

VI.C.4 Nanostructured Activated Carbon for Hydrogen Storage

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Subcontractor:

PoroGen, LLC, Boston, MA

Start Date: May 2, 2005

Projected End Date: April 30, 2009

Project Objectives

Develop and demonstrate reversible nanostructured activated carbon hydrogen storage materials with at least 7 wt% materials-based gravimetric capacity and 50 g H₂/L materials-based volumetric capacity, with the potential to meet the DOE 2010 system-level targets.

Technical Barriers

This project addresses the following On-Board Hydrogen Storage Technical Barriers outlined in the Hydrogen, Fuel Cells and Infrastructure Multi-Year Research, Development and Demonstration Plan:

- A. Cost
- B. Weight and Volume
- C. Efficiency
- D. Durability
- E. Refueling Time
- M. Hydrogen Capacity and Reversibility
- N. Lack of Understanding of Hydrogen Physisorption and Chemisorption

Technical Targets

This project is conducting R&D on novel high surface area nanostructured carbons for hydrogen storage. This project aims to address the critical need that has been recognized by the DOE, which has established a national effort to develop new and advanced high-capacity hydrogen storage materials and technologies. This project is applied toward the synthesis of inexpensive carbon-based high surface area sorbents that can be combined with chemical-interacting organic, and/or inorganic materials. These new materials and concepts have been designed to meet the DOE 2010 goals concerning the production of low-cost, high specific energy density hydrogen storage materials.

Table 1. On-Board Hydrogen Storage System Targets (**Data is based on material only, not system value)

Storage Parameter	Units	2010 System Target	FY 2005 materials**
Specific Energy	kWh/kg (wt. % H ₂)	2.0 (6 wt.%)	0.93 (2.8 wt. %)
Volumetric Energy Capacity	kWh/L	1.5	0.56
Desorption Temperature	K		77
Plateau Pressure	bar		1

**Without metal in dope

Approach

State University of New York and PoroGen, LLC have initiated a collaborative effort to develop superior high surface area nanostructured carbons for hydrogen storage. The synthesis of the carbon starts with the preparation of a nanoporous semicrystalline oriented polymer precursor having nanosize pores, with uniform pore size distribution and high surface area. The semicrystalline nanoporous polymer material is tailored to form activated carbons with slit-like microporous (0.1-2 nm) structure and high surface area. The high surface area of the polymeric precursor aids in preparation of this unique carbon (>3000 m²/g) and enables doping initial material with chemical agents which, upon carbonization, introduces specific interaction sites that significantly increase the hydrogen storage capacity of the nanostructured carbon material.

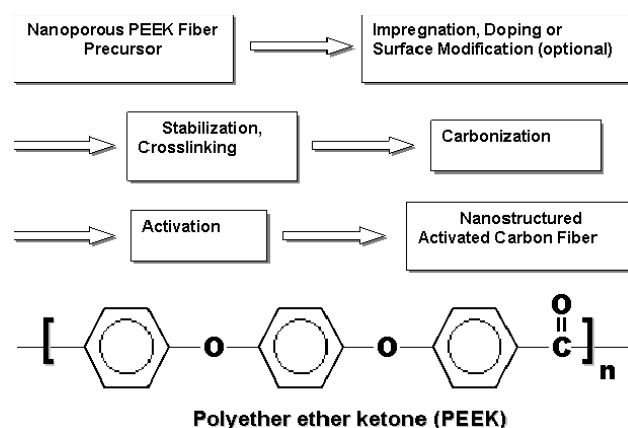


Figure 1. Processing of Nanoporous PEEK Carbon Materials

Initially the process uses a polyether ether ketone (PEEK)/polyetherimide (PEI) precursor (see Figure 1) which is spun at high melt shear rates to control the morphology and orientation of crystalline regions. Highly oriented lamellae crystals in the nanoporous PEEK material are achieved by extruding the PEEK/PEI blend at high draw ratios. High orientation of polymeric chains and the alignment of crystalline lamellae regions lead to formation of porous material with oriented nanosize pores and are expected, upon carbonization to produce activated carbon with angstrom-size slit-like pores. Reactive sites can be incorporated into the pores of active carbon/PEEK to promote significant increase in hydrogen sorption. The incorporation organometallics and metal oxide doped carbon in to catalytic sites containing heteroatoms such as N, P, S and B are being investigated. Large quantities of materials can be synthesized on a laboratory scale.

