Hydrogen Desorption Study of As-Synthesized Carbon Nanotubes Using Artificial Neural Network

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Abstract

Carbon nanotubes are considered for hydrogen storage due to their low density, high strength, and hydrogen adsorption characteristics. Reports suggest that the total surface area of carbon affects the hydrogen storage capacities in carbon nanotubes. Based on the experimental data of as-synthesized carbon nanotubes, an artificial neural network (ANN) model was developed to study the relationship between the surface area of carbon and the hydrogen desorption. The model was also used to study the effect of carbon and alumina content to the hydrogen desorption. A feedforward ANN was used for the prediction. The ANN was trained using the Levenberg-Marquardt training algorithm.

Keywords: Carbon nanotubes; Neural network; Modeling; Surface area

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1. Introduction

The discovery of carbon nanotubes (CNT) by Sumio Iijima [1] in 1991 has attracted many researchers to study and explore the material. The unique characteristics that carbon nanotubes possess include excellent properties for energy production and hydrogen storage. Researchers found that carbon nanotubes have the potential to adsorb hydrogen due to their low density, high strength, and hydrogen adsorption characteristics.

Among methodsof storing hydrogen, physisorption method is said to be the most promising for fuel cell powered vehicle [2, 3]. The storage of hydrogen can rely on physisorption because the adsorbed gas can be released (the process is reversible) [4]. However, a detailed understanding of the hydrogen storage mechanism and the effect of materials processing on this mechanism is still needed. Researchers have studied different mechanisms that affect the gas adsorption on CNT, such as CNT geometries [5,6], surface area of CNT [7], methods to open the tubes [8,9] and the purification of the adsorbent [10].

In spite of various model calculations [2,11-13] that have been carried out using a variety of computational techniques, the actual mechanism of the hydrogen storage in CNT is still unknown [14]. Although interest in applications of artificial neural network (ANN) in chemistry has increased tremendously [15], it has not been employed comprehensively in hydrogen desorption studies in CNT.

In this work, we investigated the capability of ANN model to predict hydrogen desorption in CNT. Based on the reports that suggest total surface area of carbon affect the hydrogen storage capacities in carbon nanotubes [16-20], we employed the model to study the relationship between surface area and the hydrogen desorption in CNT.

2. Artificial Neural Network Modelling

2.1 Artificial neural network concept

Artificial neural network is composed of a large number of highly interconnected processing elements called neurons. There are five basic elements which make up an artificial neuron: input, weights, summing function, activation function and output. The neurons are connected to each other by links with their own weight factors. ANN learns by example. A learning process in the ANN context can be viewed as the problem of updating network architecture and connection weights so that a network can efficiently perform a specific task.

Two important features of neural networks are the ability of supplying fast answers to a problem and the capability of generalizing their answers, providing acceptable results for unknown patterns [21]. The network usually must learn the connection weights from available training patterns.

Multi-layer perceptron is one of the most well known neural network architecture generally used for prediction problems. Fig. 1 shows a simple multi-layer perceptron structure with only one hidden layer. The numbers of neurons in input and output layers are constrained by the problem and the outputs required by the problem, respectively. The input layer consists of neurons that receive input from the user while the output layer consists of neurons that communicate the output of the system to the user. There are usually a number of hidden layers between these two layers.

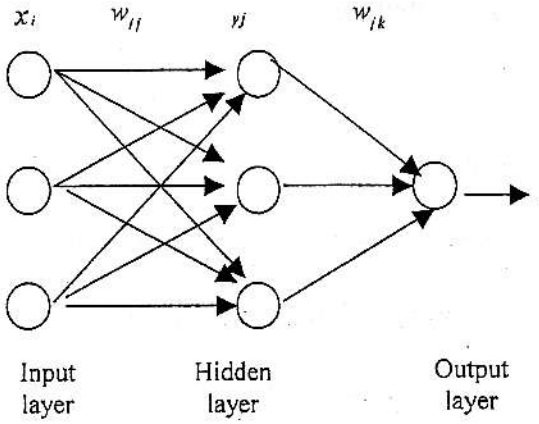

Fig. 1. Neural Network Architecture

The summation is obtained by multiplying each input with its corresponding weights and then adding up all the products:

$$y_j = \sum_{i=1}^{n} x_i w_{ij} \qquad (1)$$

2.2 Model description

Apart from predicting the hydrogen desorption in CNT, ANN is also used to study the relationship between carbon surface area and hydrogen storage. Various aspects are considered before a satisfactory model of neural network is developed. The development of a neural network model includes database collection, analysis and pre-processing of the data, design and training of the neural network, test of the trained network and use of the trained neural network for simulations and predictions [22]. A feed forward architecture is used for the design of the network.

Training sets consisting of input/output pattern pairs are used to train the network. Surface area, carbon content and alumina content are used as the input of the network and

labeled as *A*, *B* and *C*, respectively. The output of the network is hydrogen desorption. To train the network, a back propagation algorithm, namely the Levenberg-Marquardt algorithm, is used. Note that a back propagation algorithm is based on the supervised learning procedures, which allows prediction of an output object for a given input object.

