Diamond nanoparticles with functionalized surface –a NMR study

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Nanodiamond (ND) particle consists of a mechanically stable and chemically inert diamond core and a chemically active surface. On-purpose functionalization of the ND surface with targeted species allows preparation of NDs with specified chemical, physical and electronic properties. Here we review our recent NMR studies of structure, chemical bonding and properties of fluorinated (F-ND), hydroxylated (OH-ND) NDs and those with surface decorated by transition metal ions (Cu-ND and Co-ND).

In F-ND, we obtained formation of different fluorocarbon groups on the nanodiamond surface, which substitute for hydrocarbon and hydroxyl groups. Our data provide detailed information about the structure and bonding in both diamond core and surface of the F-ND particle. The NMR data are supported by EPR, XPS and Raman findings. F-ND sample has a significant number of paramagnetic defects located mainly near the diamond surface, resulting in faSt ^{19}F and ^{13}C nuclear spin-lattice relaxation.

NMR studies of Cu-ND and Co-ND exhibit that chemical modification results in appearance of paramagnetic Cu^{2+} and Co^{2+} complexes at the ND surface. This conclusion comes from the increase in the ^{1}H and ^{13}C nuclear spin-lattice relaxation rates of the surface hydrocarbon and hydroxyl groups and of the diamond core carbons obtained in the experiment, revealing appearance of paramagnetic Cu^{2+} and Co^{2+} complexes at the ND surface and their interaction with the hydrogen and carbon nuclear spins. Subsequent annealing of the modified samples up to 900°C results in an inverse process, i.e., a reduction of the relaxation rate, indicating that these complexes are destroyed, and metal ions join each other forming copper and cobalt nanoclusters.

OH-ND reveals complex spectra consisting of several components coming from the diamond core, surface CH_x and C-OH groups and adsorbed moisture.