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"Single-Walled Carbon Nanotubes By Arch Discharge: Optimization and computational simulation"

J. R. Vega-Baudrit [(1, 2)]*, M. R. Sibaja-Ballestero[(1)] and S. A. Ramírez[(2)]

(1) Polymers Laboratory, National University. Heredia, Costa Rica. jvegab@gmail.com
(2) National Laboratory of Nanotech. San José, Costa Rica. samador@cenat.ac.cr
* Corresponding author

Abstract: Single-Walled Carbon Nanotubes (SWCNT) were obtained by electric arc-discharge. This is a simple, inexpensive, energy-efficient method to obtain high quality carbon nanotubes. It does not employ catalysts. In this research, methodology was optimized using different flow and kind of gas and amperage. Finally, it was made a computational simulation using DL POLY and NWChem.

Carbon nanotubes (CNT) are one of the most commonly mentioned building blocks of nanotechnology. They have one hundred times the tensile strength of steel, thermal conductivity better than diamond, and electrical conductivity similar to copper, but with the ability to carry much higher currents. They seem to be an exceptional material. There are many kinds of methods to produce CNT. In this case, a single-walled carbon nanotube (SWCNT) by conventional arc discharge method was used. It is a non-catalytic process, an arch discharged is created between carbon electrodes and CNT`s are produced [1-6].

The variables considered in the optimization process were: gas, gas flow and amperage. Gas was used to produce plasma (helium, argon). It was found that the argon at 40 psi with an amperage of 19 A yielded the best results as shown in Transmission Electron Microscopy (TEM) image (Figure 1).

Also, SWCNT produced by arch discharged have a lot of impurities. The main impurities are graphite, amorphous carbon and the smaller fullerenes. These impurities will interfere with most of the desired properties of the SWCNT. Purification was made using a suspension in methanol and ultrasonic cleaner [2]. The SWCNT were characterized by TEM, Scanning Electron Microscope (SEM) and Atomic Force Microscopy (AFM).

Finally, to simulate the production of SWCNT, computational programs were used. DL POLY and NWChem shown better results compared with similar programs.

Figure 1: TEM image of SWCNT

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