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论文

支化高分子溶胶-凝胶相变的热力学

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摘要:

以典型的Aa-Bb型缩聚反应为例, 应用统计力学和热力学的基本原理对反应体系的一些平衡特征进行研究. 基于从两种不同角度所构造的正则配分函数, 导出反应体系的平衡自由能以及质量作用定律的解析形式, 同时指出获得数量分布函数的新方法, 并通过计算反应体系的等温压缩系数从而得到反应体系的凝胶化条件. 进一步利用数量分布函数的不变性, 给出临界点后溶胶相和凝胶相的平衡自由能, 探讨了溶胶-凝胶相变的相关问题.

关键词: 平衡自由能 质量作用定律 数量分布函数 溶胶-凝胶相变

Thermodynamics Theory for Sol-gel Transition of Branched Polymers

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Abstract:

Several equilibrium properties of typical polycondensation system of Aa-Bb type were studied by the principle of statistical thermodynamics. Starting with the canonical partition functions constructed from two viewpoints, the explicit expressions of the equilibrium free energy and the law of mass action are obtained. Meanwhile, two new methods were proposed to derive the equilibrium size distribution, and the gelation condition was carried out by the isothermal compressibility. Furthermore, based on the invariant property of the equilibrium size distribution, the equilibrium free energies of sol and gel phases in postgel regime were given, and the relevant issues on the sol-gel phase transition were discussed.

Keywords: Equilibrium free energy Law of mass action Size distribution Sol-gel phase transition

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