POLY: Division of Polymer Chemistry

343 - Calculating initial lattice configurations to enhance computational efficiency for polydisperse polymer simulations

View Session Detail

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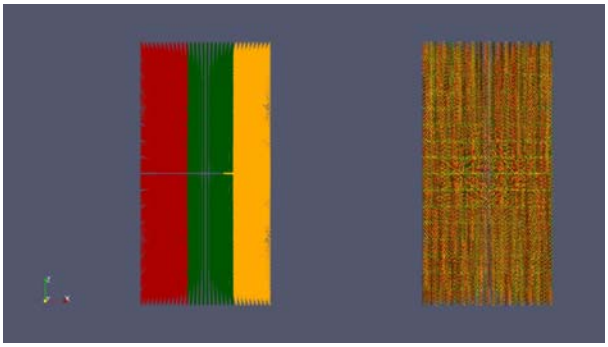
Abstract: Computer simulation as a scientific tool has been implemented for problems in virtually every field of scientific research. Polymer science has particularly profited by the use of computational simulations that are capable of predicting molecular scale properties. Monte Carlo (MC) is an extremely powerful tool to study the structural and thermodynamic properties of polymer melts. Much experimental evidence demonstrates that polydispersity plays a significant role in the physics of polymer melts. Despite its fundamental role in the behavior of polymers, polydispersity has not yet been fully extended to systems typical of industrial polymers.

A new algorithm is developed to place polymer chains of differing length into an initial configuration on a face-centered-cubic lattice. Simulations with no flow biasing are performed on two different initial configurations to show differences in reaching equilibrated configurations. Monte Carlo simulations presented here are performed on a fully occupied face-centered cubic lattice by using the p-COMOFLO algorithm, a variant of the cooperative motion algorithm of Pakula. This algorithm allows for a realistic polymer melt density by modeling lattices at full density.

System properties including the chain size, segmental density distributions and chain-end density distribution are investigated as function of Monte Carlo time. The simulation results show that the initial configuration generated by this new algorithm comes to equilibrium significantly faster with respect to chains size, segmental densities, and chain end densities. At equilibrium, the longer chains reside away from the walls and the shorter chains are preferred near the walls. Meanwhile, there is a preference for chains ends to locate at the wall. This newly developed algorithm offers the advantage of speeding up computational equilibrium and thus less computational time is needed. Accordingly, it represents an important advancement in pursuing the simulation of systems of true practical importance.



Visualization of Mapping Three Different Chains to the Lattice Using Two Different Placement Methods