Journal of Chemical Physics 2017 vol.146 N22

Segmental dynamics of polyethylene-alt-propylene studied by NMR spin echo techniques

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Abstract

© 2017 Author(s). Segmental dynamics of a highly entangled melt of linear polyethylene-al--propylene with a molecular weight of 200 kDa was studied with a novel proton nuclear magnetic resonance (NMR) approach based upon 1 H → 2 H isotope dilution as applied to a solid-echo build-up function I SE (t), which is constructed from the NMR spin echo signals arising from the Hahn echo (HE) and two variations of the solid-echo pulse sequence. The isotope dilution enables the separation of inter- and intramolecular contributions to this function and allows one to extract the segmental mean-squared displacements in the millisecond time range, which is hardly accessible by other experimental methods. The proposed technique in combination with time-temperature superposition yields information about segmental translation in polyethylene-alt-propylene over 6 decades in time from 10 -6 s up to 1 s. The time dependence of the mean-squared displacement obtained in this time range clearly shows three regimes of power law with exponents, which are in good agreement with the tube-reptation model predictions for the Rouse model, incoherent reptation and coherent reptation regimes. The results at short times coincide with the fast-field cycling relaxometry and neutron spin echo data, yet, significantly extending the probed time range. Furthermore, the obtained data are verified as well by the use of the dipolar-correlation effect on the Hahn echo, which was developed before by the co-authors. At the same time, the amplitude ratio of the intermolecular part of the proton dynamic dipole-dipole correlation function over the intramolecular part obtained from the experimental data is not in agreement with the predictions of the tube-reptation model for the regimes of incoherent and coherent reptation.

http://dx.doi.org/10.1063/1.4984265

References

[1] V. A. Kargin and G. L. Slonimskii, J. Fizhimii (USSR) 23, 563 (1949).
[2] P. J. Rouse, J. Chem. Phys. 21, 1272 (1953). 10.1063/1.1699180
[3] N. Fatkullin, R. Kimmich, and H. W. Weber, Phys. Rev. E 47 (6), 4600 (1993). 10.1103/physreve.47.4600
[4] N. Fatkullin and R. Kimmich, J. Chem. Phys. 101 (1), 822 (1994). 10.1063/1.468139
[5] S. F. Edwards, Proc. Phys. Soc. 92, 9 (1967). 10.1088/0370-1328/92/1/303
[6] P. G. de Gennes, J. Chem. Phys. 55, 572 (1971). 10.1063/1.1675789
[7] M. Doi and S. F. Edwards, J. Chem. Soc., Faraday Trans. 2 74, 1789 (1978). 10.1039/f29787401789
[8] M. Doi and S. F. Edwards, The Theory of Polymer Dynamics (Clarendon, Oxford, 1986).
[9] K. S. Schweizer, J. Chem. Phys. 91, 5802 (1989). 10.1063/1.457533
[10] K. S. Schweizer, J. Chem. Phys. 91, 5822 (1989). 10.1063/1.457534

[11] K. S. Schweizer, Phys. Scr. T49A, 99 (1993). 10.1088/0031-8949/1993/t49a/017

[12] A. Abragam, The Principles of Nuclear Magnetism (Clarendon, Oxford, 1961).

[13] C. P. Slichter, Principles of Magnetic Resonance, 3rd ed. (Springer-Verlag, Berlin, Heidelberg, New York, 1990).

[14] R. Kimmich and N. Fatkullin, Adv. Polym. Sci. 170, 1 (2004). 10.1007/b12766

[15] R. Kimmich, N. Fatkullin, R.-O. Seitter, and K. Gille, J. Chem. Phys. 108, 2173 (1998). 10.1063/1.475597

[16] M. Kehr, N. Fatkullin, and R. Kimmich, J. Chem. Phys. 126, 094903 (2007). 10.1063/1.2435357

[17] M. Kehr, N. Fatkullin, and R. Kimmich, J. Chem. Phys. 127, 084911 (2007). 10.1063/1.2773732

[18] R. Kimmich and N. Fatkullin, Prog. Nucl. Magn. Reson. Spectrosc. 101, 18 (2017). 10.1016/j.pnmrs.2017.04.001

[19] E. A. Rössler, S. Stapf, and N. Fatkullin, Curr. Opin. Colloid Interface Sci. 18 (3), 173 (2013).

[20] S. Kariyo, A. Brodin, C. Gainaru, A. Herrmann, J. Hintermeyer, H. Schick, V. N. Novikov, and E. A. Rössler, Macromolecules 41, 5322 (2008). 10.1021/ma702758j

[21] S. Kariyo, A. Herrmann, C. Gainaru, H. Schick, A. Brodin, V. N. Novikov, and E. A. Rössler, Macromolecules 41, 5313 (2008). 10.1021/ma702771s

[22] A. Herrmann, B. Kresse, J. Gmeiner, A. F. Privalov, D. Kruk, F. Fujara, and E. A. Rössler, Macromolecules 45, 6516 (2012). 10.1021/ma301099h

[23] M. Hofmann, B. Kresse, A. F. Privalov, L. Heymann, L. Willner, N. Aksel, N. Fatkullin, F. Fujara, and E. A. Rössler, Macromolecules 49 (20), 7945 (2016). 10.1021/acs.macromol.6b01860

