Molecular Deuterion crystallisation under cuasi-1D confinement

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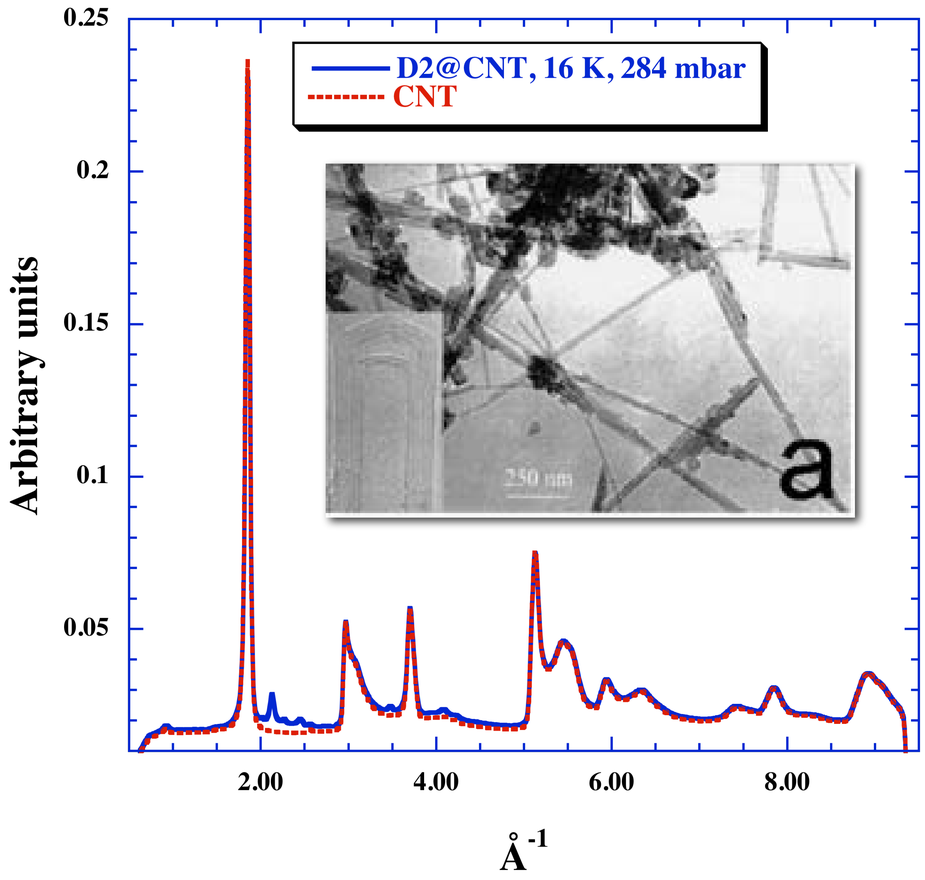
A particularly interesting aspect of Carbon Nanotubes is their use as nearly one-dimensional nano-containers. Apart of their possibilities for controlled chemistry in nano-fluidics devices new phenomena induced by confinement are also expected, such as liquid–like ordered structures [1] or exotic crystalline phases [2]. Here, we present a series of neutron diffraction measurements (instrument D20, ILL, Grenoble) of molecular deuterium confined within Multiple Wall Carbon Nanotubes (MWCTNs). Bulk liquid D_2 at its vapour pressure crystallises in an hcp structure at ~18.7 K. At low uptakes we have found a clear depression of the solidification temperature down to ~13.25 K. Interestingly, at the lowest uptake the diffraction pattern is consistent with the minimal fcc lattice compatible with a cylindrical symmetry.

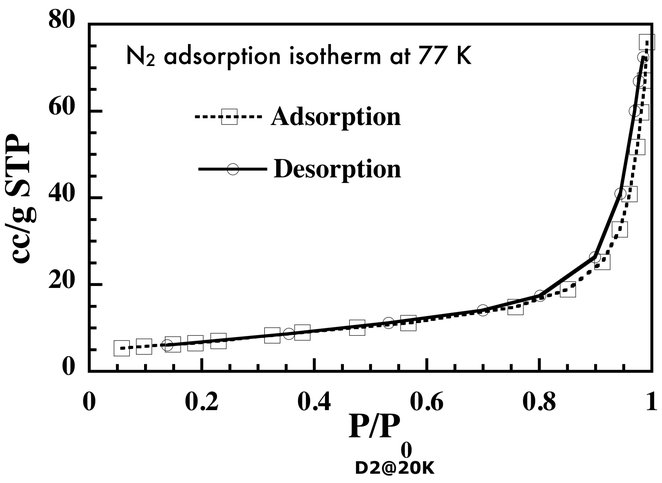
-. MWCNTs synthesized at the Group of Carbon Nanostructures and Nanotechnology (G-CNN), Instituto de Carboquímica, CSIC, by W. K. Maser and collaborators (arc discharge method).

