V-K Development of Broadband Solid-State NMR Spectroscopy

Ordinary NMR probes employs resonant circuits, which can be tuned only over bandwidth of a few 100 kHz. Most of the NMR probes have been well developed and are commercially available, although they are very expensive. However, solid samples often have much larger line width than the bandwidth of the resonant probe. Such examples are many of quadrupole nuclei (examples Cl, Br, I, Nb *etc.*) and metal nuclei (Pt, Rh, Hg, Pb *etc.*) having large Knight shifts. The samples containing these nuclei have been studied by rather simple methods as Hahn echo measurements or relaxation measurements by irradiating only a part of the spectral region. The whole spectra is obtained either by changing static magnetic field or by changing a carrier frequency and probe tuning. Only in a few cases, more than one carrier frequencies were employed to correlate different spectral regions.[1,2] Broadband NMR probe that does not use the resonant circuits may be necessary to conduct two-dimensional NMR experiments or automated experiments over the whole spectral range. Lowe and coworkers proposed transmission line NMR probe in 70s and it is expected to have much larger bandwidth than a normal resonant circuit.[3,4] In our study we reexamined the transmission line probe by numerical simulations and experiments.

References

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V-K-1 Numerical Simulations of the Transmission Line Probe

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The transmission line probe resembles to a circuit of a low-pass filter, which consists of π sections with a coil and two capacitors, which connect the ends of the coil to ground. To simulate the real transmission line probe, we need to include the inductive coupling between all the coils in the different π sections, which was taken into account as a parameter in the Lowe's analyses. In our analysis, we calculated the self and mutual inductance explicitly by using the Neumann's formula. The method of the simulation is based on the moment method.[1] We calculated the effective impedance, the propagation constants and the scattering matrix, which characterize the probe circuit.[2] We also calculated the strength of the rotating magnetic field as a function of carrier frequency and position. It is interesting to note that the scattering matrix is also employed in other fields as conductance of carbon nanotubes and an optical resonator.

We compared our numerical results with the analytical equations derived by Lowe. We found that their equations agree well with our numerical results, if the self-inductance of the low-pass filter was replaced by the average inductance, which is defined as the total inductance divided by the number of π sections. We considered a rectangular flat coil with a pitch p, wire length $l \gg d$ (d is the length along static magnetic field), number of turns N_i and cable impedance Z_0. We modified one of Lowe's equations and found that the rotating field at the coil center becomes an exponentially decaying function of carrier frequency ν,

$$|B_+| = (\mu_0 V_{\rm in}/2Z_0 p)\exp(-\nu/\nu_d),$$

where $\nu_d = (2Z_0/\pi\mu_0 l)(p/d)^2$ and $V_{\rm in}$ is the input voltage. To obtain large RF field, the pitch of the coil or the impedance of the probe must be small. The latter need the impedance transformation from the cable impedance of 50 Ω. The above equation also requires that ν_d must be much larger than the observed frequency, which restricts the dimensions of the coil.

We also found that the reflection of wave takes place near both ends of the coil. Since the coil near the ends have only one neighbor, their total inductance is smaller than that at the center. The reflection causes the undulation of magnitudes of currents over different π sections and also the undulation of the field strength, thus spoils the homogeneity of the magnetic field. We could also see the effect of diffraction at the carrier frequencies where the phase delay through the probe becomes close to integer multiples of π. Near these frequencies, the effective impedance showed a dispersion curve and the propagation constant became real positive, which means that the circuit absorbed the energy. Next we varied the pitch of the coil and made it smaller near both ends. This treatment suppressed the undulation of currents and thus improved the homogeneity of the RF field in the coil.

References

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