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Order-N electron transport calculation from ballistic to diffusive regimes by time-dependent wave-packet diffusion method -Application to carbon nanotubes-[1] HIROYUKI ISHII, University of Tokyo, NOBUHIKO KOBAYASHI, University of Tsukuba, KENJI HIROSE, NEC Corporation — Using a time-dependent wave-packet diffusion method[1], which treats the quantum electron transport problems of huge systems of up to 80 million atoms, combining with molecular dynamics simulations, we study the electron transport of carbon nanotubes from ballistic to diffusive regimes from an atomistic viewpoint in the unified way. We can simulate the effects of electron- phonon couplings on the transport properties of the nanotubes at various temperatures. We confirm that the obtained mean free path and mobility agree well with recent experimental observations and theoretical calculations, and succeed in evaluating the resistance in entire regime between ballistic and diffusive transport limits. We clarify the resistance is remarkably different from that at the two transport limits, when the length of nanotubes is comparable to the mean free path. [1]H.Ishii, N.Kobayashi, and K.Hirose, Appl.Phys.Express 1(2008) 123002.

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