Unconventional Electronic and Magnetic Features of Nanodiamond and Nanographite

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Nanocarbon has been an important target in cutting-edge nanotechnology and nanoscience, in which fullerenes and carbon nanotubes have been intensively investigated. Among these nanocarbon systems, nanodiamond and nanographene/nanographite are also important partners, which have electronic features essentially different from those of fullerenes and carbon nanotubes, although they have not been well investigated. Nanodiamnod consisting of sp^3 bond network is expected to have a variety of electronic features when its surface is modified by different chemical species or different carbon structures. Nanographite/nanographene is characterized by a nanosized flat sp^2/π hexagon network having edges around its periphery, in contrast to the closed π-bond structure in fullerenes and carbon nanotubes.

We investigated the electronic and magnetic features of nanodaimond with its surface modified and nanogarphite. The surface of nanodiamond particles with the mean size of ca.5 nm is terminated with hydrogen atoms by hydrothermal treatment in supercritical water at 650°C and 100 MPa. The hydrogen content increases as the treatment time is elongated up to 40 h, and then it is lowered after a discontinuous drop. The increase in the hydrogen content works to increase the localized spin concentration in the first stage (<40 h) of the hydrothermal treatment. The treatment above 40 h decreases the spin concentration. These experimental findings are suggestive of the presence of a surface structural reconstruction around 40 h. The temperature dependence of the susceptibility indicates an antiferromagnetic short range ordering having a strong exchange interaction. This proves that localized spin clusters are created in collective defects of hydrogen-terminated surface. The surface structural reconstruction is considered to be caused by the electronic instability of the diamond surface.

Nananographene, whose periphery is described in terms of a combination of zigzag and armchair edges, has unconventional electronic structure depending on its edge shape. According to theoretical prediction, the zigzag edge has nonbonding π-electron state having localized nature (edge state), which makes nanographite strongly magnetic in essential contrast to diamagnetic bulk graphite. Using UHV-STM/STS observations, where the edge carbon atoms are hydrogen-terminated, the edge state was successfully observed as a large local density of states localized around the zigzag edges and a sharp density-of-state peak located?around the Fermi energy, superimposed upon the bonding π- and antibonding π^*-states, in spite of the absence of the edge state in the armchair edges.