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Title of Thesis: Functionalization of Carbon Nanotubes and Their Device Applications

Abstract

The study of matter at nanometer scale is extremely significant as materials synthesized at nano scale exhibit drastically different properties compared to their properties on macro scale. Nanotechnology is the application of the principles of nanoscience to create new, useful and functional materials, devices and systems. This is achieved through the control and manipulation of the matter at the nano scale and the exploitation of novel material properties. Upto early 1980s, only three forms of carbon were known to exist, namely; graphite, diamond and amorphous (non-crystalline) carbon. The worldwide enthusiasm came in 1991 when Japanese scientist Sumio Iijima unexpectedly discovered some needle shaped material which he called “microtubules” of carbon during the arc- discharge synthesis of fullerenes. This by-product material obtained in the synthesis of fullerenes, later, came to be known as carbon nanotubes. Despite their extraordinary properties the tremendous potential of carbon nanotubes is often hindered due to their chemical inertness which causes their agglomeration. This agglomeration makes them unprocessable which poses a major challenge for their successful utilization in several applications. Functionalization is the procedure which involves the attachment of functional groups on the ends and sidewalls of carbon nanotubes. Thus functionalization enhances their dispersibility, processability and compatibility and enables the translation of their remarkable properties to other matrices leading to the creation of highly functional materials.

In the present thesis an attempt has been made to functionalize carbon nanotubes and to explore their application potential as (a) an anti-static material (b) a thermoelectric (TE) material and (c) a supercapacitor electrode material. Chemical oxidative route (by nitric acid treatment) has been employed to graft functional groups (COOH groups) on the ends and side walls of carbon nanotubes. The improved properties of carbon nanotubes caused by functionalization have been further complemented by synthesizing their composite with one of the most versatile conducting polymers; the polyaniline. This

synergy between the two materials has been exploited to broaden the application potential of carbon nanotubes.

We study the functionalization of MWCNTs through nitric acid refluxing followed by the coating of the aqueous dispersion of functionalized CNTs on cotton fiber for antistatic application. The 8h acid refluxing introduces sufficient carboxylic groups on CNTs surfaces with retention of basic structural features of CNTs which is confirmed by the appearance of corresponding peak in the FTIR spectrum. Raman spectroscopy further validates this by exhibiting an increase in D band intensity. The acid refluxing is able to functionalize the CNTs without deteriorating their structure which is backed by FESEM images and XRD patterns. The improved dispersion results as a consequence of functionalization. A facile dip coating method is used to coat the aqueous dispersion of functionalized CNTs on cotton fibers. Functionalized CNTs can be considered as a promising anti-static material as their surface coating on insulating polymeric fiber brings their resistivity down to ~10^{10} Ω/square.

We also make an attempt to study the synthesis of polyaniline/functionalized MWCNTs nanocomposite and its use for thermoelectric applications. The morphological features were observed using scanning electron microscopy (SEM). The electrical conductivity, Seebeck coefficient and thermal conductivity values were measured to calculate thermoelectric figure of merit (ZT). Our obtained room temperature figure of merit ZT value ~0.001 is comparable to previous works, which along with simplicity & scalability of the process reflects its potential for development of efficient TE devices and generators.

We also study the synthesis of polyaniline/functionalized MWCNTs nanocomposite and its use for supercapacitor electrode application. It has been found that the polyaniline/functionalized CNTs composites display higher capacitance compared to either FCNTs or PANI alone, such that the capacitance increases upto10 wt% FCNTs loading and decreases afterwards. Accordingly, PCNT10 shows a good charge storage capacity with maximum specific capacitance of 406 F/g and capacity retention of about 89% after 1000 charge-discharge cycles. Besides, it also shows the maximum energy density of 44 Wh/kg and the power density of 2445 W/kg. Such a combination of large capacitance, high rate capability and good capacity retention along with appreciable energy and power density for PCNT10, reflects greatly improved electrochemical capacitance compared with the pure PANI and FCNTs, thereby demonstrating its potential as electrode material for supercapacitors.