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# $^{7}$Li Field-Cycling NMR as Powerful Tool for Investigating Li Ion Conductors

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Solid-state nuclear magnetic resonance (NMR) spectroscopy subsumes a couple of powerful techniques to investigate the diffusion of Li ions on the microscopic scale. Understanding of these diffusion processes, besides being essential for fundamental aspects, helps in the development of Li ion battery materials. Since conventional NMR spectroscopy measures, e. g., the spin-lattice relaxation time $T_1$ as a function of temperature, this can be a disadvantage for instance in the case of temperature-sensitive samples. Using mainly $^{1}$H as probe, field-cycling NMR has been extensively used to study in particular 'soft matter' systems (see, *e.g.*, [1]-[3]). This method covers a wide range of frequencies (commonly $\omega/2\pi = 10^3 \ldots 10^7$ Hz) and the temperature can be varied optionally. The dependencies measured for the spin-lattice relaxation time $T_1$ can be compared with various models reflecting, *e.g.*, the crystal structure, the dimensionality of the diffusion pathways, and correlation effects. $^{7}$Li field-cycling NMR spin-lattice relaxometry is applied here to reinvestigate Li metal [4, 5]. This model system shows isotropic diffusion, but Li movement is also dependent on the type of lattice and the prevailing defects (see Fig. 1). It is evident that field-cycling NMR is not limited to 'soft matter' or, using $^{7}$Li, to model systems, but has also the capabilities to help understanding diffusion processes in more complex Li ion conductors relevant for, *e.g.*, batteries [6].

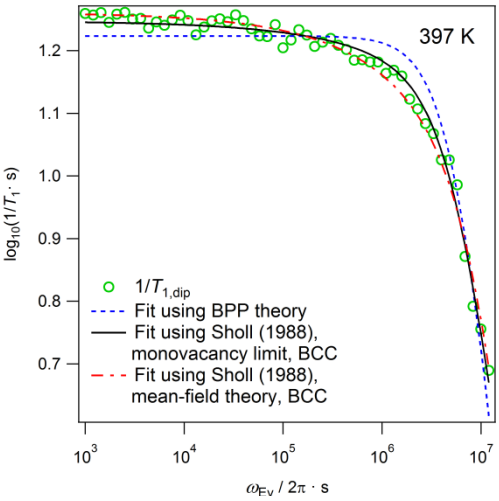


Fig. 1: Comparison of various models fitted to field-cycling $^{7}$Li NMR spin-lattice relaxation data for Li metal.

## References

[1] F. Noack, Prog. Nucl. Mag. Res. Spectr. **18** (1986) 171-276
[2] R. Kimmich, E. Anoardo, Prog. Nucl. Mag. Res. Spectr. **44** (2004) 257-320
[3] D. Kruk, F. Fujara, P. Gumann, W. Medycki, A. F. Privalov, C. Tacke, Solid State Nucl. Mag. Res. **35** (2009) 152-163
[4] R. Messer, F. Noack, Applied Physics **6**, (1975) 79-88
[5] P. Heitjans, A. Körblein, H. Ackermann, D. Dubbers, F. Fujara, H.-J. Stöckmann, J. Phys. F. Met. Phys. **15** (1985) 41-54
[6] M. Graf, B. Kresse, A. F. Privalov, M. Vogel, Solid State Nucl. Magn. Res. **51-52** (2013) 25-30