# Computational Study of Tacticity and Branch Length Effects on the Shape and Stiffness of Polymer Chains Using Monte Carlo Simulations

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# Abstract

 Polymers exhibit a variety of molecular architectures and configurations, resulting in different characteristics. Concerning these complex molecular structures, stereochemistry of polymer chains plays a decisive role. Key parameters of stereochemistry are tacticity and branching of a chain. The main methods of molecular simulations are the method of Molecular Dynamics (MD) and the Monte Carlo method. If Flory’s unperturbed coil hypothesis is applied, a single unperturbed chain can be efficiently simulated, leading to conclusions for the whole amorphous polymer. In this diploma thesis the effect of tacticity on the conformation and the shape of specific polymer systems has been studied, as well as the effect of branching on the stiffness of polymer chains. More specifically, this study is based on a single unperturbed chain Monte Carlo algorithm that was developed by Tzounis, Anogiannakis et al. [9]. In order to examine tacticity effect, the systems studied were polypropylene chains varying in tacticity and chain length, polyethylene, mainly for comparison, and polyethylene-polypropylene copolymers with different polypropylene content. Moreover, as far as the branching effect is concerned, short chain branched copolymers of ethene and higher α-olefins, such as 1-butene, 1-hexene, etc., have been studied.