

Multiscale Molecular Simulation of some important Polymers for Thailand

Visit Vao-soongnern*

Laboratory of Computational and Applied Polymer Science, School of Chemistry, Institute of Science,
Suranaree University of Technology Nakhon Ratchasima 30000,
Phone +66 44224639, Fax +66 44224185, *E-Mail: visit@sut.ac.th

Abstract

In this talk, I will present my past experience on development a multiscale molecular simulation method and apply these simulation techniques to study some important polymers for Thailand. Two selected systems will be presented namely (1) natural rubber derivative and (2) poly(lactic acid), PLA. For the first system, it is possible to modify natural rubber to have better mechanical and physical properties. One such example is the preparation of hydrogenated natural rubber (HBR) or a perfect ethylene-propylene alternating copolymer (PEP) by homogeneous catalytic hydrogenation [1]. Our simulation work is to predict material properties of hydrogenated natural rubbers based on the multiscale molecular simulation method [2] which was recently applied for poly(propylene) melts [3] and blends with poly(ethylene) [4]. Coarse-grained (CG) model of bulk amorphous PEP was first generated and then fully atomistic model can be obtained by the reverse mapping procedure to recover the missing atoms. Prediction for properties including cohesive energy density and solubility parameter, pair correlation function of carbon atoms and static scattering structure factor, surface energy and mechanical properties are presented and compared with experimental results.

For the second system, to design a more efficient plasticizer for PLA based on PEG derivative, the miscibility enhancement of PLA/PLA-PEG-PLA blends were investigated by both atomistic and mesoscale simulations. Flory-Huggins interaction (χ) parameters of these blends were calculated using molecular dynamic (MD) simulation to determine the miscibility. Based on the calculated χ -parameters and radial distribution functions, PLA/PLA-PEG-PLA is better miscible compared to PLA/PEG at the same blend composition. The χ -parameters of all PLA/PLA-PEG-PLA blends are always lower than those of PLA/PEG blends at the same PEG concentration and are increased as a function of PLA block fractions. The mesoscale properties of PLA/PLA-PEG-PLA blends were determined by dissipative particle dynamic (DPD) simulation. Smaller PEG domain of PLA/PLA-PEG-PLA blends compared to that in PLA/PEG blend is observed implying the PLA blocks in PLA-PEG-PLA should contribute to better miscibility. Miscibility of PLA/PLA-PEG-PLA blends was also investigated by experiment using DSC and rheological measurements [5-6]. We also try to investigate a possibility to apply PLA-PEG-PLA in drug delivery application as a micelle for nanocarrier. DPD was employed to investigate PLA-PEG-PLA copolymer micelles. Critical micelle concentration (cmc), micelle size and small molecule encapsulation of these triblock copolymer micelles with different hydrophobic/ hydrophilic (LA/EG) block ratios. Only the appropriated LA/EG block ratio can induce the formation of spherical micelle in a dilute solution. The cmc and micelle size were decreased and increased, respectively, as a function of the LA/EG block ratio. Upon adding small solubilize molecules, a larger micelle size was formed. Fluorescence spectroscopy and light scattering techniques were also employed to provide results for comparison [7].

Keywords: Molecular simulation, Monte Carlo Simulation, Mesoscale Simulation, Natural rubber, Poly(lactic acid)

References

- [1] Inoue, S.; Nishio T. *J. App. Polym. Sci.*, 103, 3957-3963 (2007).
- [2] Vao-soongnern, V. *Polymer Science A: Polymer Physics*, 56, 928-935 (2014).
- [3] Piniymontree, T.; Choi, P.; Vao-soongnern, V. *Macromolecular Research*, 22, 187-193 (2014).
- [4] Takhulee, A.; Vao-soongnern, V. *Polymer Science A: Polymer Physics*, 56, 936-944 (2014).
- [5] Takhulee, A.; Takahashi Y. *Vao-soongnern, V. J Polym Res*, 24(1), (2017).
- [6] Vao-soongnern, V.; Takhulee, A.; Takahashi Y. *In Preparation*.
- [7] Chansuna M.; Pimpha N.; Vao-soongnern, V.; *J Polym Res* (2014) 21:452