Rheological Characterization and Molecular Modeling of Poly(n-butyl acrylate)

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Abstract:
We propose an exhaustive experimental characterization of a series of poly(n-butyl acrylate) samples that were synthesized by controlled radical polymerization and have different molecular weights. We focus on the rheological behavior of these polymers and propose a model of their rheological behavior using a molecular model based on the reptation concept. We report the principal rheological parameters for these homopolymers and demonstrate good agreement between model predictions and experimental data.

Zusammenfassung:
Wir stellen die Ergebnisse einer umfassenden experimentellen Charakterisierung mehrerer Poly(n-butylacrylat)-Proben vor, die mittels kontrollierter radikalischer Polymerisation synthetisiert wurden und unterschiedliche Molekulargewichte besitzen. Schwerpunkt der Untersuchungen ist das rheologische Verhalten dieser Polymere. Wir präsentieren ein Modell, welches das rheologische Verhalten mit einem molekularen Ansatz basierend auf dem Reptationskonzept beschreibt. Für die untersuchten Homopolymere werden die wesentlichen rheologischen Parameter genannt und gezeigt, dass eine gute Übereinstimmung zwischen den Modellvorhersagen und den experimentellen Daten herrscht.

Résumé:
Nous avons caractérisé de manière exhaustive une série homologue de poly(n-butyl acrylate) de différentes masses molaires synthétisée par polymérisation radicalaire contrôlée. Nous proposons une étude expérimentale complète des propriétés rhéologiques de cette série pour laquelle nous validons un modèle moléculaire basé sur le concept de la reptation. Nous reportons ainsi les principaux paramètres rhéologiques de ces homopolymères et montrons la bonne adéquation entre les données expérimentales et la modélisation.

Key words: poly(n-butyl acrylate), rheological behavior, molecular modeling, controlled radical polymerization, pressure sensitive adhesives

1 INTRODUCTION

Block copolymers based on an "acrylate" soft block, including poly(n-butyl acrylate), are good candidates for Pressure Sensitive Adhesives (PSA) formulations [1]. Due to larger molecular weight between entanglements, they exhibit lower elasticity than classical elastomers. To model the behavior of such block copolymers, data from the homopolymers are required, and these are surprisingly scarce for poly(n-butyl acrylate) [2]. This study rectifies the information gap, works to develop more complete knowledge of this polymer, and provides reliable rheological data for samples over a large range of molecular weights. To this end, we synthesized a series of poly(n-butyl acrylate) samples and determined their rheological parameters.

To develop "virtual formulations" for PSA applications, it is crucial to model the rheological behavior of the polymer basis [3–5]. Simulation of rheological behavior by means of molecular models is critical to establishing a link between

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de Recherches de Lacq to synthesize the polymers studied. This work was supported by the Conseil Général des Pyrénées Atlantiques.

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