

MOLECULAR MODELING OF FREE RADICAL POLYMERIZATION OF DIACRYLATES

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Photocurable systems have become very popular in the last years, however, little is known on the molecular structure of the formed polymer networks and its influence in the ultimate properties of the materials. During photopolymerization the liquid monomer polymerizes in a few seconds via strongly branched polymers to a solid polymer network. Description of the kinetics is a challenging task as the rates of the reaction decrease by orders of magnitude due to increasing diffusion limitation. Still mathematical modeling is required to predict the network topology and the associated properties. In order to obtain better understanding of this extremely complex reaction process and to describe the evolution and the final characteristics of the polymer network, we use molecular simulations to generate several polymer networks at an atomic level for different diacrylate monomers (1,6-hexanediol diacrylate, 1,4-butanediol diacrylate, 1,10-decanediol diacrylate and 1,6-hexanediol dimethacrylate). Furthermore, we use graph theory tools to analyze the topological properties of the networks and their influence in the thermo-physical properties of the polymer network. The simulations are successfully compared with both, experimental and mathematical modeling results. The results highlight the influence of the monomer flexibility and functionality in the network topologies and properties.

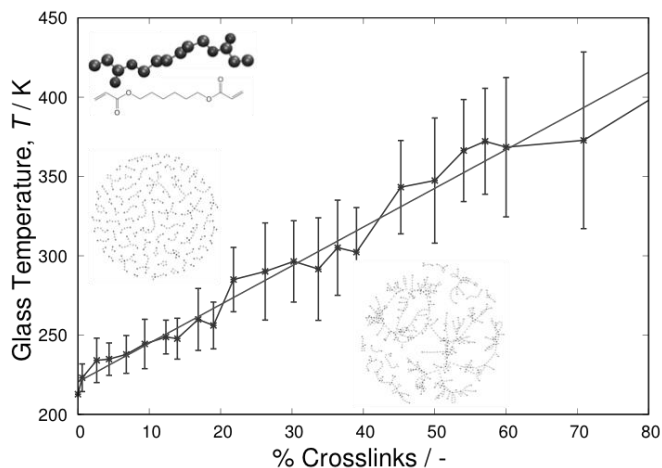


Figure 1 – Glass transition temperature as a function of crosslinks for pHDDA