Investigating the Mechanism for the Covalent Chemical Modification of Multiwalled Carbon Nanotubes Using Aryl Diazonium Salts

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Abstract

The mechanism involved in the modification of carbon nanotubes (CNTs) funtionalised using diazonium salts has been investigated. Bamboo-like and hollow-tube multiwalled carbon nanotubes (MWCNTs) were covalently modified using 4-nitrobenzenediazonium tetrafluoroborate. The MWCNTs were derivatised in the presence and absence of hypophosphorous acid as a mild reducing agent and the resulting materials were characterised using cyclic voltammetry. The observed peak potentials for the modified materials were found to differ depending on the derivatisation conditions (presence / absence of hypophosphorous acid, diazonium salt concentration and temperature) and these defferences were interpreted mechanically. The experimental results suggest that, in the absence of hypophosphorous acid, the derivatisation mechanism likely proceeds through a cationic intermediate, whilst in the presence of the hypophosphorous acid the mechanism probably involves either a purely radical intermediate or a mixture of radical and cationic species depending on the concentration of the hypophosphorous acid reducing agent and the reaction temperature. Polymerisation of the nitrophenyl groups on the surface of nanotubes was studied using different concentrations of 4-nitrobenzenediazonium tetrafluoroborate and was found to increase with increasing concentration of cationic intermediates. The effect of the reaction temperature on the derivatisation was explored over a range of temperatures from 5 to 50

0C and the optimum derivatisation temperature was determined in

the presence and absence of hypophosphorous acid. It was found to be 20

0C and 35

0C in the presence

and absence of hypophosphorous acid respectively.