March 2007

Carbide-derived carbons designed for efficient hydrogen storage

Ranjan Dash
Drexel University

Gleb Yushin
Drexel University

G. Laudisio
University of Pennsylvania

T. Yildirim
National Institute of Standards and Technology

Jacek Jagiello
Quantachrome Instruments

See next page for additional authors

Poster presented at *The Search for a Sustainable Energy Future: Challenges for Basic Research*, A Mini-Symposium sponsored by the Energy Working Group at Penn, March 9, 2007.

Carbide-derived carbons designed for efficient hydrogen storage

Abstract

Carbide-derived carbons (CDCs) with specific surface area (SSA) ~ 2000 m2/g and open pore volume up to 80% are produced by chlorine etching of metal carbides. Tuning the pore size distribution by carbide precursor selection and etching temperature yields enhanced hydrogen storage capacity at both ambient and elevated pressure. Our goal is to establish the fundamental relation between capacity and SSA, pore size and pore volume.

Comments

Poster presented at *The Search for a Sustainable Energy Future: Challenges for Basic Research*, A Mini-Symposium sponsored by the Energy Working Group at Penn, March 9, 2007.

Author(s)

Ranjan Dash, Gleb Yushin, G. Laudisio, T. Yildirim, Jacek Jagiello, John E. Fischer, and Yury Gogotsi

Carbide-derived carbons designed for efficient hydrogen storage

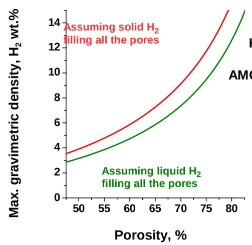
R. K. Dash[1], G. Yushin[1], G. Laudisio[2], T. Yildirim[3], J. Jagiello[4], J. E. Fischer[2] and Y. Gogotsi[1]

[1]Department of Materials Science and Engineering and A. J. Drexel Nanotechnology Institute, Drexel University, Philadelphia, PA 19104
[2]Department of Materials Science and Engineering, University of Pennsylvania, Philadelphia, PA 19104
[3]National Institute of Standards and Technology, Gaithersburg, MD 20899, USA
[4]Quantachrome Instruments, Boynton Beach, FL 33426, USA

EWGP KICKOFF SYMPOSIUM
MARCH 9, 2007

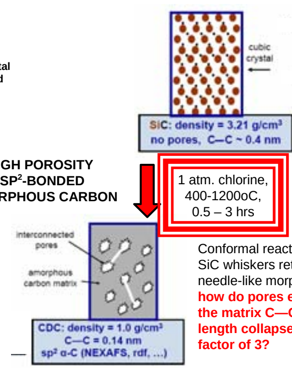
1. INTRODUCTION to CARBIDE-DERIVED CARBONS

Carbide-derived carbons (CDCs) with specific surface area (SSA) ~ 2000 m2/g and open pore volume up to 80% are produced by chlorine etching of metal carbides. Tuning the pore size distribution by carbide precursor selection and etching temperature yields enhanced hydrogen storage capacity at both ambient and elevated pressure. Our goal is to establish the fundamental relation between capacity and SSA, pore size and pore volume.



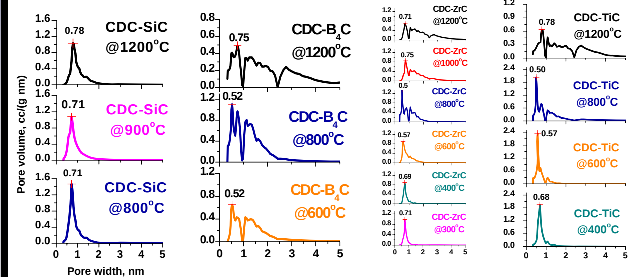
HIGH POROSITY
SP^2-BONDED
AMORPHOUS CARBON

PRECURSOR: MINERAL CARBIDE
(binary, ternary, …



Conformal reaction: e.g. SiC whiskers retain their needle-like morphology. So how do pores evolve as the matrix C—C "bond" length collapses by a factor of 3?

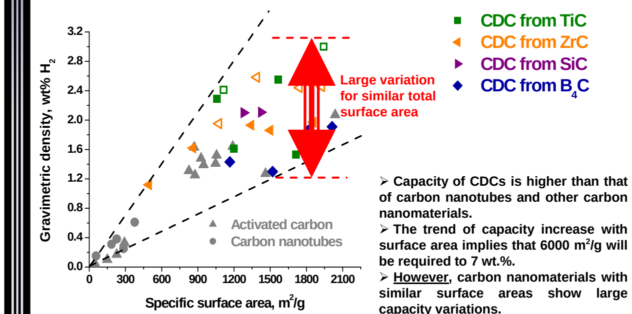
2. CDC's with TUNEABLE PORE SIZE DISTRIBUTION



➢ Pore size distribution can be tuned by changing the structure of the metal carbide precursor as well as the synthesis temperature.

