Kinetic parameters of photo-excited triplet state of pentacene determined by dynamic nuclear polarization

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A polarized proton target prepared by dynamic nuclear polarization (DNP) techniques, which is a means of transferring electron spin polarization to nuclei by microwave irradiation, has been extensively used in particle and nuclear physics experiments.[1)] However, in these studies, DNP is carried out at a cryogenic temperature of <4.2K and in a high magnetic field of several Tesla. On the other hand, DNP using photo-excited triplet states (Triplet-DNP) can produce high nuclear spin polarization without such equipment, by using the non-equilibrated electron spin polarization in the lowest photo-excited triplet state generated by laser irradiation.[2)]

In this paper, we determined kinetic parameters of the triplet electron spin of pentacene, which is mainly used as a polarizing agent in Triplet-DNP, to optimize the polarization transfer sequence for maximizing the polarization of the target. Although the polarization of the triplet electrons is initially higher than 70%, it decreases as a function of time after the optical excitation. There are two processes relevant to this phenomenon: one is the decay from the triplet state to the ground state, while the other is the relaxation to the thermal equilibrium in the triplet state. The time constants are referred to as lifetimes (τ_i, i=+1, 0, -1: i represents the sublevels in the triplet state) and spin-lattice relaxation time (T_1).

We determined the time constants of pentacene doped into p-terphenyl in 0.3 T and at room temperature, based on the NMR signal intensities of proton spins enhanced by Triplet-DNP. A continuous-wave Ar-ion laser pulsed by an optical chopper is used for optical excitation. We first measured the delay-time (the timing of microwave irradiation for polarization transfer) dependence (Fig. 1(a)). Analysis using only this data revealed a difficulty in separating the contributions of τ_i and T_1. We thus utilized the pulse-structure (the duty and the repetition rate of laser pulse) dependence data as additional information (Fig. 1(b)). The combined analysis of these data allowed us to separate the contributions of the parameters. The values of τ_0 and $\tau_\pm$ were determined to be 22.3 $\mu s^{+3.0\ \mu s}_{-1.5\ \mu s}$ and 88 $\mu s^{+13\ \mu s}_{-19\ \mu s}$, respectively (Fig. 1(c)). The value of T_1 was found to be longer than 300 μs. It was also found that the proton signal enhancement is limited at a high repetition rate owing to the partial cancellation of the electron spin polarization by the remaining population produced by the preceding laser pulses.

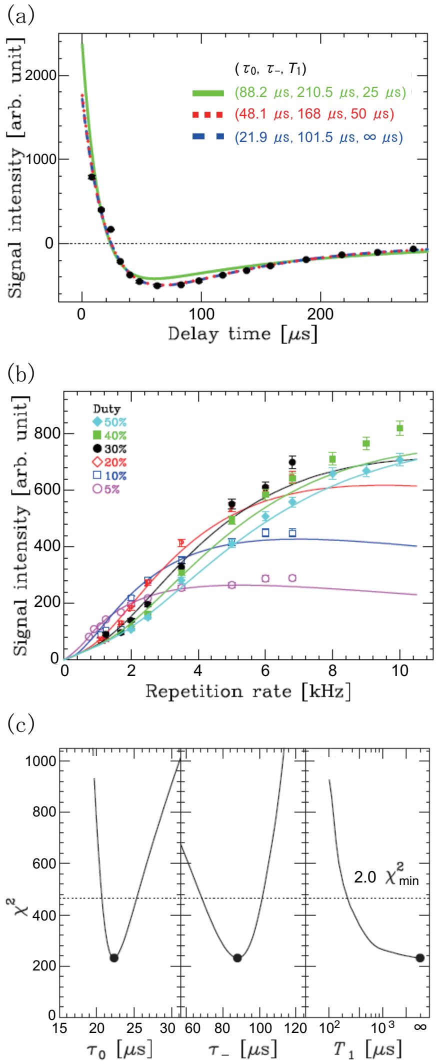

Fig. 1. (a) the delay-time dependence of the NMR signal intensities of proton spins enhanced by Triplet-DNP. (b) the pulse-structure (the duty and the repetition rate of laser pulse) dependence of the signal intensities. (c) Variation of the chi square values of τ_0, τ_-, and T_1.

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