q-SPACE, RESTRICTED DIFFUSION AND PULSED GRADIENT SPIN ECHO NUCLEAR MAGNETIC RESONANCE

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Errata

p. ii, line 5	'pervides' should read 'provides'
p. ii, line 7	'give' should read 'given'
p. 25, bottom of page	't' should read 'τ'
p. 28, eqn (3.28)	full stop is in the wrong place
p. 29, lines 5 and 9, section 3.3.2	**r'** should read **r**´
p. 36, eqn (4.6)	$\overline{P_s}(Z,\infty)$ should read $Z^2\overline{P_s}(Z,\infty)$
p. 40, line 4	'lograthmic' should read 'logarithmic'
p. 40, line 7	'ration' should read 'ratio'
p. 42, line 10, section 4.2.3	'planer' should read 'planar'
p. 42, line 3, section 4.3	'criteria' should read 'criterion'
p. 48, line 8	'on the order of' should read 'of the order of'
p. 78, line 13, section 6.6	'move' should read 'more'
p. 81, line 9, section 7.1	'hoping' should read 'hopping'
p. 93, bottom line	'However' should read 'however'
p. 94, line 10, section 7.4.3	'm^1' should read 'm^{-1}'
p. 118, line 17, section 8.3.3	'losses' should read 'loses'
p. 126, line 23	'repatative' should read 'reptative'

Abstract

The theory and technique of Pulsed Gradient Spin Echo (PGSE) Nuclear Magnetic Resonance (NMR) are presented. Particular attention is paid to the Fourier relationship between the average propagator of motion and the echo attenuation function. Using the q-space formalism, existing PGSE theory for diffusing molecules trapped between parallel barriers is extended to include the effects of relaxation at the walls. Computer simulations have been performed to test this extension to the theory and also to investigate the effect of finite gradient pulses in such an experiment.

PGSE experiments were performed on pentane inside rectangular microslides of 100 μm width. Diffraction-like effects predicted by theory for such experiments were observed where the PGSE data has a minimum when the gradient wavevector $\mathbf{q}$ is equal to the reciprocal width of the microslides. Through the use of non-linear least squares fitting techniques the PGSE data is fitted to theories for perfectly reflecting walls, partially reflecting walls and wall with variable spacings.

NMR microimaging experiments were performed on the microslide capillaries. The images revealed edge enhancement effects which can be explained through the signal attenuation expressions used in PGSE experiments. A brief theoretical discussion shows that the effect is due to the restricted diffusion of the molecules at the boundaries compared with the center of the sample.

A pore hopping technique is presented which allows analytic expressions to be found for diffusion in porous media. PGSE experiments are performed on water diffusing in the interconnecting voids formed by close packed, monodisperse, micron sized polystyrene spheres. Diffraction-like interference effects predicted by theory are obsevered where the PGSE data has a maximum when q is equal to the reciprocal lattice spacing of the porous network. Using non-linear least squares fitting techniques the PGSE data is fitted to the pore hopping theory for a pore glass with some variation in pore spacing. The use of an appropriate structure function for the pore shape is analysed by modelling the true pore shape and comparing it to the structure function for a sphere. The parameters revealed by fitting theory to data are consistent with the known dimensions and show that important structural information can be revealed by this technique.

Electron Spin Resonance (ESR) experiments are performed on the quasi-one-dimensional organic conductor $(FA)_2PF_6$. PGSE experiments on the conduction electrons show restricted diffusion effects. The PGSE data is analysed using both an impermeable relaxing wall model and a permeable pore hopping model. Fitting the data to these models show that a hopping model is more consistent with the data.

PGSE experiments are performed on semi-dilute solutions of high molecular weight polystyrene dissolved in CCl_4. The reptation model of diffusion is reviewed and features of this model relevant to PGSE experiments are detailed. PGSE experiments are performed and the mean square displacement of the entangled polymers is obtained as a function of diffusion time. Transitions from t to $t^{1/2}$ scaling of the mean square displacement are found, and a region exhibiting $t^{1/4}$ scaling is also observed, this region often being considered the signature for reptation.

The PGSE-MASSEY technique, which pervides a method to correct for gradient pulse mismatch, is described. The details of the hardware and software implementation of this technique are also give. PGSE-MASSEY experiments are performed on the semi-dilute polymer solutions and enable structure functions to be acquired. These structure functions are compared to the primitive chain structure function enabling an estimate of the Doi-Edwards tube diameter to be made.

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