Adsorption Thermal Diode Using Nonequilibrium Molecular Dynamics Simulation

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The development of thermal diodes (heat transfer preferentially in one direction) is of great interest for advanced thermal and energy applications. However, their performance is limited due to the poor thermal rectification and slow transient behavior. In this study, a fast and efficient thermal diode mechanism is demonstrated using a gas-filled, heterogeneous nanogap with asymmetric surface interactions in Knudsen regime. Non-equilibrium molecular dynamics simulation is employed to create the temperature gradient over the nanogap size of L_z = 20 nm with ΔT = 20 K (80 < T < 130 K) and different gas-sold interaction ratios, i.e. $\varepsilon_2/\varepsilon_1$ = 0.5, and 0.75. The maximum degree of rectification ($R_{max} \sim 8$) is found at T = 80 K, resulting from the significant contrast of the adsorption-controlled thermal accommodation coefficient (TAC). The results provide insights into the design of advanced thermal management systems including thermal switches/computers.