Development of data-collection and data-analysis systems for time-resolved ESR experiments

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Nuclear magnetic resonance (NMR) is a valuable tool for biochemistry and medical science. The signal strength of NMR can be boosted significantly using dynamic nuclear polarization, which transfers the electron polarization to that of the nucleus. However, the conventional and well-understood polarization molecule pentacene[1)] is not water solvable, and that limits its biological application. Various water-solvable pentacene derivatives have been synthesized (from collaborations) and their molecular structure needs to be studied via the electron spin resonance (ESR) spectrum. We are developing a data-collection system to simplify the labor of this task.

The data-collection system is illustrated in Fig. 1. The sample of pentacene derivative is placed inside a dielectric microwave chamber with a narrow resonance frequency band. A pulsed laser[2)] is fed into the chamber to excite the electrons from the ground singlet state to the excited triplet state. The laser also triggers the oscilloscope to record the time-resolved ESR signal. The strength of an external magnetic field is fixed for each measurement, but it can vary from 0.0 T to 3.8 T and is controlled by a DC voltage power supply. The DC voltage is fed to a voltage-to-current convertor to supply a steady current to the magnetic coil. The magnitude of the magnetic field is measured using a Hall probe. A typical ESR signal is show in Fig. 2.

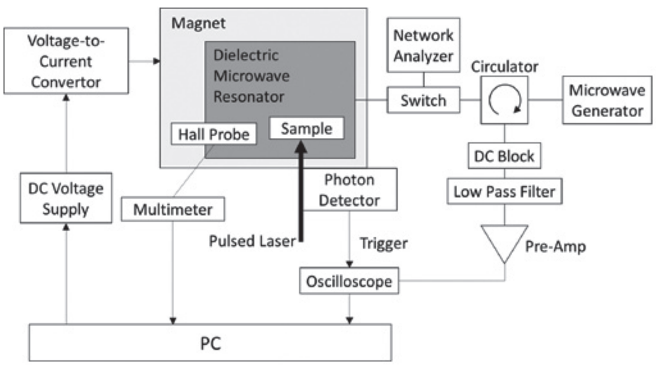

Fig. 1. Illustration of the ESR system.

A custom-built data-collection program with a graphical user interface (GUI) sets the control voltage, gets the Hall probe voltage, obtains the time-resolved ESR signal from the oscilloscope, and saves the signal into a file for analysis. Using the program, the strength of the magnetic field can be swapped and the data-collection process is fully automatic once the initial setup is done.

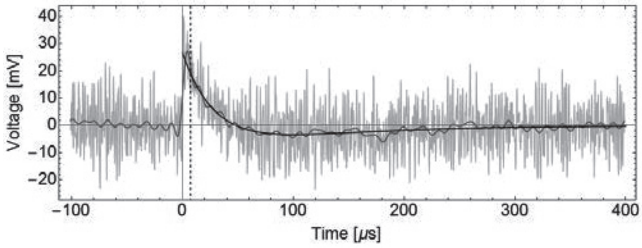

Fig. 2. Typical ESR signal (light gray). The gray line indicates the 100 kHz cutoff obtained using a Fourier transform. The black line is fit to the gray line using Eq. (1). The fitting uses the region after the dashed line.

The 2-dimensional data (time-resolved signal for each magnetic field setting) can be analyzed using a custom-built cross-platform GUI analysis program. The time-domain signal has the form

$$f(t) = a \exp\left(-\frac{t}{T_a}\right) - b \exp\left(-\frac{t}{T_b}\right), \quad (1)$$

where a and b are the relative populations of the energy levels and T_a and T_b are the lifetimes of the corresponding energy levels. The Levenberg—Marquardt algorithm is used to fit the non-linear function against the time-resolved signal. The effective magnitude of the electron polarization is

$$P = \frac{|a| - |b|}{|a| + |b|}. \quad (2)$$

The program also has other functions. It can be used as a plotting tool, for example, to plot the contour of the data. The program also provides a 2-dimensional Fourier transform[3)] and different digital filters for noise elimination, for example, a sharp-cut low/high-pass filter and conventional low/high-pass filter. The filter can be applied as many times as needed to create filters such as a band-pass filter.

We are now developing a cross-platform GUI database program. The database stores the properties of the samples and their measurements. Other denoising methods such as discrete wavelet transformation will be evaluated.

References
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3) FFTW3.35, www.fftw.org.

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