A Tensor Approach for Double Wave Vector Experiments on Microscopic Anisotropy

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Double wave-vector experiments (DWV) [1] involving two diffusion-weightings applied successively in a single experiment have been shown to be successful for the investigation of tissue micro-structure [2,4]. For short mixing times τ_m between the two wave vectors, the cell or compartment size can be estimated and a theoretical description was provided in terms of a tensor model [3] generalizing the early work of Mitra [1]. For long mixing times, the DWV experiment is able to detect microscopic anisotropy, e.g. pore eccentricity, in a macroscopically isotropic sample. As pointed out by Mitra, this effect appears in the fourth order of the wave vector amplitude $q = \delta\ \gamma\ G$. In this work, a signal expression for arbitrary orientation distributions is derived by expanding Mitra's result to fourth order which yields rather complex terms. This approach can be written in a tensor formalism using a rank-2 tensor with 12x12 elements. The rotationally invariant trace of this tensor which can be determined from 15 measurements, reflects a measure of the microscopic diffusion anisotropy which is independent of the underlying orientation distribution of the pores. To verify the results, Monte Carlo simulations were performed.

Methods

The echo amplitude for fully restricted diffusion is given by $M = \sum_i |\rho_i(\boldsymbol{q_1})|^2\, |\rho_i(\boldsymbol{q_2})|^2$ derived by Mitra [1], where $\boldsymbol{q_i}$ are the wave vectors and $\rho_i(\mathbf{q})$ is the Fourier transform of the spin density of pore *i*. The expansion of this equation to fourth order for one wave vector is proportional to $\Sigma_{i,j,k,l}\ q_i\, q_j\, q_k\, q_l\ \rho(r))\, r_i\, r_j\, r_k\, r_l + \Sigma_{i,j}\, (q_i\, q_j\, \rho(r)\, r_i\, r_j)^2$ integrated over each pore where *i,j,k,l* are summed over the three spatial directions *x,y,z*. Considering the two wave vectors as independent variables yields a fourth order expansion which can be written in a tensor form. The corresponding equation can be written using a 12x12 rank-2 tensor and a 12-component vector consisting of the inner products of the components $q_i\, q_j$ of each wave vector. The rotationally invariant trace of the tensor represents a measure of the microscopic anisotropy of the pore that vanishes for spherical pores and increases with the eccentricity of ellipsoidal pores. It can be determined from the signals observed for an appropriate wave vector scheme consisting of 15 combinations of wave vector directions.

Monte Carlo simulations of the DWV experiment were performed to verify the theoretical considerations for simple cell geometries such as oblate, prolate, and ball spheroids. The explicit tensor expressions were fitted to the simulated signal modulation using a Levenberg-Marquardt algorithm. The microscopic anisotropy was calculated from signals simulated for three different spatial orientations of the wave vector scheme to compare it with the theoretical value and investigate its rotational invariance. For the simulations, a ratio of $\tau_m / \tau_D = 70$ - where τ_D represents the time a spin typically needs to diffuse along the longest axis - and gradient amplitudes of G = 500 mT/m (pulse duration 0.1 ms) were chosen.

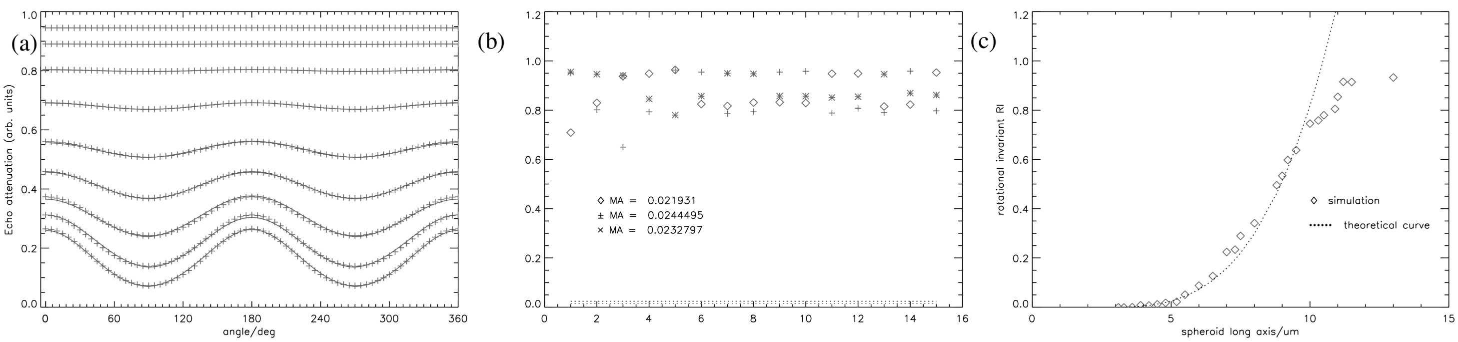

Figure 1: Simulations of the MR signal in a DWV experiment for spin diffusion in ellipsoidal cells. (a) Signal modulation (symbols) vs. the angle between the two wave vectors upon variation of the long axis (from 3µm to 15µm) and corresponding fits of the tensor model (solid lines). (b) Signals for the 15 wave vector combinations of the three different schemes and values of the microscopic anisotropy (MA) calculated from them (theoretical value 0.02529, long axis 5µm). (c) Calculated MA (symbols) for different values of the long axis in comparison to the theoretical results (dotted). For all simulations shown the other ellipsoid axes were 3µm.

Results and Discussion

Examples of the Monte Carlo simulations are sketched in Figure 1a. With increasing length of the long axis, the simulated signal modulation (symbols) observed upon variation of the angle θ between the two wave vectors increases and it is in accordance with the predictions of Mitra [1]. The fits of the tensor formulation to these data (solid lines) yield pore axes within ±5% of the nominal values for all data sets. Figure 1b shows the signals simulated for the 15 wave vector combinations of each of the schemes. The value for the anisotropy is within ±5% for the three schemes (mean 0.02322) and close to the nominal value of 0.02529. Considering the anisotropy for a large range of the long axis of the ellipsoids yields a good agreement with the theoretical values (Fig. 1c) except for rather long axes where the simulated signal approaches zero for some wave vector combinations at the chosen wave vector amplitudes and higher order terms cannot be neglected. To remove this distortion, the wave vector amplitude could be adjusted to avoid excessive signal decay. In summary, the simulated data are well described by the derived tensor model. The trace of the tensor represents a measure of the cell anisotropy for unknown cell configurations.

References

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