Systematic and Simulation-Free Coarse Graining of Polymer Melts

Delian Yang and Qiang Wang [C, S]
Department of Chemical and Biological Engineering, Colorado State University, Fort Collins, CO, U.S.A.
q.wang@colostate.edu

Full atomistic simulations of many-chain systems such as polymer melts are not feasible at present due to their formidable computational requirements. Coarse-grained (CG) models have to be used instead, where each segment represents, for example, the center-of-mass of a group of atoms/monomers. Such models, however, reduce the chain conformational entropy, which plays an essential role in the thermodynamic behavior of polymeric systems. On the other hand, in most work on coarse graining, molecular simulations are used to obtain the structural and/or thermodynamic properties of both original and CG systems that need to be matched, which is not only computationally very expensive but also non-transferable. Here we present a systematic and simulation-free strategy for both structure- and relative-entropy-based coarse graining of homopolymer melts. We use integral-equation theories, instead of molecular simulations, for both original and CG systems, and examine in detail how the CG potential varies with *N* (the number of CG segments on each chain) and how well the CG models can reproduce the structural and thermodynamic properties of the original system. The structure-based approach reproduces the structural but not thermodynamic properties of the original system due to the information loss of coarse-graining, and the relative-entropy-based approach minimizes such information loss. Our systematic and simulation-free coarse-graining strategy is much faster than those using molecular simulations, and provides a quantitative basis for choosing small *N*-values that can still capture the chain conformational entropy, a characteristics of polymers.