Accomplishment

- A process has been developed to obtain an inexpensive carbon matrix, with a very narrow (“sharp”) pore diameter average in the microporous range that is associated with a large surface area. The preparation of nanoporous PEEK carbons with a surface area in excess of 3000 m²/g has been demonstrated (Figures 1 and 2). The relationship between average pore diameters to surface area in carbon samples prepared in different conditions is shown in Figure 2. (*Sample size measured 1g; large quantity of the material can be easily prepared!*)

- A linear correlation between pore diameter and hydrogen adsorption per unit area has been obtained and is shown in Figure 3; note that no metal was mixed with the dope! *(This result indicates that improvement of the process calls for reduction of the pore diameter for the further increase of hydrogen adsorption. However, this carbon matrix can be used as a carrier for metal hydride, or other metals that would complex with hydrogen.)*
- The relationship between surface area and hydrogen adsorption (Figure 4) demonstrate that ~3 wt% of H₂ is adsorbed on PEEK-carbon (~2 nm dia.) with a surface area of 3000 m²/g and more. *(The results indicate that carbon, with a surface area in excess of 2000 m²/g, is required for an elevated H₂ adsorption.)*

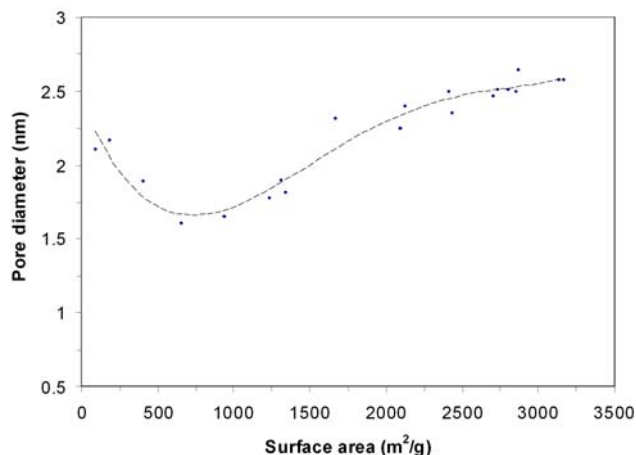


Figure 2. Change of Average Pore Size with Surface Area of Activated PEEK Carbon

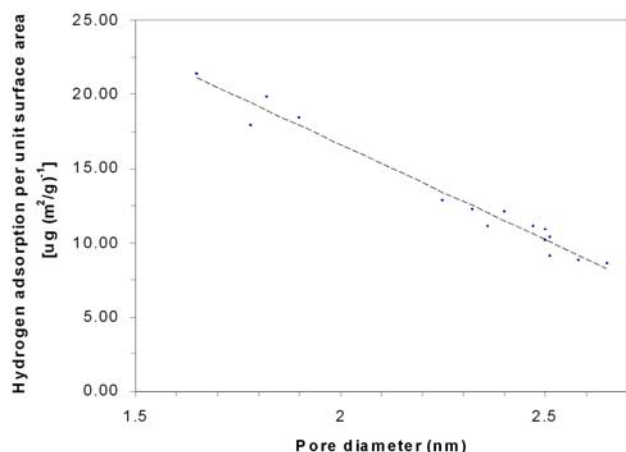


Figure 3. Effect of Pore Size on the Hydrogen Adsorption per Unit Surface Area of Activated PEEK Carbons

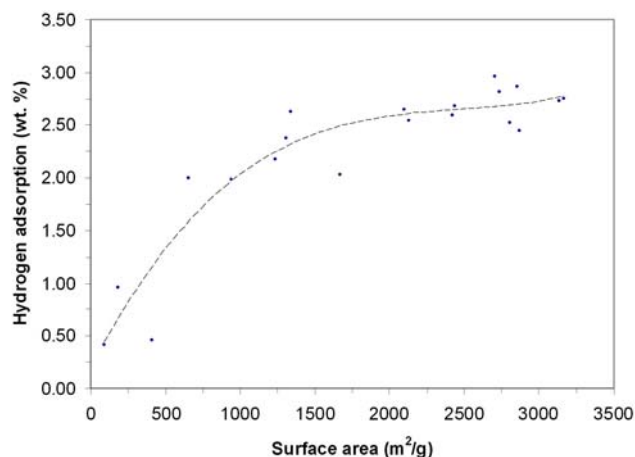


Figure 4. Change of Hydrogen Adsorption at 77 K and 1 Bar With the Specific Surface Area of Activated PEEK Carbons