Abstract

The exceptional properties of Carbon Nanotubes (CNTs) have attracted much attention in recent years for their small dimensions, high electrical and thermal conductivities and unique morphologies [1]. It is important to control the structure of these CNTs if we want to control the properties they exhibit for mass-production purposes. The methodology is basically correlating the morphology of the structure, which is extracted using image processing techniques of Scanning Electron Microscope (SEM) images, and Raman Spectroscopy analysis with the mechanical properties of the structure using Artificial Neural Network modeling technique. The model will play a significant role in analyzing and predicting the CNTs’ properties, which will eventually help in designing the desired CNT structure.

Introduction

Properties

- Large aspect ratio (>1000).
- Atomically Sharp tips.
- High temperature and chemical stability.
- High electrical and thermal conductivity.
- Can be either Metal or semiconductor.

Problems in the Field

- Experimental data doesn’t match the theoretical expectations due to quality issues.
- Comprehensive theoretical models are still an approximation, which doesn’t involve the distinctiveness of every sample.
- Methods for deterministic (controlled) synthesis and assembly of carbon nanostructures for novel devices and materials have not been developed.
- “Nanotube suppliers accused of selling shoddy goods” by Jim Giles “ Researchers who buy products such as carbon nanotubes are frequently being sold defective materials, according to a survey of nanotechnology companies.” [News@nature published online: 10 December 2004 [doi:10.1038news041206-15]

Raman Spectroscopy

Nondestructive, lots of information content (wavelength, polarization, batch average over macro scale). Research has proven that some geometrical information are embedded in Raman Spectrum [2].

Image Processing

- 2D FFT (Fast Fourier Transform) analysis.
- 2D Stereological Relations:
  - Area Fraction: \( A = \sum A_i / \sum A_n \)
  - Perimeter length per unit area: \( P_i = \sum P_i / \sum A_n \)
  - Line intercept count: \( L_i = \sum L_i / \sum A_n \)
- Relative Alignment measurements
  Measured based on the variance of the distance between each nuclei, \( d \), and each two nuclei, \( d_i \).
  \[
  \begin{align*}
  \text{Average distance} & = \frac{1}{N} \sum_{i=1}^{N} d_i \\
  \text{Relative distance} & = \left( \frac{d_i}{d} \right) ^2 \\
  \text{Relative distance} & = \left( \frac{d_i}{d} \right) ^2 \\
  \end{align*}
  \]

- Relative Curvature measurements:
  The curvature is calculated as the ratio of radius, \( r \), of the circle that tangential the curve as the point moves along the segment length, \( s \).

Artificial Neural Networks

Backpropagation training methodology is used in training the type of neural network [3].

Characterization

Image Processing

- Raman Spectroscopy
  - FFT was applied to both real images and ideal images, to understand the meaning of the results based on CNTs alignment, curvature, orientation, and thickness properties.
  - Fig. 2: Raw portion of Raman signal (a) D, (b) 2D peak positions.
  - Fig. 13: Effect of excitation wavelength on (a) D, (b) 2D peak positions.

- FFT Analysis
  - Peaks info.
  - Fig. 12: Model output for (a) sample I and (b) sample 2 alignment estimations, (c) sample I and (d) sample 2 curvature estimations. Insets are the SEM images of the analyzed samples.

- Raman Spectrum
  - Filtering using Wavelet data processing [4]
  - Fig. 10: Raw portion of Raman signal (a) DWT and IDWT data processing (b) Filtered Raman signal.
  - Fig. 8: Different FFT patterns of correct ideal images (a-e) and SEM images (d-f).

- Empirical Modeling
  - Artificial Neural network model for CNTs quality classification

Discussion

- Understanding the correlation between CNT growth aspects and its properties is the key factor to develop quality control methods for controlled synthesis and assembly of carbon nanotubes.
- The system is built to model and estimate CNTs quality based on Raman Spectroscopy, morphology information extracted from SEM images using in-house image processing algorithms.
- A neural network model for CNTs alignment classification using image processing results shows an accurate categorizing technique for CNTs with an acceptable range of approximation.
- ANN was able to model the Raman data and extract the influence of the given inputs. The effect of the excitation wavelength and CNT morphology was intensely studied.

Conclusion

Modeling using Raman Spectroscopy analyses and SEM image processing will link CNT properties with growth conditions, which could be used later to manipulate the nucleation factors such that the CNT desired properties in large quantities will be achieved.

Neural networks classifier is very helpful to categorize the images based on alignment and purity characteristics. Empirical modeling is a powerful tool to predict, explain, and model materials behavior, especially when the analytical modeling is not achievable.

References