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Diffusion mechanism of DNA in agarose gel – NMR Studies and Monte Carlo Simulations

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This work reports on thorough studies of the diffusion of DNA molecules in agarose gels. Agarose gels are of great importance in gel electrophoresis to separate DNA molecules according to their size and charge. However, the interaction mechanism between DNA molecules and agarose gels is not yet clear. Here we report on precise pulsed field gradient nuclear magnetic resonance (PFG-NMR) measurements of the diffusion of single-stranded DNA containing up to 100 nucleobases in agarose gels of concentrations up to 2%. PFG-NMR is a powerful tool to measure the diffusion coefficients directly, i.e. without the need for a fluorescent label and independent of any diffusion-model assumptions. The diffusion coefficients measured by PFG-NMR decrease both with increasing length of the DNA strand and increasing gel concentration. The experimental data were compared with the results of Monte Carlo simulations we performed for DNA diffusion in the network of polymer chains. This successful combination of precise PFG-NMR diffusion measurements with Monte Carlo simulations allowed us to obtain detailed information about the interaction of DNA molecules with agarose gels. The reduction of the diffusion coefficients is related to a temporary adhesion of the DNA molecule at the surface of the gel fibers. The average adhesion time to a gel fiber increases with the length of the DNA strands. The corresponding magnitude of the binding enthalpies of DNA strands to gel fibers indicate that a mixture of Van der Waals interactions and hydrogen bonding contributes to the decreased diffusion of DNA in agarose gels.

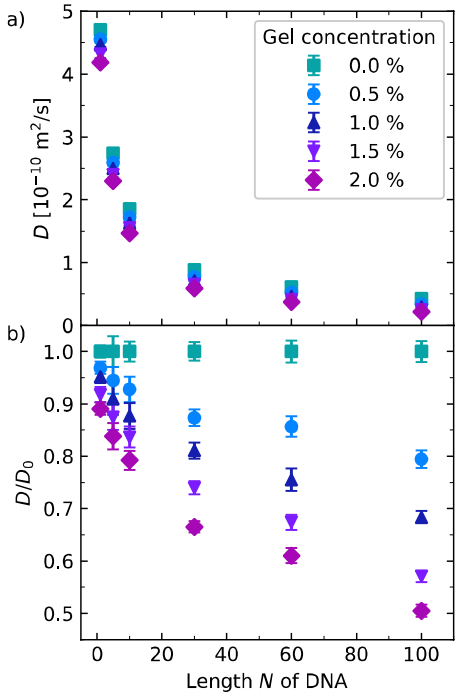

Figure 1: Diffusion coefficients D of polyT DNA molecules in agarose gels measured by PFG-NMR (a), and after normalization to diffusion coefficient D_0 in pure TBE buffer (b).