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ARTIFICIAL NEURAL NETWORK MODELING OF HYDROGEN UPTAKE BASED ON CARBON SURFACE AREA

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ABSTRACT

The discovery of carbon nanotubes (CNT) by Sumio Iijima in 1991 has attracted many researchers worldwide to study and explore the newly found materials. CNT are considered for hydrogen storage due to their low density, high strength, and hydrogen adsorption characteristics. Recent reports suggest that total surface area of carbon affect the hydrogen storage capacities in carbon nanotubes. An Artificial Neural Network model was created to study the relationship between the surface area of carbon and the hydrogen adsorption.

Keywords: carbon nanotubes; neural network; modeling; surface area

1. INTRODUCTION

Hydrogen is the cleanest fuel and is expected to replace the conventional fossil fuel. Hydrogen is the most promising candidate to replace the current fossil fuel since it is not only environmentally compatible (pollution-free), but it also can be produced from renewable energy sources, thus eliminate the net production of greenhouse gases [1]. Despite tremendous efforts to use hydrogen as a source of energy, a safe and efficient on board storage technology has never been easily accessible. Due to its explosiveness, an efficient storage method is needed for hydrogen to become a replacement for fossil fuels. The ability to store hydrogen onboard vehicles is a key technological issue for the development of fuel cell powered vehicles. The technique of hydrogen storage has to meet the benchmark set by the US Department of Energy (DOE) Hydrogen Plan for the volumetric and gravimetric density of the stored hydrogen. According to DOE, a material needs to store 6.5% of its own weight in hydrogen to make fuel cells practical for commercial used.

In general, there are four main technologies being explored for hydrogen storage [1]: Compressed gas, liquefaction, metal hydrides and physisorption (gas-on-solid adsorption). Although nowadays all of these options are investigated extensively and

progress is gained, none of these technologies is fully developed. There are still some significant disadvantages which exist. For example, the critical issue connected with compressed gas storage may be tank volume and safety, while liquefying hydrogen wastes at least 1/3 of stored energy and suffers from potential losses due to evaporation and the hydride-based approach suffers from weight and cost concerns [1]. The storage based on physisorption potentially may have a higher energy density [2]. Research reports suggested that physisorption is the most promising hydrogen storage method for meeting the goals of the DOE Hydrogen Plan for fuel cell powered vehicle [3,4]. Physisorption is an inherently safe and potentially high energy density H_2 storage method that could be extremely energy efficient [5]. The storage of hydrogen can rely on physisorption because the adsorbed gas can be released reversibly [6].

Researchers worldwide have studied different types of adsorbent such as silica, graphite, activated carbon, carbon nanofiber and carbon nanotubes in their physisorption research. Carbon is well known as one of the better adsorbents for gases. This is due to (i) the ability of this material to exist in a very fine powdered form with highly porous structure and (ii) the existence of particular interactions between carbon atoms and gas molecules [7]. The discovery of carbon nanotubes (CNT) by Sumio Iijima [8] in 1991 has attracted many researchers worldwide to study and explore the materials. Carbon nanotubes possess unique characteristics such as low density, high strength, and hydrogen adsorption characteristics that make them suitable for hydrogen storage. Because of these characteristics, carbon nanotubes are said to be a good adsorbents for adsorption. Recent reports suggest that there was a dependence of the storage capacity on the specific area of the carbonic adsorbents [9-11].

2. METHODS

Artificial neural network (ANN) was used to study the relationship between carbon surface area and hydrogen storage. Among the adsorbents used were carbon nanotubes and activated carbon. ANN is a type of Artificial Intelligence that is inspired by the way the brain process information. A neural network consists of simple synchronous processing elements, called neurons. The neurons are connected to each other by links with their own weight factors. 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. The network usually must learn the connection weights from available training patterns. Performance is improved over time by updating the weights in the network iteratively. ANN appears to learn the underlying rules from the given collection of representative examples. Various aspects have to be considered before a satisfactory model of neural network is developed. The development of neural network model is including 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 [12]. A feed forward architecture was used for the design of the network. Such architecture is shown schematically in Fig. 1, where the number of neurons in input and output layers is constrained by the problem and the outputs required by it, respectively. The neurons are ordered in layers and the information is processed in one direction, from input to output

The input layer consists of neurons that receive input from the user. 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 shows a simple structure with only one hidden layer. When the input layer receives the input, its neurons produce output, this becomes input to the other layer of the system. he process continues until a certain condition is satisfied or until the desired output is reached.

