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

Follow this and additional works at: http://repository.upenn.edu/pennergy_posters

Dash, Ranjan; Yushin, Gleb; Laudisio, G.; Yildirim, T.; Jagiello, Jacek; Fischer, John E.; and Gogotsi, Yury, "Carbide-derived carbons designed for efficient hydrogen storage" (2007). Energy Research Group Posters. 2.
http://repository.upenn.edu/pennergy_posters/2


This paper is posted at ScholarlyCommons. http://repositoryupenn.edu/pennergy_posters/2
For more information, please contact libraryrepository@pobox.upenn.edu.
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

Author(s)
Ranjan Dash, Gleb Yushin, G. Laudisio, T. Yildirim, Jacek Jagiello, John E. Fischer, and Yury Gogotsi
**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 and pore volume for CDCs with tunable pore size distribution is achieved by varying the chlorination temperature. For example, CDC-ZrC with a surface area of ~ 2000 m²/g and open pore volume up to 80% is produced by chlorine etching of metal carbides. Tuning the pore size and pore volume for CDCs with tunable pore size distribution is achieved by varying the chlorination temperature. For example, CDC-ZrC with a surface area of ~ 2000 m²/g and open pore volume up to 80% is produced by chlorine etching of metal carbides.

**2. CDC’s with TUNABLE PORE SIZE DISTRIBUTION**

- **PRECURSOR: MINERAL CARBIDE**
  - Chloride reaction: C → C → C bonding, 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?
  - Conformal reaction: e.g., CDC from B4C, CDC from SiC, CDC from TiC, CDC from ZrC.

- **SYNTHESIS TEMPERATURE, °C**
  - Hypothetical reaction: 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?
  - Conformal reaction: e.g., CDC from B4C, CDC from SiC, CDC from TiC, CDC from ZrC.

- **ETCHING TEMPERATURE**
  - Hypothetical reaction: 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?
  - Conformal reaction: e.g., CDC from B4C, CDC from SiC, CDC from TiC, CDC from ZrC.

**3. EFFECT OF SURFACE AREA ON H₂ CAPACITY**

- **Assuming solid H₂ filling all the pores**
  - Volume of pores below 1 nm, cc/g
  - Volume of pores above 1 nm, cc/g
  - Large variation for similar total surface area
  - Capacity of CDCs is higher than that of other carbon materials.

**4. SMALL PORES ARE CRUCIAL FOR HIGH CAPACITY**

- Specific surface area: only 2600 m²/g needed to achieve 6.1 wt.% at 277K, 1 atm. if all pores were 0.6 nm.
  - B₃C - 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.
  - Assuming liquid H₂ filling all the pores
  - Volume of pores below 1 nm, cc/g
  - Volume of pores above 1 nm, cc/g

**6. CONCLUSIONS AND REFERENCES**

- Reversible hydrogen storage capacity of CDC is 10 times that of multi-walled nanotubes, 3.5 times that of single-walled nanotubes and 2 times that of metal-organic frameworks (MOF-5).
  - At 1 atm. and 77K, gravimetric capacity > 3.0 wt.% with > 24 kg/m³.
  - 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, CDC capacities > MOF-5, SWNT, MWNT.
  - 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, CDC capacities > MOF-5, SWNT, MWNT.