ABSTRACT

Carbon nanotubes, due to their unique properties, such as: large surface wettable by electrolyte, very good electrical conductivity and high chemical, mechanical and electrochemical stability, are potentially a good electrode material, e.g., in lithium-ion batteries. In addition to the conductive properties, the excellent tensile and flexural strength of CNTs can also be used. However, despite their exceptional properties, a major limitation in their use is their low chemical reactivity and hydrophobicity, and the formation of agglomerates. To solve these problems, many methods of covalent and non-covalent modification of the CNT surface are used, thus improving the dispersion and processing/ application possibilities of nanotubes.

The aim of the study was to obtain new, functional materials based on multi-wall carbon nanotubes functionalized with phosphoroselenoates derivatives for use as potential components of lithium-ion cells. The method of synthesizing new electrode materials was carried out in several stages. In the first step, sodium and lithium *O,O*-dialkyl(aryl) phosphoroselenoates were synthesized by reaction with metal alkoxides or hydrides. The next step was the covalent attachment of bromine to MWCNTs in order to improve their chemical activity. Then, chemical functionalization of brominated MWCNTs with phosphoroselenoates was performed. The resulting products were identified and characterized by the following methods: scanning and transmission electron microscopy imaging (SEM and TEM), X-ray microanalysis (EDS), X-ray photoelectron spectroscopy (XPS), Fourier transform infrared spectroscopy (FT-IR) and Raman and nuclear magnetic resonance (NMR) spectroscopies, X-ray diffraction (XRD), thermogravimetric analysis (TG/DTG). The ability to store energy was tested in three-electrode cells (Swagelok® type) and coin cells by performing chronopotentiometry and cyclic voltammetry analyzes. Additionally, by determining the potentiokinetic polarization curves of the electrode materials, an assessment of their susceptibility to corrosion was made.

As a result of the conducted reactions, it was possible to obtain sodium and lithium *O,O*-dialkyl(aryl) phosphoroselenoates and brominated MWCNTs, which were used to synthesize their new organoselenophosphorus derivatives. Cells composed of nanotubes modified in this way were characterized by greater stability of work and higher capacity in relation to native nanotubes. This gives the possibility of the potential use of the new electrode materials as a component of lithium-ion batteries, replacing the commercially used graphite in anodes.

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