➢ Metal carbides, which have a uniform carbon distribution such as ZrC, TiC and SiC, can yield CDC with narrowly distributed small pores, whereas carbide with a non-uniform carbon distribution, such as B_4C, yield CDC with widely distributed larger pores.

3. EFFECT OF SURFACE AREA ON H_2 CAPACITY

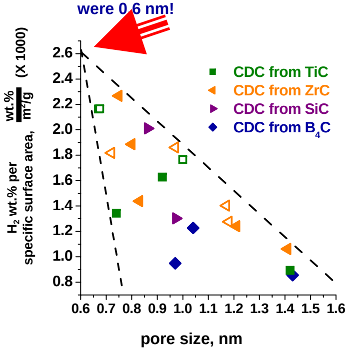


Gas sorption measurements were performed using argon at 77K using Quantachrome Autosorb-1. Pore size distributions were calculated using Non Local Density Functional Theory (DFT).

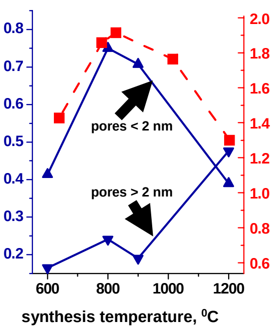
➢ Capacity of CDCs is higher than that of carbon nanotubes and other carbon nanomaterials.
➢ The trend of capacity increase with surface area implies that 6000 m²/g will be required to 7 wt.%.
➢ However, carbon nanomaterials with similar surface areas show large capacity variations.
➢ Possibility: This traditional plot of wt.% vs SSA could be obsuring something important.

4. SMALL PORES ARE CRUCIAL FOR HIGH CAPACITY

Specific surface area: only 2600 m²/g needed to achieve 6.1 wt.% at 77K, 1 atm. if all pores were 0.6 nm!

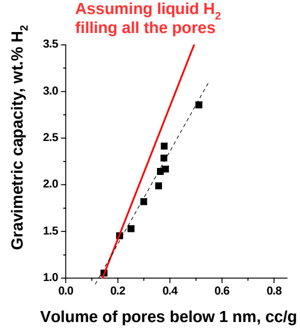


B_4C - CDC: reduced capacity correlates with increasing pore size when the chlorination temperature is too high.

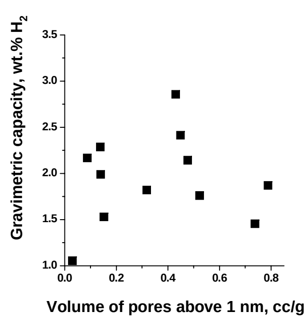


5. CAPACITY CORRELATED W/VOL. OF SMALL PORES

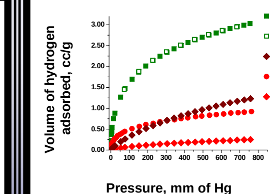
Hydrogen storage increases linearly with pore volume for pores less than 1 nm.



No correlation between hydrogen storage and pore volume for pores greater than 1 nm.



6. CONCLUSIONS and REFERENCES



CDC from TiC (Adsorption)
CDC from TiC (Desorption)
Metal organic framework (MOF-5)
Single-walled carbon nanotubes
Multi-walled carbon nanotubes

Reversible hydrogen storage capacity of CDC is 10 times that of multi-walled nanotubes, 3.5 times that of single-walled carbon nanotubes and 2 times than that of metal organic framework (MOF-5) at 1 atm pressure and 77K.

➢ Nanoporous CDC's with tunable pore size provide SSA up to 2000 m²/g, pore volume > 1 cc/g available for hydrogen storage.
➢ At 1 atm. and 77K, gravimetric capacity > 3.0 wt.%, volumetric > 24 kg/m³.
➢ At 1 atm. and 77K, CDC capacities > MOF-5, SWNT, MWNT.

Y. Gogotsi, A. Nikitin, H. Ye, W. Zhou, J.E. Fischer, B. Yi, H.C. Foley, and M.W. Barsoum, *Nature Mat'ls*, **2**, p. 591-594 (2003).
Y. Gogotsi, R.K. Dash, G. Yushin, T. Yildirim, G. Laudisio, J.E. Fischer, *J. Am. Chem. Soc.*, **127**, p. 16006-16007 (2005).
R. K. Dash, G. Yushin, Y. Gogotsi, *Micro. and Meso. Mat'ls,* **86**, p. 50-57 (2005).
G. Yushin, Y. Gogotsi, and A. Nikitin, Carbide Derived Carbon, in *Handbook of Nanomaterials*, Y. Gogotsi, Editor, CRC Press (2006).
G. Laudisio, R. K. Dash, J. P. Singer, G. Yushin, Y.Gogotsi, J. E. Fischer, *Langmuir* **22**, 8945-8950 (2006).