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ESR and Magnetic Susceptibility Studies of Graphite Nanoparticles: Density of States Anomaly Near the Fermi Level

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The presence of open edges around the peripheral region can result in occurrence of specific features in nanographites, which are different from bulk graphite and their closed-surface counterparts [1]. The calculations show that one dimensional graphite ribbons with zigzag edges possess localized edge states with energies close to the Fermi level [1]. In a general finite graphene sheet consisting of several types of edges, even a few zigzag sites per sequence also are lead to the non-negligible edge-state effects, resulting in an enhancement in the electronic density of states around the Fermi energy [1]. In this report, we present ESR and magnetic susceptibility research work results of nanographites - the structural blocks of activated carbon fibers (ACFs), in order to clarify their structure and electronic properties near the Fermi level.

According to our X-ray diffraction data in ACFs studied, the nanographites consist of 3-4 graphen sheets and have an average in-plane size of L_a ~ 20 Å. The distance between carbon layers d_c in nanographite is equal to 3.75 Å that is much more, than in bulk graphite (3.354 Å).

The ESR spectra of ACFs reveal two Lorentzian signals. At temperatures above ~150 K one broad signal from conduction electrons with a linewidth ~40 mT is observed. Below ~150 K, a second narrow signal from localized states appears with a linewidth ~3 mT. The g values are estimated at g=1,98 and 2,01 for the signals from conduction electrons and localized states, respectively. The conduction ESR (CESR) signal is practically symmetric, that specifies a weak anisotropy of the g-factor. At lowering of the temperature the CESR signal linewidth increases at constant values of the g-factor and integral intensity.

The magnetization curve shows the absence of the residual magnetization at different constant magnetic fields. The temperature dependence of the magnetic susceptibility χ_g for ACFs investigated is well described by the expression χ_g=1.318e-5/(T+0.9)-0.61e-6. From this low, it follows that approximately one localized spin per 2500 carbon atoms (or ~1 localized spin per 10 nanographites) are presented in fibers at low temperatures.

From comparison of integral intensities of signals from conduction electrons and localized spins (the concentration of latter is known from the magnetic susceptibility data), the density of states near the Fermi level in nanographites was estimated. Such calculations show, that it is more than two orders of magnitude larger than in bulk regular graphite at the same value of Fermi energy. The results obtained unambiguously indicate the presence of an additional band around the Fermi energy in nanographites.

At adsorption by ACFs of water and some other molecules, the d_c and the stacking order of graphen sheets in nanographite reversibly decreases and increases, respectively. Simultaneously, the CESR linewidth reversibly increases. The correlations found between changes of structural, electronic and magnetic parameters of nanographites are discussed.

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1) O.E. Andersson et al.: Phys. Rev. B, **58**, 16387, **1998**.