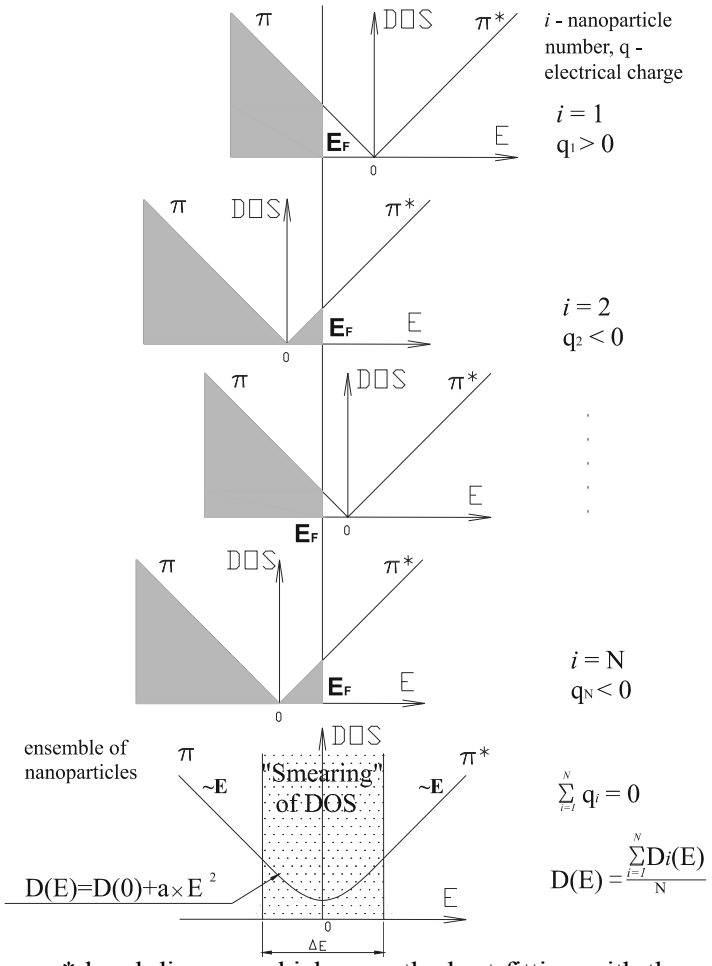
"Smearing" of density-of-states in nanographite

V.Yu. Osipov[1], T. Enoki[2], K. Takai[2], A. Volgaev[1], and A.Ya. Vul'[1]

[1]*Ioffe Physico-Technical Institute, Polytechnicheskaya 26, St.Petersburg, 194021 Russia*
[2]*Tokyo Institute of Technology, 2-12-1 Ookayama, Meguro-ku, Tokyo 152-8551, Japan*

The temperature dependence of orbital diamagnetic susceptibility in nanographite derived from detonation nanodiamonds (mean size 5 nm) is very weak in comparison with the same one for bulk graphite [1]. This weak temperature dependence is well described by the phenomenological Kotosonov (K) equation [2,3] and not by well known McClure equation proposed for infinite sheets of quasi-two dimensional (2D) qraphite. The microscopic reason of that why K-equation works well was not understood well before and was an unresolved question for the theory. In this paper we try to resolve this problem. We apply the model of ensemble of individual nanographite particles with different position of Fermi level respecting the point (0,0) on the π-π* band diagram for DOS and ordinary McClure equation for each individual nanographite particle in order to describe the temperature dependence of orbital susceptibility. The origin of different positions of Fermi levels in the individual nanoparticles is a different discrete electrical charge of a few number of π-electrons or holes. In general, the exact position of Fermi level at fixed temperature in the each nanoparticle of the ensemble can be found from the condition of charge neutrality of the whole system. We found the shape of statistical distribution of the Fermi lever around the cone point (E=0) on the π-π* band diagram which gave the best fitting with the experimental data followed to Kotosonov equation. This shape of statistical distribution of the Fermi level has a peak at $E_F = 0$ and the width around 60 meV. Because the absolute position of the Fermi level on the energy scale for all of nanographite particles should be the same, it leads to the "smearing" of DOS function around the contact point between the valence and conductive bands for the whole ensemble of nanoparticle and is a one of the microscopic reasons responsible for the weak temperature dependence of orbital susceptibility in nanographite. Thus, the "smearing" of DOS (ΔE) is determined by the lineshape of statistical distribution of Fermi energy. The results of computer simulations which were done are analyzed in this paper.



[1] V.Yu. Osipov, T. Enoki, K. Takai, K. Takahara, M. Endo, T. Hayashi, Y. Hishiyama, Y. Kaburagi, A.Ya. Vul', *Carbon.* **44**(7), 1225-1234 (2006).
[2] A.S. Kotosonov, *Carbon.* **259**(5), 613-615 (1987).
[3] A.S. Kotosonov, *Carbon.* **26**(2), 189-195 (1988).