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Multiscale simulation for long chain polymer using MD/continuum hybrid method

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Summary

Atomistic molecular dynamics simulation for"polymer melts has been performed inten-sively and revealed the dynamical behavior of atomistic"chain structure in the melt. These atomistic"calculations, however, have been limited by the massive computational costs because of macroscopic properties of long chain polymer. It would be highly de-sirable to use a multiscale approach covering atomistic and macroscopic behavior of the polymer melt.

We have developed computational method coupling atomic model and continuum model [1] and applied the method to polymer melt consisted of the long chain polymers. The polymer molecule is coarse-grained into meso-scopic model by so-called spring- beads model. This spring-beads model is coupled with an elastic continuum model using our hybrid method. The mean square end to end distance of polymer is calculated, and it was shown that the hybrid model leads fast convergence into the equilibrium state. This result shows that our hybrid model is useful in a large-scale system.

References

1. G. Kim and Y. Senda, Journal of Physics: Condensed Matter Vol.19 246203 (2007)