

论文

高分子在受限稀溶液中的结构和动力学性质

何彦东, 尤莉艳, 王晓琳, 吕中元, 李泽生

吉林大学理论化学研究所, 理论化学计算国家重点实验室, 长春130021

摘要:

利用平衡态及非平衡态耗散粒子动力学模拟方法, 分别研究了平衡态和流场作用下受限高分子在稀溶液中的链结构和动力学. 采用没有滑移和密度涨落的边界条件模拟纳米管道环境, 进而研究了高分子回转半径和扩散系数对受限强度及高分子与溶剂间相互作用的依赖关系. 在非平衡态模拟中, 分别考虑了Poiseuille和Couette两种流场. 研究发现, 在这两种流场作用下, 高分子都随着溶剂与高分子排斥作用的降低而向管道中心迁移. 在强流场下, 在Poiseuille流场中高分子密度呈现出双峰分布, 而在Couette流场中则呈现为单峰分布.

关键词: 耗散粒子动力学 受限高分子 稀溶液 Poiseuille流场 Couette流场

Structure and Dynamics of Confined Polymer Chain in Dilute Solution

HE Yan-Dong, YOU Li-Yan, WANG Xiao-Lin, LÜ Zhong-Yuan*, LI Ze-Sheng

State Key Laboratory of Theoretical and Computational Chemistry, Institute of Theoretical Chemistry, Jilin University, Changchun 130021, China

Abstract:

The structure and dynamics of confined single polymer chain in dilute solution, either in equilibrium or subjected to different flow fields, are investigated by means of dissipative particle dynamics simulations. The no-slip boundary condition without density fluctuation near the wall is taken into account to mimic the environment of a nanochannel. The dependence of the radius of gyration and the diffusion of the chain on the strength of the confinement and the solvent quality is studied. In non-equilibrium systems, both the Couette flow and the Poiseuille flow acting on a dilute polymer solution are investigated. The effect of the interaction between polymer and solvent under these two flow conditions are found to be the same: the polymer migrates to the center of the channel when the interaction was reduced. With increasing the flow strength, there are two peaks with a dip in the center of the polymer density profile in the Poiseuille flow and only one peak in the center in the Couette flow, which are in agreement with the previous investigations.

Keywords: Dissipative particle dynamics Confined polymer Dilute solution Poiseuille flow Couette flow

收稿日期 2008-06-11 修回日期 1900-01-01 网络版发布日期

DOI:

基金项目:

扩展功能

本文信息

Supporting info

PDF(441KB)

[HTML全文](OKB)

参考文献[PDF]

参考文献

服务与反馈

把本文推荐给朋友

加入我的书架

加入引用管理器

引用本文

Email Alert

文章反馈

浏览反馈信息

本文关键词相关文章

▶ 耗散粒子动力学

▶ 受限高分子

▶ 稀溶液

▶ Poiseuille流场

▶ Couette流场

本文作者相关文章

▶ 何彦东

▶ 尤莉艳

▶ 王晓琳

▶ 吕中元

▶ 李泽生

▶ 何彦东

▶ 尤莉艳

▶ 王晓琳

▶ 吕中元

▶ 李泽生

PubMed

Article by

Article by

Article by

Article by

Article by

Article by

Article by

Article by

Article by

Article by

通讯作者: 吕中元

作者简介:

参考文献:

