COARSE-GRAINED SIMULATION OF MOLECULAR ORDERING IN POLYLACTIC BLENDS UNDER UNIAXIAL STRAIN

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Studying mechanical properties of polymer systems by aids of computer experiments requires simulations on large time and spatial scales. In many cases, such simulations can be made feasible only by switching to coarse-grained molecular dynamics. The earlier developed coarse-grained model of polylactic acid (PLA)[1] was used to estimate the mechanical properties and ordering of pure PLA caused by uniaxial straining above the glass transition temperature, as well as the effect of oligolactic acid (OLA) content in the mixtures of PLA and OLA.

It was shown that the values of the elastic modulus observed in the coarse-grained simulations are in the same range as those observed experimentally. The coarse-grained model qualitatively reproduces the dependence of the elastic modulus on the strain rate and content of OLA molecules.

The coarse-grained model also reproduces the high degree of orientation of the macromolecules and its dependence on strain rate. In the mixtures with the OLA content of 40%, the segregation between PLA and OLA chains was observed at certain strain rates.

The coarse-grained samples can be converted to all-atom representation using the reverse mapping algorithm[2]. The coarse-grained approach provides an efficient way to speed-up molecular dynamics simulations without compromising the validity of the results.

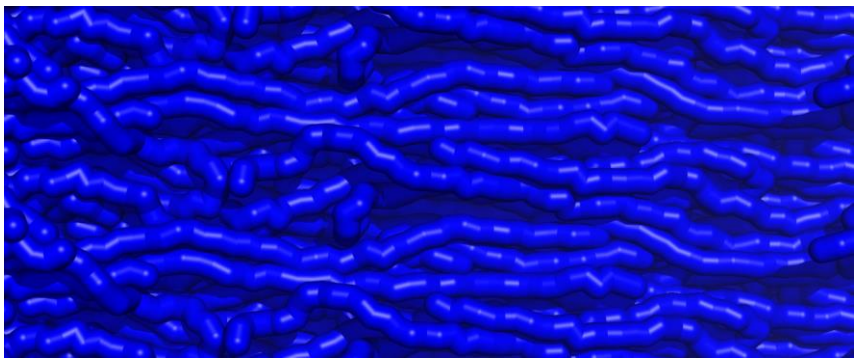

Figure 1. Backbones of PLA chains in neat PLA sample at 500% strain.

Acknowledgments

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References

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2. M. Glagolev, V. Vasilevskaya, *Supercomputing Frontiers and Innovations* **2018**, *5*, 103.