Structure and electronic properties of single-walled carbon nanotubes intercalated by transition metal halogenides

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Single-walled carbon nanotubes (SWCNTs) are studied intensively during laSt decade due to their unusual electronic, chemical and structural properties accompanied by extraordinary mechanical behavior with all these features being strongly dependent on the diameter and conformation of tube. Currently, the researchers are focused on finding tools to govern the electron structure of nanostructures designed on the basis of single-walled carbon nanotubes (SWCNT) [1]. One of the approaches is given by filling the internal channels of nanotubes with inorganic one-dimensional nanocrystals. In some cases, this approach makes it possible to get the material with well-defined electron structure and properties even without separating of SWCNTs on their size and chirality [2].

The aims of our study were the controllable growth of 1D nanocrystals (AgHal, CuHal and $MHal_2$, where Hal=Cl, Br, I and M=Mn, Fe, Co, Ni, Zn) in channels of single-walled carbon nanotubes with inner diameter 1-1.4 nm and investigation of structure and electronic properties of these nanostructures. The synthetic strategy was based on the impregnation of pre-opened SWCNTs by molten salts in vacuum.

The atomic structure of Ag and Cu halides within SWCNTs was found to correspond to distorted two-layer *hcp* of halide atoms arranged laterally with respect to the SWCNT and metal atoms located in incomplete octahedral positions. EXAFS data revealed the metal atoms coordination with nanotube walls in nanocomposites, and it was also proved by HAADF HRTEM imaging. According to work function measurements, Fermi level downshift of SWCNTs was observed for all composites. XPS data exposes an acceptor behavior of metal halides accompanied by partial charge increase on halogen atoms while no noticeable alteration of charge was observed on metal atoms. Raman spectroscopy performed under an electrochemical charging enabled the direct determination of charge transfer efficiency for selective-chirality metallic SWCNTs intercalated by metal halogenides.

[1] Tans S.J., Verschueren A.R.M., Dekker C., *Nature* **393**, 49 (1998).
[2] Dresselhaus M.S., Dresselhaus G., Saito R., *Carbon* **33**, 883 (1995).