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THE APPLICATION OF NONLOCAL THEORY METHOD IN THE COARSE-GRAINED MOLECULAR DYNAMICS SIMULATIONS OF LONG-CHAIN POLYLACTIC ACID**

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ABSTRACT The micro-capsules used for drug delivery are fabricated using polylactic acid (PLA), which is a biomedical material approved by the FDA. A coarse-grained model of long-chain PLA was built, and molecular dynamics (MD) simulations of the model were performed using a MARTINI force field. Based on the nonlocal theory, the formula for the initial elastic modulus of polymers considering the nonlocal effect was derived, and the scaling law of internal characteristic length of polymers was proposed, which was used to adjust the cut-off radius in the MD simulations of PLA. The results show that the elastic modulus should be computed using nonlinear regression. The nonlocal effect has a certain influence on the simulation results of PLA. According to the scaling law, the cut-off radius was determined and applied to the MD simulations, the results of which reflect the influence of the molecular weight change on the elastic moduli of PLA, and are in agreement with the experimental outcome.

KEY WORDS polylactic acid, molecular dynamics simulation, nonlocal theory, scaling law

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