Carbide-derived carbons designed for efficient hydrogen storage

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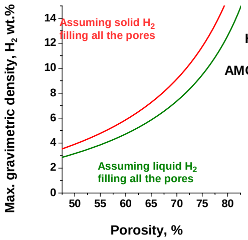
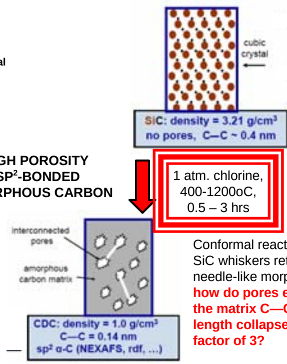
1. INTRODUCTION to CARBIDE-DERIVED CARBONS

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.

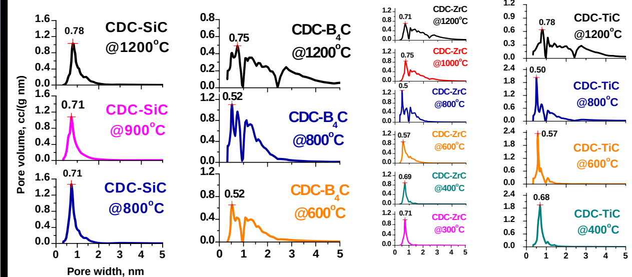


PRECURSOR: MINERAL CARBIDE (binary, ternary, …)



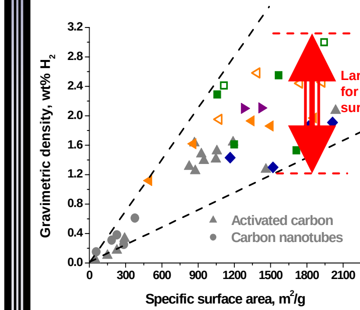
Conformal reaction: e.g. SiC whiskers retain their needle-like morphology. So **how do pores evolve as the matrix C—C "bond" length collapses by a factor of 3?**

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

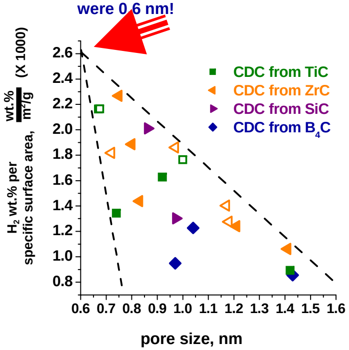


Gas sorption measurements were performed using argon at 77K using Quantachrome Autosorb-1. Pore size distributions were calculated using Non Local Density Functional Theory (DFT).

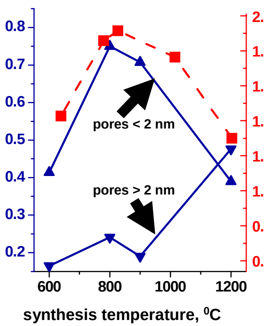
- Capacity of CDCs is higher than that of carbon nanotubes and other carbon nanomaterials.
- The trend of capacity increase with surface area implies that 6000 m²/g will be required to 7 wt.%.
- <u>However</u>, carbon nanomaterials with similar surface areas show large capacity variations.
- <u>Possibility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

4. SMALL PORES ARE <u>CRUCIAL</u> 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!

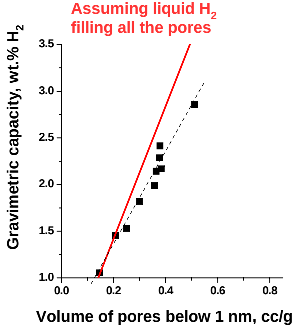


B_4C - CDC: reduced capacity correlates with increasing pore size when the chlorination temperature is too high.

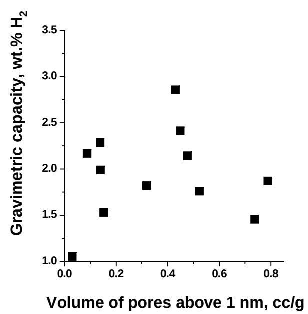


5. CAPACITY CORRELATED W/VOL. OF <u>SMALL</u> PORES

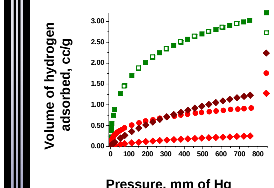
Hydrogen storage <u>increases linearly</u> with pore volume for pores <u>less than 1 nm.</u>



<u>No correlation</u> between hydrogen storage and pore volume for pores <u>greater than 1 nm.</u>



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 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.**

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