical, and thermal properties[2-6]. In the field of nanofluids, CNTs have often been employed as molecular channels because of their special geometrical structure. Experimental evidences of particles passing through CNTs have been reported[7, 8].

Using molecular dynamics simulation, Hummer et al.[9] found that water can pass through CNTs rapidly. Skoulids et al.[10-14] did a lot of researches and got a conclusion that the diffusion of gas in CNTs is orders of magnitude quicker than that in other microporous materials such as ZSM-12 and silicalite, because of their super smooth surface. Duren et al.[15] explained the effects of molecule mass and Lennard-Jones (L-J) parameters (σ and ε) on transport diffusion characteristics. Later, Mutat et al.[16] studied the self-diffusion and transport diffusion of gas by using equilibrium molecular dynamics (EMD) and non-equilibrium molecular dynamics (NEMD) methods. They presented that the former is much lower than the latter. They also found that rigid CNT is a reasonable model only when the pressure difference is very low. Xu et al.[17, 18] studied the transport diffusion in CNTs in one dimension and three dimensions. Their results show that Fick's law has an invalid region in the nano-channel. Recently, similar experimental studies have been carried in transport diffusion [19-21].

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