THE COVALENT THEORY OF METALLIZATION AND MAGNETIC ORDER OF CARBON NANOTUBES

Mitsek A. I.*, Pushkar V. N., Mitsek V. A.
Department of Solid State Theory, G. V. Kurdyumov Institute for Metal Physics, N.A.S.U.,
36 Academician Vernadsky Blvd., UA-03680 Kyyiv-142, Ukraine
* *Fax: +(380) 44 4242561; E-mail: tatar@imp.kiev.ua*

The quantum theory must take into account the covalent bonds. It is built in the many-electron operator spinors (MEOS) representation for C-ions. The localization condition of electrons on covalent orbits allows to define correctly the MEOS in the Fock spaces.

Fullerene (FUL) and carbon nanotube (CNT) C^{12} are considered as two-dimensional closed semiconductors (s/c) with covalent bonds of C^{4+} ions. The chemical bonds fluctuations (CBF) lead to appearance of C^{3+} and band electron (hole). The ionization energy decreased by them causes narrowed forbidden band $E_g \leq 1$ eV. 3*d*-ions placing (Fe^{3+} ions with spin $S = 3/2$ are considered) creates another channel for band fermions. C–Fe covalent bonds with energy $|\Gamma| \sim E_0$ create admixture band of FUL and CNT. The conditions of conduction band formation from it are defined.

FUL and CNT metallization depends strongly on correlation between E_0 for 2*p*-electrons of C^{12} and delocalization energy Γ. When $|\Gamma| < E_0$, FUL or CNT systems (films, for example) are in s/c state and $E_g \sim E_0 - |\Gamma|$. The covalent bond, strong enough $|\Gamma| > E_0$ favours the delocalization of hybridized 2*p*–3*d*-electrons (holes). The Fermi energy $\varepsilon_F \sim (|\Gamma| - E_0) << 1$eV. The tensor of hole effective mass m_h is defined by $\Gamma(\mathbf{k})$ dispersion. Electron effective mass m_e is defined by dispersion of hopping integral $t(\mathbf{r} - \mathbf{R})$ between ions in the sites **r** and **R**.

3*d*-ions clusters in CNT are considered as ferromagnetic (FM) particles for the case of FM exchange between 3*d*-ions. Its value is $A_{11}/k_B \sim 10^3$K for Fe^{3+}-ions. Indirect exchange interaction Fe–C–Fe of covalent nature $|A_{12}| << A_{11}$ create magnetic order of CNT. The consideration of CNT system (for example, film) with exchange interaction between CNT ($|A_{13}| << |A_{12}|$) allows to calculate the magnetization $M(T,\mathbf{B})$ as a function of temperature T and magnetic field **B**. The results of numeral calculation are given for FM signs of exchange integrals. The obtained theoretical dependences $M(T,\mathbf{B})$ allow interpreting the experimental data for any systems of FM nanoparticles.

The theory allows taking into account magnetic anisotropy (MA) of nanoparticles. Numeral results for $M(T,\mathbf{B})$ of CNT system with MA alternate signs ($K_1 > 0$ or $K_1 < 0$) differ noticeably from results for superparamagnetic systems. The nature of exchange integrals A_{1n} ($n = 1, 2, 3$) and one-ionic MA of CNT system is discussed.