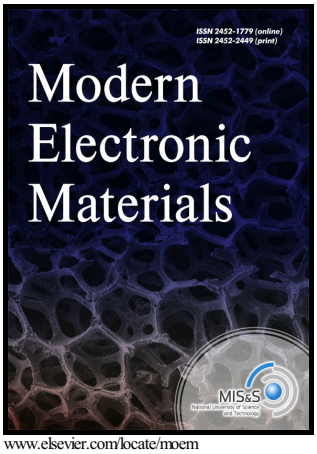

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METAL-CARBON NANOCOMPOSITES BASED ON PYROLYSED POLYACRYLONITRILE

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Abstract. The electronic structure and geometry of metal−carbon nanocomposites based on pyrolyzed poliacrylonitrile (PPAN) with Cu, Si, Fe, Co and Ni atoms using the DFT method have been theoretically studied. The effect of nitrogen on the stability of PPAN and its conductivity has been determined. The electrophysical properties and structure of metal nanocomposites have been studied using the XFA method. The composites have been produced by IR heating. We suggest that metal−carbon nanocomposites form due to the special processing of the (PAN−MeR) samples. Metal nanoparticles are regularly dispersed in the nanocrystalline matrix of PPAN. The conductivity of these metal−carbon nanocomposites has an activation character and varies from 10^{-1} to 10^{3} Om/cm depending on synthesis temperature (T = 600—900 °C). The results of theoretical and experimental research are in a good agreement.

Keywords: pyrolyzed polyacrylonitrile, transition metals, metalcarbon nanocomposites.

Introduction

Advanced electronics demonstrate a blistering technical progress causing an exponential decrease (in time) of the sizes of objects and the development of nanotechnology. Nanotechnology deals with objects of nanometer size (at least one dimension of which is less than 100 nm) and methods of their fabrication and implementation [1]. Advanced electronics may find use for new materials in the form of metal-carbon nanocomposites which at the nanoscale are dispersions of organic materials (with particle sizes of approx. 1 to 100 nm) in a carbon matrix and combining the practically useful advantages of organic and inorganic materials. For example, metal-carbon nanocomposites can be used as efficient screens reducing the electromagnetic emission of cell phones. For example, introduction of a copper containing composite in a layer of 3 mm thick non-screening phone coating is capable of screening electromagnetic radiation at 1-2 GGz frequencies with a 65 dB efficiency.

Currently there is intense research of metal-carbon nanocomposites based on organic semiconductors. Much attention is paid to the pyrolysis of poliacrylonitrile (PAN) resulting in a carbon material having very promising physical, chemical and mechanical properties. An efficient method was proposed for the application of carbon coatings using intense IR irradiation (IR heating) [2-9]. The chemical transformations occurring during IR heating of PAN lead to the formation of poly-conjugate structures. The ordering degree of these structures is determined by the intensity of IR radiation (temperature of IR heating) and the duration of treatment. The resultant coatings have a complex multiphase structure the main component of which is a graphite-like carbon phase. In the presence of metal compounds the chemical transformations in the PAN undergo a number of changes resulting in lower formation temperatures of the cyclic polymer structure and eventually in the formation of metal nanoparticles homogeneously distributed and intercalated in the structure of the carbon matrix. The properties of metal-carbon nanocomposites depend on the nature of interaction between the phases and the structure of the interphase regions the volume fraction of which may be as large as 50%. The interphase regions have specific mechanical properties that differ from those of both the matrix and the metallic nanoparticles. In nanocomposites, the surface of nanoparticles is bonded with the carbon matrix and forms ionic and coordination bonds that limit the mobility of molecular chains and their segments.