Microscopic Anisotropy Revealed by Double-PFG NMR

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The multiple scattering generalizations [1] of the pulsed field gradient (PFG) experiments have been predicted to be sensitive to restricted diffusion even at long wavelengths [2], i.e., when $\gamma\delta Ga\ll 1$. Here, γ is the gyromagnetic ratio of the spins, G and δ are, respectively, the strength and duration of the applied magnetic field gradients, and a is a characteristic pore size. Such a pulse sequence is illustrated in Fig. 1.



Fig. 1: The double-PFG experiment considered in this work. Two consecutive PFG blocks are separated by a mixing time $t_{\rm m}$. The separation between the two gradient pulses of each PFG block is denoted by Δ . The angle between the two gradients **G**₁ and **G**₂ is denoted by Ψ .

We calculate the exact form of the quadratic term of the NMR signal attenuation, obtained via NMR double-PFG experiments with arbitrary timing parameters (t_m , Δ , and δ), from spins diffusing between two parallel plates, as well as in cylindrical and spherical pores. As shown in Fig. 2a, when t_m is short, there is significant variation of the signal intensity with varying values of ψ ; this is a manifestation of the sensitivity of the double-PFG experiment to microscopic anisotropy induced by the restricting walls of the spheres.

In Fig. 2b, we consider a pack of coherently oriented infinitely long cylinders. The φ dependence of the signal when $\theta=90^{0}$ is due to microscopic anisotropy whereas its θ dependence when $\varphi=90^{0}$ is indicative of ensemble anisotropy due to the coherence in the cylinders' orientations. When the cylinders are isotropically distributed, similar to the case of spherical pores, only microscopic anisotropy can be observed. However, unlike in the case of spheres, signal attenuation can be enhanced significantly by increasing the diffusion time (Δ), eventually leading to a qualitatively different angular pattern (see Fig. 2c).



Fig. 2: NMR signal attenuation (*E*) vs. angle curves from (a) spherical pores of radius *a*; (b) cylindrical tubes of radius *a* coherently oriented along the z-axis where the orientations of the gradients are shown on the left; (c) isotropically distributed cylinders of radius *a*. D_0 denotes the bulk diffusivity.

Our results can be used to design experiments with many degrees of freedom and to obtain accurate information on pore microstructure using double-PFG acquisitions, including compartment size and fiber orientation distributions—all from the long wavelength regime of the NMR signal attenuation, i.e., using small gradient strengths. Therefore, the double-PFG technique, along with our quantitative findings, are expected to be useful in characterizing geometric features of small pores with possible biological and clinical applications.

References:

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2. P. P. Mitra, Phys. Rev. B. 51 (1995) 15074.

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