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Empirical relationship between band gap and synthesis parameters of chemical vapor deposition-synthesized multiwalled carbon nanotubes

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Abstract

In this study, an empirical relationship between the energy band gap of multi-walled carbon nanotubes (MWCNTs) and synthesis parameters in a chemical vapor deposition (CVD) reactor using factorial design of experiment was established. A bimetallic (Fe-Ni) catalyst supported on $CaCO_3$ was synthesized via wet impregnation technique and used for MWCNT growth. The effects of synthesis parameters such as temperature, time, acetylene flow rate, and argon carrier gas flow rate on the MWCNTs energy gap, yield, and aspect ratio were investigated. The as-prepared supported bimetallic catalyst and the MWCNTs were characterized for their morphologies, microstructures, elemental composition, thermal profiles and surface areas by high-resolution scanning electron microscope, high resolution transmission electron microscope, energy dispersive X-ray spectroscopy, thermal gravimetry analysis and Brunauer-Emmett-Teller. A regression model was developed to establish the relationship between band gap energy, MWCNTs yield and aspect ratio. The results revealed that the optimum conditions to obtain high yield and quality MWCNTs of 159.9% were: temperature ($700^{\circ}C$), time (55 min), argon flow rate ($230.37 mL min^{-1}$) and acetylene flow rate

(150mLmin−1) respectively. The developed regression models demonstrated that the estimated values for the three response variables; energy gap, yield and aspect ratio, were 0.246 eV, 557.64 and 0.82. The regression models showed that the energy band gap, yield, and aspect ratio of the MWCNTs were largely influenced by the synthesis parameters and can be controlled in a CVD reactor.

Keywords

- multi-walled carbon nanotubes; factorial design; energy gap; regression model; scanning electron microscopy; transmission electron microscope; chemical vapor deposition

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