Thermal Conductivity of a Gas in a Nanoporous Structure

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The thermal conductivities of nitrogen gas in a nanoporous structure have been calculated by the equilibrium molecular dynamics simulations and the kinetic theory of gases, through building a nanoscale cubic pore model. The thermal conductivities of nitrogen in different size pores calculated by the equilibrium molecular dynamics simulations are compared with those obtained by the kinetic theory of gases. The compared results indicate good agreement when the wall size of the pore is larger than 20 nm, but bad agreement when the wall size is smaller than 20 nm. With the decrease of the wall size of the pore, the thermal conductivities of nitrogen obtained from the equilibrium molecular dynamics simulations and kinetic theory of gases are both reduced, and are much smaller than that of nitrogen in free space under the same conductions.