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Reaction-mediated entropic effect on phase separation in a binary polymer system

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Abstract

We present a computer simulation to study the phase separation behavior induced by polymerization in a binary system comprising polymer chains and reactive monomers. We examined the influence of interaction parameter between components and monomer concentration on the reaction-induced phase separation. The simulation results demonstrate that increasing interaction parameter (enthalpic effect) would accelerate phase separation, while entropic effect plays a key role in the process of phase separation. Furthermore, scanning electron microscopy observations illustrate identical morphologies as found in theoretical simulation. This study may enrich our comprehension of phase separation in polymer mixture.

Keywords

reaction-induced phase separation, entropic effect, enthalpic interaction, conformation, Flory-Huggins interaction parameter

1. Introduction

Mixture of polymers can yield complex and highly ordered composites for new functional materials, such as nanodevices and photoelectric materials [1–5]. These kinds of materials may provide great opportunities in industry applications. The unique function and specific morphology of these materials

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