PROPERTIES OF POLY(LACTATE ACID) CHAINS VIA MULTI-SCALE DYNAMIC SIMULATIONS, USING ATOMISTIC AND COARSE-GRAINED MODELS

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ABSTRACT

We present results from hierarchical multi-scale Molecular Dynamics (MD) simulations of poly(lactate acid), PLA, chains. First, a fully atomistic OPLS-based force field, PLAFF3[1], has been utilised to build amorphous structures of atactic PLA and isotactic L-PLA of various molecular weights from decamer to 100-mer. The structures have been relaxed and subsequently simulated at the isothermal-isobaric ensemble at atmospheric pressure and temperatures from 200 ºC down to 100 ºC, covering a range between commonly employed conditions of PLA synthesis and target specifications for the pilot plant production system, respectively. Then, a coarse-grain, CG, model of PLA, in which D- and L- monomers are represented as single interaction sites, has been developed by analyzing the atomistic data *via* the Iterative Boltzmann Inversion technique[2] as implemented in an in-house software package. The CG force field was employed in order to explore longer time scales and larger systems that would require excessive computational resources when simulated with atomistic resolution; the atomistic force field, on the other hand, can capture PLA properties with higher accuracy. The CG PLA model was compared to the detailed atomistic model, and also with a previous CG model obtained from the literature[3], in terms of predicted structural (static structure factor, radius of gyration), dynamic (self-diffusion, viscosity) and thermodynamic (density, isothermal compressibility) properties as functions of PLA molecular weight. The glass transition temperature has also been determined by gradually lowering the temperature below the above mentioned range and looking at the change in slope of specific volume with temperature. In all cases simulation results are compared against available experimental data.

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