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Nanoscale Organisation and Dynamics Group

NMR relaxometry as a fingerprint of the mechanisms of molecular motion

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Abstract

Nuclear Magnetic Resonance (NMR) relaxometry is one of the most prominent methods to study dynamical processes in condensed matter. Standard NMR relaxation experiments are performed at a single resonance frequency (magnetic field) versus temperature. Profiting from Fast Field Cycling (FFC) technology, relaxation studies can be carried out in a remarkably broad frequency range encompassing five orders of magnitude, from about 1 kHz to 120 MHz (referring to ^{1}H resonance frequency). Frequency dependent relaxation studies possess the exceptional potential to reveal the underlying mechanisms of ionic motion (not only their time scale)

The principle of NMR relaxometry can be outlined as follows. The sample is initially polarized in a high magnetic field. The polarization stems from a difference in the populations of the two protons energy levels in an external magnetic field, associated with its magnetic spin quantum numbers ±1/2 and determined by Boltzmann distribution. Then the field is reduced to a lower value, B_{rel} , which is kept for a given time. The system adjusts to the new conditions – *i.e*. the nuclear spin energy levels repopulate according to Boltzmann distribution. This leads to a magnetization decay (single or multi-exponential) which is monitored versus time. The time constant describing the magnetization decay is referred to as spin-lattice relaxation time, T_1. It depends on the magnetic field, B_{rel}, which determines the resonance frequency of the nucleus, $\omega = \gamma B_{rel}$ (γ - nuclear gyromagnetic ratio). The frequency dependence of the spin-lattice relaxation rate, $R_1(\omega) = 1/T_1(\omega)$, is referred to as relaxation dispersion profile. The relaxation rate (rates for multi-exponential relaxation processes) reflects the probability of transitions between the energy levels of the system. The transitions (i.e. the nuclear spin relaxation) are induced by stochastic fluctuations of spin interactions. The interactions are modulated by molecular dynamics, like rotational and translational diffusion. Relaxation rates are given as linear combinations of spectral density functions (Fourier transform of time correlation function) of the motion modulating the interactions causing the relaxation process. Mathematical forms of spectral densities characterizing different kinds of dynamics are essentially different – in consequence relaxation dispersion experiments unambiguously reveal the mechanism of molecular motion.

The possibility of inquiring into the mechanism of molecular and ionic motion will be demonstrated for molecular and ionic liquids, as well as solid electrolytes. However, to fully profit from this “recognition tool” an appropriate quantum-mechanical theory of the relaxation processes is needed, the theory has to take into account spin interactions between different kinds of NMR active nuclei combined with complex dynamics, including many relaxation pathways. This subject will be discussed as well and illustrated by examples.

References

[1] Kruk, D.; Meier, R.; Rössler, E.A. *J. Phys.Chem.* B **115**, 951, 2011

[2] Kruk, D.; Meier, R.; Rössler, E.A. *Phys. Rev. E* **85**, 020201, 2012
[3] Kruk, D.; Herrmann, A.; Meier, R.; Rössler, E.A. (2012b) *Prog. Nucl. Magn. Reson. Spectr*. **63**, 33, 2012

Profile
Danuta Kruk: professor of physics at the University of Warmia and Mazury in Olsztyn, Poland.
Scientific interest:

- Theory of spin resonances and relaxation processes
- Dynamics of viscous liquids and glass-forming systems
- Relaxation process in condensed matter and solid state
- Dynamical properties of macromolecular systems (proteins, polymers)
- Transport phenomena and dynamics of solid and liquid electrolytes
- Relaxation processes in paramagnetic and superparamagnetic systems
- Novel contrast agents for Magnetic Resonance Imaging
- Nuclear Magnetic Resonance relaxometry for medical diagnosis

Staff and students at all levels are welcome to attend.

Venue and Time:
This talk will be held on Wednesday 21 August at 11 am at the Campbelltown Campus in Lecture Theatre 5 (CA-21.G.03). Also via **Zoom** https://uws.zoom.us/j/165195355

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