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微纳技术与精密机械

不同映射中心的PMMA粗粒化分子动力学模型

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摘要： 建立了基于分子动力学的聚合物粗粒化模型,用于从介观尺度分析聚合物在微纳通道内的流动状态。首先，采用Materials Studio软件构建了全同异构的聚甲基丙烯酸甲酯（PMMA）全原子模型，并基于该模型建立了不同映射中心的粗粒化初始模型。对全原子模型进行结构优化和动力学分析，获得了体系的势能统计规律，并采用高斯拟合函数与玻尔兹曼变换方程得到粗粒化力场的初始参数。随后，根据键伸缩势、键弯曲势、非键结势等各项势能的相对强度和相互影响关系，依次迭代并修正力场解析式，获得优化后的粗粒化模型。最后，统计了粗粒化模型中的均方末端距和均方回转半径等静态特性，并与全原子模拟进行对比验证，结果显示二者之间的相对偏差分别为0.68%和6.6%。研究结果表明，映射中心的选取对模型参数有较大影响；优化后的粗粒化模型能很好地吻合全原子模拟下的统计规律，能用于分析和解释纳注射成型中的流动传质问题。

关键词： 粗粒化力场 分子动力学 聚甲基丙烯酸甲酯 纳注射成型

PMMA Coarse-Grained Molecular Dynamics Models of Different Mapping Centers

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Abstract: Coarse-grained (CG) models based on molecular dynamic were developed to analyze the flowing process of polymer melt in nano-sized channels on a mesoscale. Firstly, atomistic models of amorphous isotactic Polymethyl Methacrylate(PMMA) were built by Materials Studio， and initial CG models of different mapping centers were then developed based on the models mentioned above. After the structure optimization and kinetic analysis of the atomistic models, the statistic law of potential energy of the system was obtained and the initial force field forms were calculated by Gaussian fitting function and Boltzmann inversion method. Then, the formula of force field was iterated and modified according to the relative strength and the relation of bond, angle and nonbonded potentials and an optimized CG model was obtained successively. Finally, the static properties of the CG model, such as mean square end-to-end distance and mean square radius of gyration, were compared to those of atomistic simulation, and obtained relative deviations are 0.68% and 6.6%, respectively. The results demonstrate that the mapping center has impact on the models and the optimized CG model reproduces the atomistic model well. It can be used to analyze and explain the flow and mass transfer behaviors in the nano-injection molding process.

Keywords: Coarse Grained Molecular Dynamics Polymethyl Methacrylate(PMMA) Nano-Injection Molding

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