Solid State Nuclear Magnetic Resonance Study of Nanocarbons

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In this paper, we review solid-state nuclear magnetic resonance (NMR) investigations of different nano-carbon compounds. The NMR spectra and chemical shielding tensors in nano-graphite, pure and doped fullerenes, carbon nanotubes, nanodiamonds and onions and their application for the characterization of the compounds are discussed.

The NMR study of ultrananocrystalline diamond (UNCD) materials produced by detonation technique, which is carried out under financial support of New Energy Development Organization of Japan (grant # 04IT4), is reported in more detail. Analysis of the static and MAS ^{13}C and ^{1}H NMR spectra, spin-spin and spin-lattice relaxation time in crude and purified UNCD compounds is presented. The crude sample (detonation soot) is a mixture of UNCD particles and turbostratic graphite. The latter is significantly reduced as a result of purification. Our measurements show that UNCD particles consist of diamond core that is covered (at least partially) by a fullerene-like sp^2-carbon shell.

Significant increase in the spin-lattice relaxation rate (in comparison with that of natural diamond), as well as stretched exponential character of the magnetization recovery, are attributed to the interaction of nuclear spins with paramagnetic centers, which are likely fabrication-driven dangling bonds with unpaired electrons. Our NMR data, along with the EPR measurements, show that these centers are located mainly at the interface between the diamond core and shell. The outer surface comprises a number of hydrocarbon groups that saturate the dangling bonds. The origin of the aforementioned hydrocarbon groups is discussed in connection with the preparation, purification and surface treatment procedures and calculations of the stability of hydrogenated and dehydrogenated nanodiamond surfaces.

Investigation of the structure modification due to hydrothermal treatment of the UNCD compounds is also reported.