[24] M. Hofmann, B. Kresse, L. Heymann, A. F. Privalov, L. Willner, N. Fatkullin, N. Aksel, F. Fujara, and E. A. Rössler, Macromolecules 49 (22), 8622 (2016). 10.1021/acs.macromol.6b01906

[25] B. Kresse, M. Hofmann, A. F. Privalov, N. Fatkullin, F. Fujara, and E. A. Rössler, Macromolecules 48 (13), 4491 (2015). 10.1021/acs.macromol.5b00855

[26] E. Fischer, R. Kimmich, N. Fatkullin, and G. Yatsenko, Phys. Rev. E 62, 775 (2000). 10.1103/physreve.62.775

[27] D. Richter, M. Monkenbusch, A. Arbe, and J. Colmenero, Adv. Polym. Sci. 174, 1 (2005). 10.1007/b99835

[28] A. Wischnewski, M. Monkenbusch, L. Willner, D. Richter, and G. Kali, Phys. Rev. Lett. 90 (5), 58302 (2003). 10.1103/physrevlett.90.058302

[29] D. Richter, R. Butera, L. J. Fetters, J. S. Huang, B. Farago, and B. Ewen, Macromolecules 25 (23), 6156 (1992). 10.1021/ma00049a011

[30] R. Graf, A. Heuer, and H. W. Spiess, Phys. Rev. Lett. 80, 5738 (1998). 10.1103/physrevlett.80.5738

[31] F. Furtado, J. Damron, M.-L. Trutschel, C. Franz, K. Schröter, R. C. Ball, K. Saalwaechter, and D. Panja, Macromolecules 47 (1), 256 (2014). 10.1021/ma4021938

[32] F. Vaca Chávez and K. Saalwächter, Phys. Rev. Lett. 104 (19), 198305 (2010). 10.1103/physrevlett.104.198305

[33] F. Vaca Chávez and K. Saalwächter, Macromolecules 44 (6), 1549 (2011). 10.1021/ma1025708

[34] N. Fatkullin, C. Mattea, and S. Stapf, J. Chem. Phys. 139, 194905 (2013). 10.1063/1.4830410

[35] N. Fatkullin, A. Gubaidullin, C. Mattea, and S. Stapf, J. Chem. Phys. 137, 224907 (2012). 10.1063/1.4769977

[36] P. W. Anderson and P. R. Weiss, Rev. Mod. Phys. 25, 269 (1953). 10.1103/revmodphys.25.269

[37] J. P. Cohen-Addad and M. Domard, J. Chem. Phys. 75 (8), 4107 (1981). 10.1063/1.442517

[38] M. G. Brereton, Macromolecules 22 (9), 3667 (1989). 10.1021/ma00199a028

[39] M. G. Brereton, Macromolecules 23, 1119 (1990). 10.1021/ma00206a034

[40] R. Kimmich, E. Fischer, P. Callaghan, and N. Fatkullin, J. Magn. Reson., Ser. A 117, 53 (1995). 10.1006/jmra.1995.9973

[41] A. Lozovoi, C. Mattea, A. Herrmann, E. A. Rössler, S. Stapf, and N. Fatkullin, J. Chem. Phys. 144 (24), 241101 (2016). 10.1063/1.4954664

[42] J. P. Cohen-Addad and R. Vogin, Phys. Rev. Lett. 33 (16), 940 (1974). 10.1103/physrevlett.33.940

[43] J. Collignon, H. Sillescu, and H. W. Spiess, Colloid Polym. Sci. 259 (2), 220 (1981). 10.1007/bf01381764

[44] P. T. Callaghan and E. T. Samulski, Macromolecules 30 (1), 113 (1997). 10.1021/ma960784u

[45] R. C. Ball, P. T. Callaghan, and E. T. Samulski, J. Chem. Phys. 106, 7352 (1997). 10.1063/1.473696

[46] J. P. Cohen-Addad, Prog. NMR Spectrosc. 25, 1 (1993). 10.1016/0079-6565(93)80004-D

[47] J. T. Gotro and W. W. Graessley, Macromolecules 17, 2767 (1984). 10.1021/ma00142a058

[48] L. J. Fetters, D. J. Lohse, D. Richter, T. A. Witten, and A. Zirkel, Macromolecules 27 (17), 4639 (1994). 10.1021/ma00095a001

[49] M. Flämig, M. Becher, M. Hofmann, T. Körber, B. Kresse, A. F. Privalov, L. Willner, D. Kruk, F. Fujara, and E. A. Rössler, J. Phys. Chem. B 120, 7754 (2016). 10.1021/acs.jpcb.6b05109

[50] B. Schmidtke, M. Hofmann, A. Lichtinger, and E. A. Rössler, Macromolecules 48 (9), 3005 (2015). 10.1021/acs.macromol.5b00204

[51] K. Halbach, Nucl. Instrum. Methods 169 (1), 1 (1980). 10.1016/0029-554x(80)90094-4

[52] N. Fatkullin, A. Gubaidullin, and S. Stapf, J. Chem. Phys. 132, 094903 (2010). 10.1063/1.3336832

[53] M. Mehring, Principles of High Resolution NMR in Solids, 2nd ed. (Springer-Verlag, Berlin, Heidelberg, New York, 1983).