Experimental data are divided into training and test sets. The training set is used to train the network while the test data is used to assess the performance of the network after training. Using one single hidden layer and starting with five neurons, the network topology was varied by increasing the number of neurons. Logistic and tangential sigmoidal activation functions were independently used in neurons of the hidden layer.

3. Results and Discussion

It is found that eight neurons in the hidden layer with logistic sigmoidal activation function and Levenberg-Marquardt training algorithm can predict the experimental data close to the test set.

Using the same model to study the effect of surface area of CNT, carbon content and alumina content, we found that was a correlation between surface area and hydrogen desorption. When the surface area of our sample increased, the hydrogen desorption also increased, a finding similar to that of Zuttel et al. [16-19] and Strobel [20]. We also found that the hydrogen desorption increased as well when the carbon content of the sample increased. However, hydrogen desorption decreased when alumina content increased. Together the study thus shows that the it was the carbon content which contributed to hydrogen desorption, not the alumina content. The results are shown in Fig. 2.

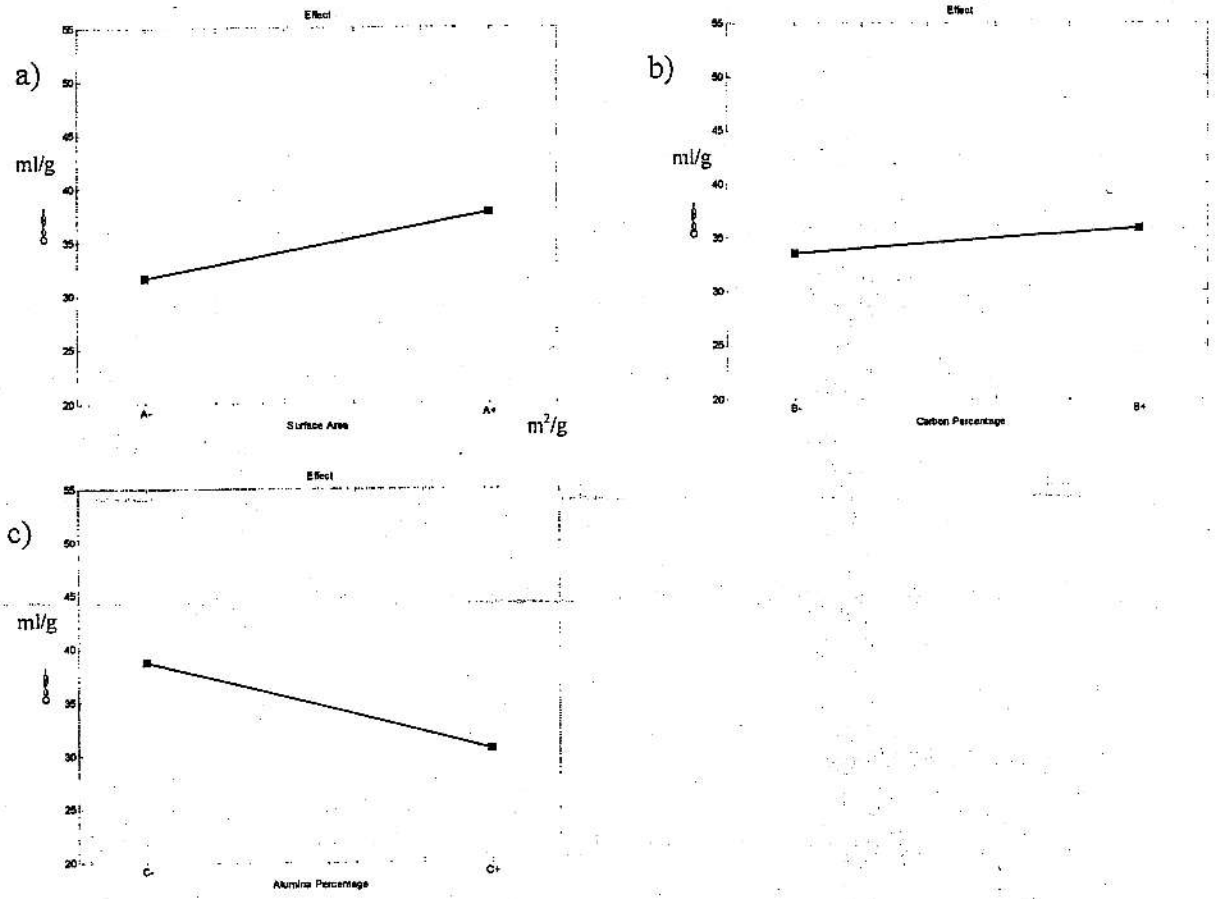

Fig. 2. Individual graphs of the effects of (a) surface area, (b) carbon content, (c) alumina content to the hydrogen desorption

4. Conclusions

This work shows that ANN can be used as an alternative approach to predict the hydrogen desorption in carbon nanotubes. However our model is not recommended to be employed in the prediction of the hydrogen desorption beyond the range of the input used in overall experimental data.

We would like to point out that our study into the use of ANN models is still at a preliminary stage and the model is subject to further refinement.

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