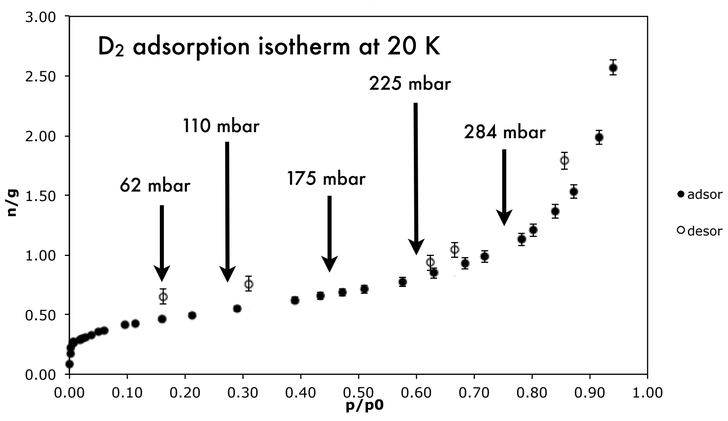
-. Oxidized at 700 C during 30' (expected to open the tubes).

-. Annealed at 900 C in Ar atmosphere during 12 h.

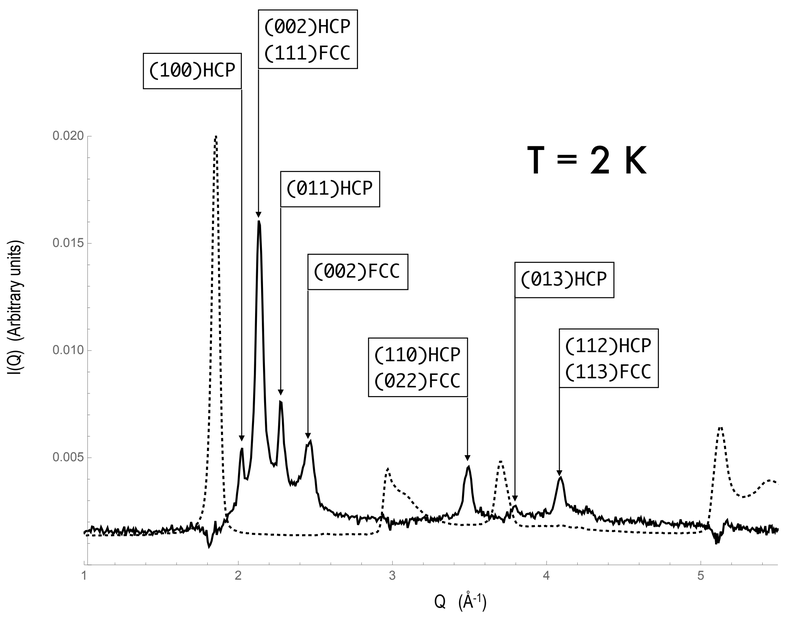
-. External Diameter: ~ 20 - 40 nm



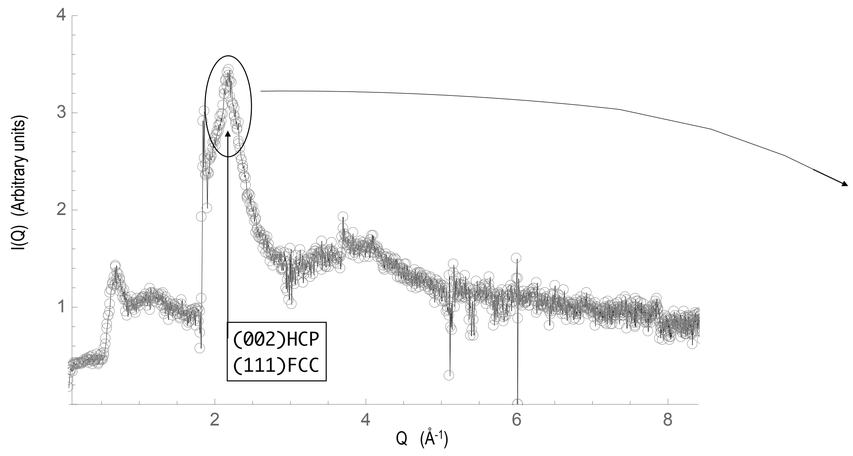


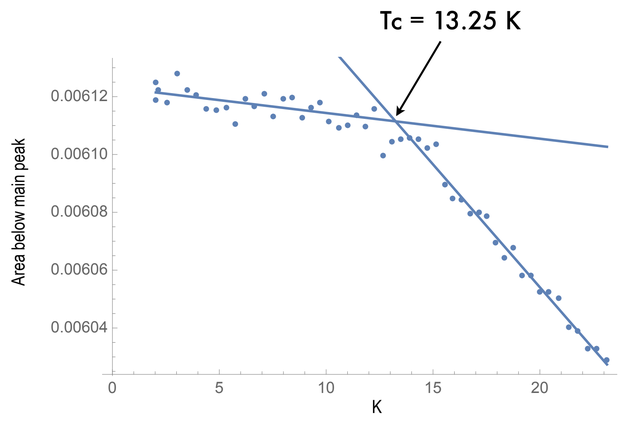


D_2 load: 225 mbar at 20 K

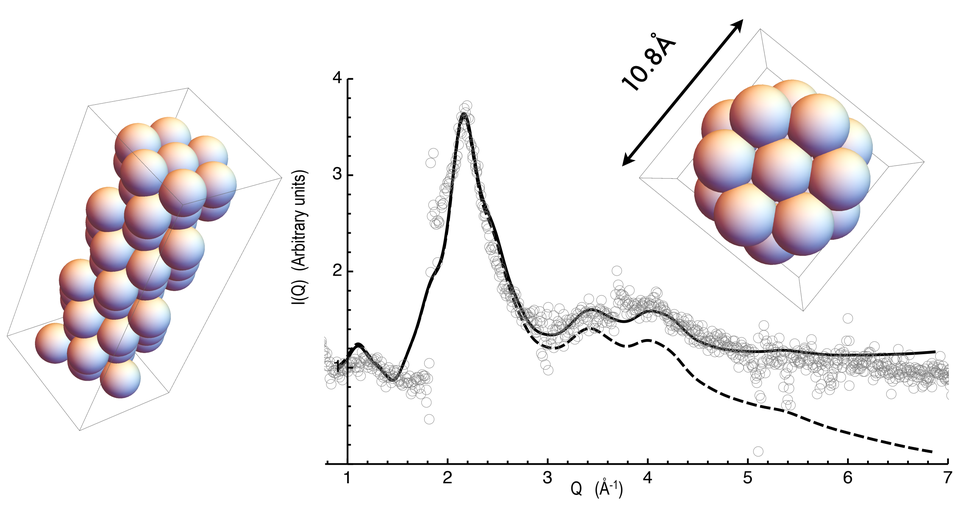


D_2 load: 62 mbar at 20 K

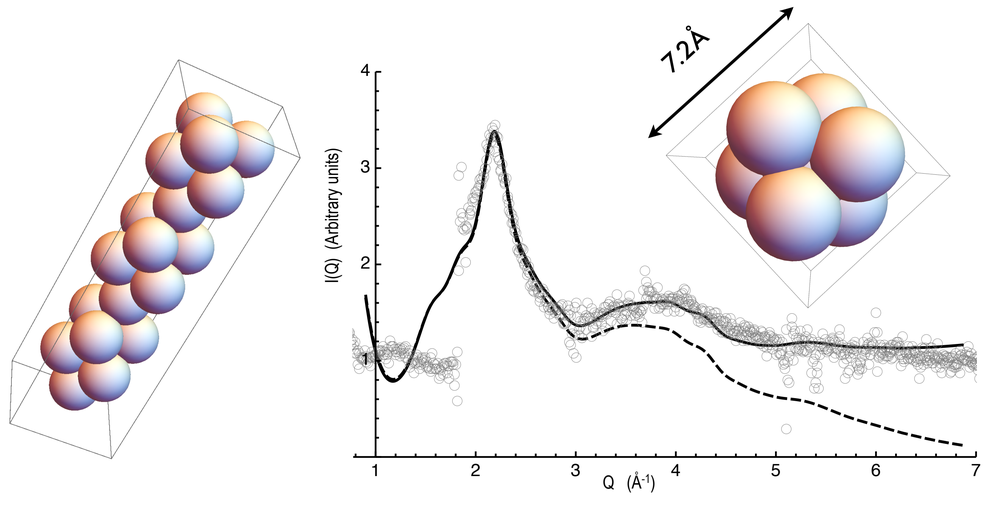




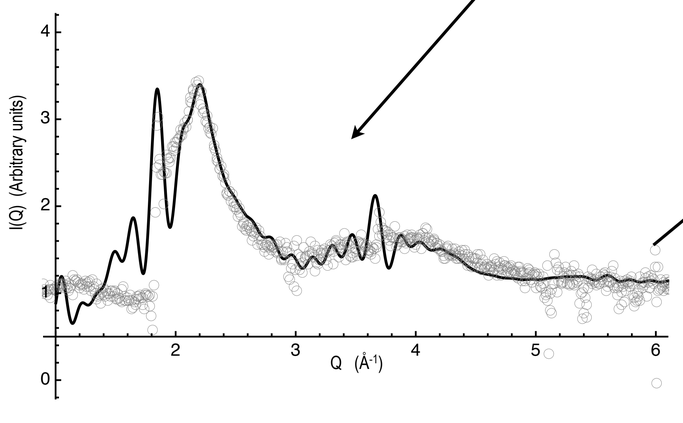
Comparison with calculated ND of the smaller FCC crystals with maximal cylindrical symmetry



Solid line: full quantum scattering calculation
Dashed line: S-wave scattering
Fitted rms molecular displacement: 0.15 Å



Mininal FCC crystal



Solid line: Minimal nanocrystal full scattering + interference term with a MWNT of ten continuos layers of infinite length

Bibliografía:
1] W. H. Noon et al, Chem. Phys. Lett **355**, 445 (2002).
[2] K. Koga er al, Nature **412**, 802, (2001).