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Estimation of elastic modulus of confined polymer near interface by molecular dynamics simulation

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ABSTRACT

Recently, confined polymers have drawn increasing attention due to their large deviations in various physical properties compared with bulk behavior. In particular, increase or decrease of the mechanical, electrical, and other physical properties have been reported via different experimental technologies. In this discussion, we present a new method to explore the local elastic modulus of a coarse-grained polymer near the interfacial region and free surface based on the deformation–fluctuation hybrid scheme in conjunction with semi-NVT ensemble. The developed method has been verified by comparing with several crystal structures, including Ar and Cu. Simulation results on the coarse-grained polymer prove that enhancements of elastic constants have been discovered near surface and interfacial regions, independent of the interaction between the polymer and its substrate. Therefore, this new algorithm is applicable for validating various experimental measurements and providing a means to investigate effects of confinement on stiffness-related behavior in polymers.