Supporting information

Correlation between Molecular Weight and Confined Crystallization Behavior of Polymers Grafted on Zero-dimensional Filler

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The conventional Metropolis sampling algorithm was used for each attempt of segment motion. The corresponding change of the potential energy is

$$\Delta E = \Delta c \cdot E_c + \Delta p \cdot E_p$$

where E_c is the potential energy change due to non-collinear connection of consecutive bonds along the chain, which can be used to reflect chain flexibility, E_p is the potential energy change due to each pair of nonparallel packed bonds, reflecting molecular driving force for polymer crystallization, Δc is the net change of the number of non-collinear connection pairs of bonds and Δp is the net change of the number of pairs of nonparallel packed bonds. In the current simulations, the ratio of nonparallel-packed bonds potential to non-collinear potential, i.e., E_p/E_c, was set to 1

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to achieve a proper flexibility of chains at crystallization temperatures, and kT/E_c (k is the Boltzmann's constant and T is the temperature) represents the reduced system temperature (below simplified as T^*).