1. Fang L., Hu H., Larson R. G.. J. Rheol.[J], 2005, 49: 127-138
2. Nykypanchuk D., Strey H. H., Hoagland D. A.. Science[J], 2002, 297: 987-990
3. Maier B., Rdlar J. O.. Phys. Rev. Lett.[J], 1999, 82: 1911-1914
4. Reisner W., Morton K. J., Riehn R., *et al.* Phys. Rev. Lett.[J], 2005, 94: 196101(1)-196101(4)
5. Tegenfeldt J. O., Prinz C., Cao H., *et al.* Proc. Nat. Acad. Sci.[J], 2004, 101: 10979-10983
6. Riehn R., Lu M., Wang Y. M., *et al.* Proc. Nat. Acad. Sci.[J], 2005, 102: 10012-10016
7. Doyle P. S., Bibette J., Bancaud A., *et al.* Science[J], 2002, 295: 2237-2240
8. Han J., Graighead H. G.. Science[J], 2000, 288: 1026-1029
9. Hu G., Gao Y., Sherman P. M., *et al.* Microfluid Nanofluid[J], 2005, 1: 346-355
10. Gorman B. R., Wikswo J. P.. Microfluid Nanofluid[J], 2008, 4: 273-285
11. Balducci A., Mao P., Han J., *et al.* Macromolecules[J], 2006, 39: 6273-6281
12. Chen Y. L., Graham M. D., de Pablo J. J., *et al.* Macromolecules[J], 2005, 38: 6680-6687
13. Ma H., Graham M. D.. Phys. Fluids[J], 2005, 17: 083103-1-13
14. Jendrejck R. M., Schwartz D. C., de Pablo J. J., *et al.* J. Chem. Phys.[J], 2004, 120: 2513-2529
15. Berk Usta O., Ladd A. J. C., Butler J. E.. J. Chem. Phys.[J], 2005, 122: 094902-1-11
16. Berk Usta O., Butler J. E., Ladd A. J. C.. Phys. Fluids[J], 2006, 18: 031703-1-4
17. Hoogerbrugge P. J., Koelman J. M. V. A.. Europhys. Lett.[J], 1992, 19: 155-160
18. Schlijper A. G., Hoogerbrugge P. J., Manke C. W.. J. Rheol.[J], 1995, 39: 567-579
19. Espaol P.. Phys. Rev. E[J], 1995, 52: 1734-1742
20. Groot R. D., Warren P. B.. J. Chem. Phys.[J], 1997, 107: 4423-4435
21. Pivkin I. V., Karniadakis G. E.. J. Comput. Phys.[J], 2005, 207: 114-128
22. Qian H. J., Chen L. J., Lu Z. Y., *et al.* Phys. Rev. Lett.[J], 2007, 99: 068301-1-4
23. Pivkin I. V., Karniadakis G. E.. Phys. Rev. Lett.[J], 2006, 96: 206001-1-4
24. Allen M. P., Tildesley D. J.. Computer Simulations of Liquids[M], Oxford: Oxford Science, 1987
25. Lu Z. Y., Hentschke R.. Phys. Rev. E[J], 2002, 65: 041807-1-5
26. Hernández-Ortiz J. P., Ma H. B., de Pablo J. J., *et al.* Phys. Fluids[J], 2006, 18: 123101-1-12
27. Hernández-Ortiz J. P., de Pablo J. J., Graham M. D.. Phys. Rev. Lett.[J], 2007, 98: 140602-1-4
28. LIU Wei(刘伟), QIAN Hu-Jun(钱虎军), LÜ Zhong-Yuan(吕中元), *et al.* Chem. J. Chinese Universities (高等学校化学学报)[J], 2007, 28(3), 548-551

本刊中的类似文章

1. 刘伟, 钱虎军, 吕中元, 李卓, 孙家锤. 剪切场作用下环形二嵌段共聚物微相形态变化的耗散粒子动力学研究[J]. 高等学校化学学报, 2007,28(3): 548-551
2. 刘英涛, 李占伟, 吕中元, 李泽生. 梳型嵌段共聚物微观相分离的耗散粒子动力学模拟[J]. 高等学校化学学报, 2008,29(6): 1200-1204
3. 毛伟, 孔滨, 杨小震. 用耗散粒子动力学方法研究高分子链取向对形变液滴回缩法测定界面张力值的影响[J]. 高等学校化学学报, 2008,29(5): 1056-1060

文章评论

序号	时间	反馈人	邮箱	标题	内容
					ugg online ugg bc online buy ugg boot boots sale ugg boc cardy ugg boots l cardy tall ugg ugg boots ugg knightsb