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材料科学与工程

D_4/APAEDMS本体开环共聚反应的Monte Carlo模拟

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摘要 Monte Carlo方法模拟八甲基环四硅氧烷与*N*-*β*-氨乙基-*γ*-氨丙基甲基二甲氧基硅烷（D_4/APAEDMS）的本体开环共聚动力学. 在兼顾模拟精度与计算经济性基础上，模拟过程采用自由体积理论简化处理扩散效应并与本征反应动力学耦合. 本征动力学常数通过模拟主要共聚基元反应得到，基于优化的动力学常数通过模拟从分子水平揭示：（1）D_4/APAEDMS本体开环共聚存在总活性基团的“稳态”行为；（2）D_4/APAEDMS本体开环共聚反应过程的重均分子量与数均分子量以及分子量分布系数存在“突变”特性.

关键词 D_4 APAEDMS 本体开环共聚 动力学 Monte Carlo模拟

分类号

MONTE CARLO SIMULATION ON BULK RING-OPENING COPOLYMERIZATION OF OCTAMETHYLCYCLOTETRASILOXANE WITH *N*-*β*-AMINOETHYL-*γ*-AMINOPROPYLMETHYLDIMETHYOXYSILANE

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Abstract

Monte Carlo method was applied to bulk ring-opening copolymerization of octamethylcycl-otetrasiloxane with *N*-*β*-aminoethyl-*γ*-aminopropylmethyldimethyoxysilane.With consideration to the cost of computation as well as the precision of simulation results,a new computational model was established to simulate copolymerization system based on the free volume theory used to indicate diffusion influence and chemical reaction kinetic theory.The reaction rate constants were obtained by simulating main elemental reactions of the copolymerization.Based on the optimum rate constants, Monte Carlo simulation indicates:(1)the stationary state assumption of total amount of living groups is proved to be correct;(2)the average molecular mass and its distribution coefficient have a sudden change during the copolymerization process.

Key words octamethylcyclotetrasiloxane *N*-*β*-aminoethyl-*γ*-aminopropylmethyldimethyoxysilane bulk ring-opening copolymerization kinetics Monte Carlo simulation

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