

论文

两相聚合物熔体中相区粗化过程的格子Boltzmann研究

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摘要:

在自由能格子Boltzmann方法的基础上, 采用附加的作用力项描述非理想流体作用, 得到了改进自由能形式的格子Boltzmann模型. 对于高分子共混体系, 采用了Flory-Huggins自由能函数形式, 对两相聚合物熔体中的相区粗化过程进行了模拟. 首先通过格子Boltzmann方法计算得到了聚合物共混物的相分离曲线, 该曲线与两相共存曲线的解析值吻合得较好. 应用此模型, 研究了聚合物共混体系不稳分相机理的相区粗化过程. 在此基础上, 探讨了分相后期相区尺寸随时间的增长指数与高分子链长和Flory-Huggins相互作用参数的关系. 模拟结果表明, 相区的后期增长机理与高分子链长和Flory-Huggins相互作用参数关系不大, 而流体的粘度决定了相区的后期增长机理, 是影响相区后期增长指数的重要因素.

关键词: 格子Boltzmann方法 相分离 粗化

Studies on Coarsening of Microdomains in Binary Polymer Mixtures by Lattice Boltzmann Methods

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Abstract:

An improved free energy approach Lattice Boltzmann model(LBM) is proposed by introducing a forcing term instead of the pressure tensor. This model can reach the proper thermodynamic equilibrium after enough simulation time. On the basis of this model, the phase separation in binary polymer mixtures is studied by applying a Flory-Huggins-type free energy. The numerical results show good agreement with the analytic coexistence curve. This model can also be used to study the coarsening of microdomains in binary polymer mixtures at the early and intermediate stages. The simulation results are in accordance with those found in experiments. To understand the coarsening of microdomains at the late stage, we study the relationship between the growth exponent of the characteristic domain size and the interaction parameter χ and chain length N . The rescaled simulation results show that the growth exponent dependence on χ and N is trivial, while the growth exponent dependence on the fluid viscosity is dominant.

Keywords: Lattice boltzmann method Phase separation Coarsening

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