

Influence of the carbon nanoparticles structure on their lithium storage capacity

L.L. Lapteva,^{1,2} Yu.V. Fedoseeva,^{1,2} E.V. Shlyakhova,^{1,2} L.G. Bulusheva,^{1,2} A.V. Okotrub^{1,2}

¹*Nikolaev Institute of Inorganic Chemistry SB RAS, 3 Acad. Lavrentiev Avenue, 630090 Novosibirsk, Russia*

²*Novosibirsk State University, 2 Pirogova Street, 630090 Novosibirsk, Russia*

lapteva.l.l@yandex.ru

Investigation of carbon/lithium interface is an urgent task for energy storage devices such as lithium-ion batteries and supercapacitors. It has been shown that single-walled carbon nanotubes (SWCNTs) and porous carbon materials are successful for electrochemical applications. We used commercial SWCNTs by OCSiAl and porous carbon grown via CVD from ethanol, toluene and acetonitrile. To characterize the samples high-resolution transmission electron microscopy, scanning electron microscopy, Raman spectroscopy and optical absorption spectroscopy were applied. The SWCNT sample is a mixture of semiconducting and metallic single-walled nanotubes of different diameters. The average diameter of SWNTs was estimated to be 1.7 nm. In addition, we found that porous carbons synthesized from ethanol and acetonitrile have thin-layered sponge-like structure, while porous carbon grown with toluene is enriched by hollow capsules of 10 nm thickness.

We have studied the effect of vacuum thermal vapor deposition of lithium on SWCNTs and porous carbon by in situ X-ray photoelectron spectroscopy (XPS) and near-edge X-ray absorption fine structure spectroscopy. The low ratio between lithium and carbon materials means that carbon materials are incompletely covered by Li. In case of SWCNTs, two types of carbon atoms, which are located close to and away from Li atoms were emerged clearly. Quantum-chemical modeling of XPS spectra and calculation of atomic charges and molecular electrostatic potential maps showed that carbon atoms located near Li atoms are in strong positive electric field from Li, whereas Li-free regions have negative electrostatic potential. Similar effects should be for porous carbon but they can not be separated because of a large amount of defects.

Electrochemical studies were carried out in half cells, using lithium metal foil as anode and porous carbon as cathode. The cells were galvanostatically charged and discharged over the potential range from 0.01 to 2.50 V versus Li/Li⁺ at various current densities. The charge-discharge voltage curve revealed different behavior for fast and slow cycling which is explained by various conductivity, pore size and surface area of the samples.

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