Molecular Simulation of Polymer Nanofiber and Polymer Crystallization

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Molecular simulation is an interesting technique for polymer science research. These computational approaches enable predictions and provide explanations of experimentally observed macromolecular structure, dynamics, thermodynamics, and microscopic and macroscopic material properties. In this talk, the Monte Carlo simulation of coarse-grained polymer models is used to study the effect of polydispersity on the surface properties of polymer nanofiber and structural formation during an initial stage of polymer crystallization upon cooling from the melts. The method employs the modified Flory's rotational isomeric state (RIS) model and discretized version of Lennard-Jones potential; respectively, for intrachain and intermolecular interaction. The RIS chains were then coarse-grained and mapped onto the high coordination lattice.

Poly(ethylene oxide), PEO, nanofibers made up of mono- and bi-dispersed chains with diameters ranging from 7.4 to 16.4 times the radius of gyration of PEO chains were analyzed. For mono-disperse chains, as a result of increasing molecular weight, the bulk density increases and the molecular size at the surface is decreased more than the nanofibers composed of shorter chain lengths. There is a higher degree of parallel orientation of the chains and bonds at the surface and a broader region over which this bond orientation pertains. For nanofibers with mixed molecular weight, shorter chains tend to segregate at the surface and the density of short-chain components is higher in this region. Compared to mono-disperse nanofibers, the properties of longer chains do not significantly change, whereas the orientation of chains and bonds for low molecular weight polymers become more anisotropic orientation in the presence of longer chains [1].

Next, simulations of the polyethylene (PE) model were employed to investigate the structural formation of mono- and bidisperse PE chains upon stepwise cooling from the melts. Simulation data suggest that the rate of structure formation and the degree of crystallinity were decreased for the bidisperse PE mixture. In general, polymers in the mixture form a less-ordered structure, exhibit slower crystallization rates and have lower melting temperatures. For the monodisperse systems, the shorter chains exhibit an increase of the local bond properties including a fraction of trans conformation, intra- and intermolecular order parameters, but show a decrease in molecular properties such as chain orientation and chain packing. For mixed molecular weight systems, short-chain components are perturbed by the long chains resulting in a lower fraction of trans conformation, less dense structures, and a significant decrease in the degree of the bond orientation. Both short and long polymers can co-crystallize initiated at the same simulation time and finally reach the same magnitude of the chain order parameter [2].

References

[1] Nanofiber: Journal of Polymer Research (2019) 26:147

[2] Crystallization: Journal of Molecular Liquids 376 (2023) 121434

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EDUCATION

1999	Ph. D. Polymer Science, University of Akron, Ohio, USA
	with Prof. Wayne L. Mattice (Thesis Advisor)
1994	B.Sc. Chemistry (First Class Honors), Khon Kaen University, Thailand

PROFESSIONAL APPOINTMENT

1997-1999	Research Assistant, EPIC Macromolecular Modeling Center, Dept. of Polymer Science, University of Akron, Ohio, USA
2000-2002	Lecturer, School of Chemistry, Institute of Science, Suranaree University of Technology, Thailand
2002-2013	Assistant Professor, School of Chemistry, Institute of Science, Suranaree University of Technology, Thailand
2013-	Associate Professor, School of Chemistry, Institute of Science, Suranaree University of Technology, Thailand
2007-2009	Head of Research Department (equivalent to Associate Dean) Institute of Science, Suranaree University of Technology, Thailand
2009-2013	Assistant Rector for Academic Affairs (Deputy Vice-President) Suranaree University of Technology, Thailand

Research Activities

Computational Polymer Science, Physical Chemistry of Polymer, Polymer Surface and Interface (nanofiber, nanoparticle, nanocomposites), Polymeric Materials (polymer electrolytes, bioplastics, copolymer & blends), Polymer Characterization (X-Ray techniques, Thermal analysis)

Recent Publications [2020-present]

1. Visit Vao-soongnern*, Natchamon Sukhonthamethirat, Kanokporn Rueangsri, Kanjana Sirirak, Go Matsuba, Molecular simulation of the structural formation of mono-and bidisperse polyethylene upon cooling from the melts, Journal of Molecular Liquids (2023) 376: 121434
2. Kamonthira Wichai, Visit Vao-soongnern*, Khongvit Prasitnok, Wantana Klysubun, Molecular dynamics simulation and X-ray absorption spectroscopy to characterize the local structure and dynamics of calcium ion in sulfonated polystyrene (2023) 1278: 134972
3. Kanjana Sirirak, Visit Vao-soongnern*, Molecular simulation of structural properties of polymer blend nanofilms, Journal of Polymer Research (2023) 30(1): 46
4. Visit Vao-soongnern*, Molecular simulation of poly(ethylene-ran-propylene) nanoparticles with different comonomer composition, Journal of Molecular Liquids (2022) 363: 119835
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7. Natchamon , Sukhonthamethirat, Shigeru Okamoto, Shinnichi Sakurai*, Visit Vao-soongnern*, Morphology and crystallization kinetics of G-resins and isotactic polypropylene, Polymer Engineering and Science (2022) 62(6): 1775-1785
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9. Visit Vao-soongnern*, Molecular simulation of molecular and surface properties of random copolymer nanoparticle, Journal of Molecular Liquids (2021) 342:117556
10. Kamonthira Wichai, Visit Vao-soongnern*, Monte Carlo simulation of molecular and structural properties of random copolymer thin films, Journal of Molecular Modeling (2021) 27(10): 301
11. Visit Vao-soongnern*, Supanont Jamornsuriya, Molecular simulation of structural and surface properties of poly(ethylene-ran-propylene) thin films ,Journal of Polymer Research (2021) 28(9):340
12. Kamonthira Wichai, Visit Vao-soongnern*, A multiscale simulation of amorphous polystyrene, Journal of Polymer Research (2021) 28(4):109
13. Visit Vao-soongnern*, Structures and dynamics of polyethylene nanostructures with different free surface geometries: nanofilm, nanofiber and nanoparticle, Journal of Polymer Research (2020) 27(2):24