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Thermodynamic and Kinetic Study of the Production of Carbon Nanotube Yarn from Chemical Vapour Deposition Reactor

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ABSTRACT

Overcoming the low production rate of carbon nanotubes (CNTs) could be instrumental to reducing their cost of production and enhancing its wide application. Understanding the kinetics of the production of yarn from CNTs, through kinetic model development could assist in the optimisation of the production and this makes the application of yarn as a replacement to filament in incandescent bulb promising.

In this study, kinetic of the production of CNTs, an intermediate in the production of yarn, is presented. Several experiments were conducted using Ferrocene as catalyst in a CVD reactor. The reaction of CH_4 on Ferrocene catalyst is via heterogeneous catalysis because methane is in gaseous phase and Ferrocene in solid phase. Langmuir Hinshelwood was used to develop a kinetic model based on these two- phase phenomena. The effect of CH_4 concentration was investigated as well. The derived kinetic model fits the experimentally measured data with 95% confidence interval.

Good quality CNTs were obtained at methane flow rate of 125 ml/min. The CNTs produced at this flow rate has high purity, low tube diameter and spinnable long array as compared to the one produced at 100 ml/min and 150 ml/min. Yarn was produced at this flow rate (125 ml/min) at a reactor temperature of 900, 950 and 1000^{o}C. Characterisation techniques such as Scanning Electron Microscopy (SEM), Transition Electron Microscopy (TEM), Energy-Dispersive X-ray (EDX), Gas Chromatography (GC) and Raman Spectroscopy were used to analyse the product from experiments. At all studied reactor temperatures CNT yarns were synthesised as observed in SEM images.

Four Probe method was used to measure the electrical conductivity of as-produced CNTs and yarn. By using the proposed CH_4 flow rate (125 ml/min) the produced CNT yarn was found to be metallic and electrically conductive. The studied electrical conductivity of as-produced

CNTs were found to be approximately 2 times higher than their yarn. Yarn produced at reactor temperature of 950^{o}C proved to have high quality and more electrically conductive than those produced at 900 and 1000^{o}C.

The thermodynamic properties of CNTs yarn were studied using TGA/DSC equipment. Polynomial models for predicting Specific heat capacities of yarns produced in this study were developed. The results showed that the temperature at which yarn is produced has an effect on a thermodynamic property such as heat capacities, enthalpy and entropy.