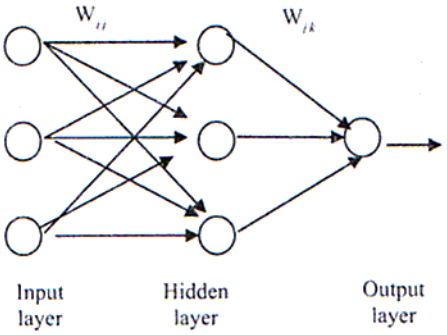

Figure 1. Neural Network architecture

Back propagation algorithm was used in our artificial neural network modeling. Back propagation algorithm is based on the supervised learning procedures. It compares the responses of the output units to the desired output, and readjusts the weights in the network. It has to build the model up solely from the examples presented, which are together assumed to implicitly contain the information necessary to establish the relation. Training sets consist of input/output pattern pairs, which are taken from real data, are used to train the network. The input data is repeatedly presented to the neural network. Output of the neural network is compared to the desired output and an error is computed, feed back and back propagated to the network and used to adjust the weight. This process is known as training. Back propagation method is often capable of modeling complex relationships between variables. It allows prediction of an output object for a given input object. Typically, it needs both training and test set of data. The training set is used to train the network while the test data is used to assess the performance of the network after training.

3. EXPECTED RESULTS

Monte Carlo simulations [3,13-16] and other calculations [17,18] have been carried out to verify and predict the adsorption capacity of hydrogen in carbon nanotubes based on the assumption of physical adsorption. It is important to notice that different factors can influence the gas adsorption such as the specific area of the materials, the method used in order to open the carbon nanotubes and the purification of the adsorbent before any adsorption measurement. Consequently, the hydrogen storage properties of high surface area carbons have been extensively studied. Nijkamp et al. [19] examined that there was a correlation between the specific surface of carbonic materials and hydrogen adsorption. Using volumetric method, Nijkamp et al. investigated different

adsorbents for hydrogen at 77 K and atmospheric pressure. They found an approximately linear correlation between the specific surface area determined by BET measurements and the hydrogen adsorption. Zuttel et al. [9] did the electrochemical measurements of the hydrogen adsorption in carbon nanotubes. They found that the electrochemically measured discharge capacity at room temperature (T = 293K) of the nanotubes samples correlate with the surface area. The linear relationship is shown in Fig. 2 [20], where the line intercepts at the axis at the origin and the slope is 1.5 mass%/1000 m^2/g. They plot their data in one plot together with the low-temperature adsorption data measured by Nijkamp et al. Their extrapolated maximum discharge capacity of carbon sample is 2 mass%.

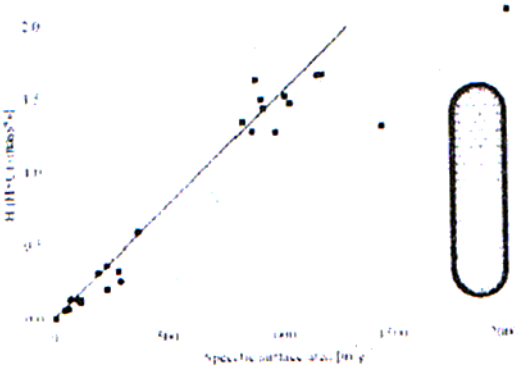

Figure 2. Desorbed amount of hydrogen versus the B.E.T. surface area

In figure 2, the round markers are few carbon nanotubes samples including two measurements on high surface area graphite (HSAG) samples together with the fitted line. The square markers are hydrogen gas adsorption measurements at 77K from Nijkamp et al. [19]. The dotted line represents the calculated amount of hydrogen in a monolayer at the surface of the substrate.

Based on the experiments performed by other researchers [9, 21] who found that there was a correlation between the specific surface area and the amount of hydrogen uptake in carbon materials, we developed an artificial neural network model to study the influence of the total surface area on the hydrogen storage capacity of carbon. The model is expected to predict that when the surface area is increased, the hydrogen uptake will also increase. The artificial neural network model is still open for constant upgrade and improvement.

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