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Double-PFG Diffusion-Diffraction in Ellipsoidal Pores

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Repeated application of diffusion gradient pulse pairs [1] in a pulsed field gradient (PFG) experiment provides important insights into pore microstructure. For example, the dimensions and eccentricity of yeast cells were measured from the fourth order term of the double-PFG signal attenuation when the mixing time between the two encoding blocks is long [2]. In this abstract, we propose an alternative double-PFG technique to address the same problem, which exploits the diffusion-diffraction phenomenon [3] in double-PFG experiments [4]. In our approach, all diffusion gradients in a single acquisition are applied along the same direction with a mixing time of 0. The experiment is subsequently repeated with diffusion gradients applied along different directions.

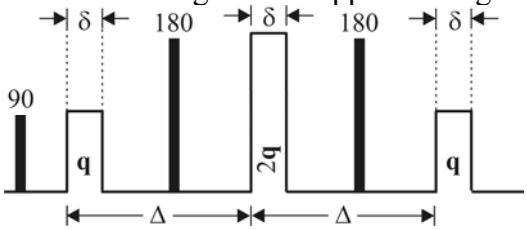

Fig. 1: The double-PFG pulse sequence considered in this work. The duration of the diffusion gradients (δ) are assumed to be very short. $q=\gamma\delta G/2\pi$, where γ is the gyromagnetic ratio and G is the gradient strength. The separation between subsequent pulses (Δ) is assumed to be long enough so that a spin can probe the largest dimension within the pore.

As demonstrated in [4], the expected signal for this pulse sequence is given by $\tilde{\rho}(q)^2\tilde{\rho}(2q)^*$, where $\tilde{\rho}(q)$ is the Fourier transform of the pore shape function. This expression for the NMR signal attenuation leads to two interesting observations: (i) the first signal minimum occurs at exactly half the q-value necessary to observe nonmonotonicity in a single-PFG experiment; (ii) the diffraction minima are replaced by zero-crossings making the diffraction pattern robust to the heterogeneity of the specimen. We calculated the NMR signal attenuation from ellipsoidal pores with different eccentricities using the expressions in [5].

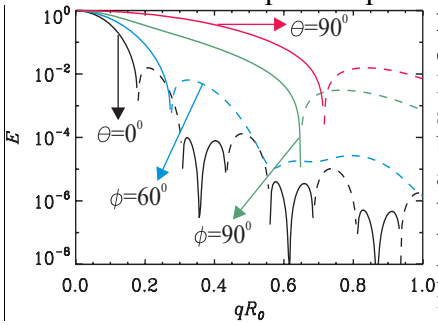

Fig. 2: The continuous and the dashed portions of each curve correspond to the positive and negative signal values, respectively. Black and red curves are computed for coherently oriented, axially symmetric ellipsoids whose ratio of major to minor axes was 4. The black curve is expected when the gradients are applied along the major axis, whereas the red curve is expected when the gradients are in the transverse plane. The blue curve shows the signal from ellipsoids whose axes are uniformly distributed over a spherical cap between the polar angles $\theta=0^0$ and $\theta=60^0$. The green curve is predicted for isotropically distributed pores.

The proposed method makes it possible to observe diffusion-diffraction phenomenon in anisotropic pores even when the pore orientations are randomly distributed. The first zero-crossings of the diffraction patterns with gradients applied along different directions can be used to quantify the compartment size as well as the pore shape anisotropy using double-PFG acquisitions with 0 mixing times, hence mitigating the effect of relaxation-related signal loss.

References:

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