

## Doped Carbon Nanotubes for Hydrogen Storage

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### Abstract

The ultimate goal of this research is to develop a low-cost high-capacity hydrogen storage material. The final product should have favorable thermodynamics and kinetics characteristics as well as stability with cycling. The material should be compatible with the DOE goals for on-board hydrogen storage for transportation applications. One of the candidates for solid hydrogen storage has been carbon nanotubes. However, simple mechanisms for hydrogen uptake and release involving physisorption and chemisorption alone can not account for the unusual sorption of hydrogen by carbon nanotubes, reported by other researcher. We believe that in some cases the unique nanotube structure and configuration can give rise to polarization and condensation inside the tubes. We believe that introducing nano-particles (dopants) to the nanotubes can enhance hydrogen bonding at the edge and inside the tubes allowing for hydrogen storage to occur. Therefore, our objective is to establish an interaction between hydrogen and carbon nanotubes based on a weak covalent bond where the electron donation from the ( $\sigma$ ) orbital of hydrogen to the doped tubes weakens but does not break the hydrogen-hydrogen bond. The relatively weak nanotubes-hydrogen bond should allow hydriding and dehydriding to occur at mild conditions of temperatures and pressures. A new method was developed to form and control characteristics of carbon nanotubes and dopants.

### Introduction

A major obstacle in the way of a transition to hydrogen economy has been the absence of a practical means for hydrogen storage. For years, the goal of researchers has been to develop a high-density hydrogen storage system that can release hydrogen at temperatures lower than 100°C. Although approaches such as compressed gas or liquefaction can have near term

applications issues such as safety and infrastructure are still subjects of concern over the implementation of these technologies. On the other hand developing a suitable solid state hydrogen storage system is expected to be simple to engineer and tremendously safer. Carbon nanotubes technology represents a new direction for solid hydrogen storage especially if these materials can be altered to store large amounts of hydrogen at room temperature. Carbon nanotubes discovery has generated much interest and created extensive research activities into the properties and application of the nano-meter scale cylindrical carbon tubes [1-3]. Persistent research activities in the US and elsewhere have been exploring the use of carbon nanotubes for hydrogen storage [4-8]. Reported results on hydrogen uptake and release by carbon nanotubes systems created much excitement and stimulated extensive interest in their potential use as hydrogen storage media. Our research is focused on modifying carbon nanotubes systems in an attempt to enhance and tune the hydrogen storage capabilities of the nanotubes. Our objective has been to introduce transition metals and hydrogen bonding clusters inside tubes. Our approach is aimed at producing consistent size dopants and structures of carbon nanotubes. Controlling the type and size of the tubes and clusters is expected to allow us to tune the material for hydrogen sorption at desired temperatures and pressures.

## **Results and Discussion**

The synthesis of different doped carbon nanotubes has been achieved using a technique we developed that allows us to control the type and amount of dopants in the tubes. We were able to produce large quantities of consistent structure carbon nanotube systems (Figure 1 shows SEM microscopic of samples prepared by the new method). The success of making doped carbon nanotubes with transition metals and alloys can allow for a weak covalent bond similar to cases of dihydrogen bond that is not restricted to pure physisorption or chemisorption bond [9,10]. Controlling the type and size of tubes and dopant is expected to tune the product for hydrogen sorption to occur at desired temperature and pressure. Preliminary results of hydrogen uptake and release showed indication of 0.5 to 1 % by weight hydrogen uptake and release from samples. A thermogravimetric system capable of operating at a wide range of temperatures was used to measure hydrogen uptake and release. Although more investigation is needed to identify the type of hydrogen bond with the carbon nanotubes the preliminary results look encouraging.

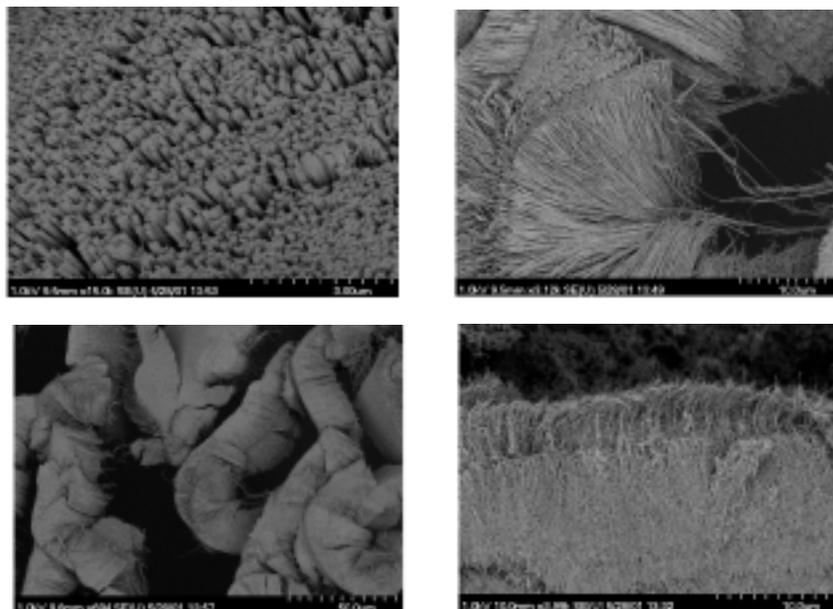
## **Conclusion**

Our original plan was to produce large quantities of consistent structures that can be modified as needed. We felt that such effort was required to avoid discrepancy in the measured data. Therefore, a novel method for producing and controlling configuration and structure of carbon nanotubes was developed and demonstrated. This method will allow us to investigate different combination of metals and structures of doped carbon nanotubes for hydrogen storage. Scanning and transmission electron microscopy were used to investigate configuration of tubes and dopants. Preliminary results, using thermogravimetric analyzer, indicated hydrogen uptake and release. We recognize that this research effort is high risk however high reward because of the potential applications that will result from developing a carbon nanotubes hydrogen storage system.

## **Future Work**

We plan to continue production of nanotubes with different dopants. In order to determine thermodynamic characteristics of hydrogen uptake and release thermogravimetric and thermogravimetric methods will be used. Different spectroscopic methods (e.g. SEM, TEM,

EDS etc. ) will be used to identify the type and size of nanotubes and clusters that result in a reversible high hydrogen capacity material. The ability to control structure will allow us to tune conditions that result in a high yield of material possessing favorable characteristics. We also plan to perform cycling tests on material and investigate the effect of contaminants on hydrogen sorption.



**Fig. 1 Consistent structure doped carbon nanotubes**

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