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Rainer Kimmich, Nail Fatkullin

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Equation Section 1

Self-diffusion studies by intra- and inter-molecular spin-lattice relaxometry using field-cycling: Liquids, plastic crystals, porous media, and polymer segments

Rainer Kimmich[a*], Nail Fatkullin[b]

[a] University of Ulm, 89069 Ulm, Germany
[b] Institute of Physics, Kazan Federal University, Kazan 420008 Tatarstan, Russia

Abstract:
Field-cycling NMR relaxometry is a well-established technique for probing molecular dynamics in a frequency range from typically a few kHz up to several tens of MHz. For the interpretation of relaxometry data, it is quite often assumed that the spin-lattice relaxation process is of an intra-molecular nature so that rotational fluctuations dominate. However, dipolar interactions as the main type of couplings between protons and other dipolar species without quadrupole moments can imply appreciable inter-molecular contributions. These fluctuate due to translational displacements and to a lesser degree also by rotational reorientations in the short-range limit. The analysis of the inter-molecular proton spin-lattice relaxation rate thus permits one to evaluate self-diffusion variables such as the diffusion coefficient or the mean square displacement on a time scale from nanoseconds to several hundreds of microseconds. Numerous applications to solvents, plastic liquids and polymers will be reviewed. The technique is of particular interest for polymer dynamics since inter-molecular spin-lattice relaxation diffusometry bridges the time scales of quasi-elastic neutron scattering and field-gradient NMR diffusometry. This is just the range where model-specific intra-coil mechanisms are assumed to occur. They are expected to reveal themselves by characteristic power laws for the time-dependence of the mean-square segment displacement. These can be favorably tested on this basis. Results reported in the literature will be compared with theoretical predictions. On the other hand, there is a second way for translational diffusion phenomena to affect the spin-lattice relaxation dispersion. If rotational diffusion of molecules is restricted, translational diffusion properties can be deduced even from molecular reorientation dynamics detected by intra-molecular spin-lattice relaxation. This sort of scenario will be relevant for adsorbates on surfaces or polymer segments under entanglement and chain connectivity constraints. Under such conditions, reorientations will be correlated with translational displacements leading to the so-called RMTD relaxation process (reorientation mediated by translational displacements). Applications to porous glasses, protein solutions, lipid bilayers, and clays will be discussed. Finally, we will address the intriguing fact that the various time limits of the segment mean-square displacement of polymers in some cases perfectly reproduce predictions of the tube/reptation model whereas the reorientation dynamics suggests strongly deviating power laws.

*corresponding author

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