Akira Naito, Materials Science and Nanotechnology

Microwave heating mechanism of liquid crystals as revealed by microwave irradiation NMR spectroscopy

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Microwave (MW) heating effects are widely used in the acceleration of organic and enzymatic reactions. These effects are primarily caused by the local heating induced by MW irradiation. However, the detailed molecular mechanisms associated with MW heating effects on the chemical reaction have not yet been well understood. This study investigated the MW heating effect of N-(4-methoxybenzyliden)-4-butylaniline (MBBA) in liquid crystalline and isotropic phases using *in situ* MW irradiation ^{1}H NMR spectroscopy. The instrument used in this study consist of a solid state NMR spectrometer, equipped with a MW generator which is capable of transmitting 1.3 kW pulsed or continuous MW at a frequency of 2.45 GHz. A 3 mm wide flat copper ribbon was used to form the capacitor of the resonance circuit, and was wound coaxially inside the radio wave circuit. MWs were transmitted from the MW generator to the vicinity of the magnet through the MW, which served a coaxial cable and finally the MW were guided to the resonance circuit at the probe head. The application of MW irradiation at 130 W for 90 s while maintaining the spectrometer temperature at 20 °C generated a small amount of isotropic phase within the bulk liquid crystal (Fig. 1 top). The partial transition to the isotropic phase can be attributed to a non-equilibrium local heating state induced by the MW irradiation. The application of MW at 195 W for 5 min to isotropic MBBA while maintaining a spectrometer temperature of 50 °C raised the sample temperature to 160 °C. However, CH_3-O, and CH=N protons showed the temperatures at 220 and 350 °C, respectively. It is revealed that the different protons indicated significantly different their temperatures within the molecule (Fig. 2 bottom). This result is realized as a distinctive microwave heating effect.

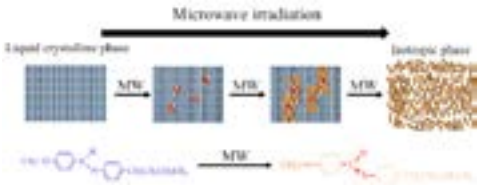

Figure 1: MW heating processes of liquid crystalline MBBA and the molecule.

Biography

Akira Naito obtained his Ph D. from the Chemistry Department of Kyoto University, Japan, working with Prof. K. Akasaka on radiation damage of disulfide radicals as studied by ENDOR spectroscopy. He later worked as a post-doctral research fellow with Prof. C.A. McDoewell, University of British Columbia, Canada. Since 2001, he has been a Prof. in Yokohama National University, Japan. His main research interests are improving the magnetically oriented bilayer system and developing microwave irradiation and photo-irradiation solid-sate NMR spectrometers. He applied the microwave irradiation NMR to liquid crystal systems to reveal the microwave heating mechanisms and initiated state correlated 2D NMR spectroscopy [1,2]. He also applied photo-irradiation NMR to biological systems such as photoreceptor membrane proteins [3] to reveal the photoreaction processes.

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