# Cronfa -  Swansea University Open Access Repository

_____

This is an author produced version of a paper published in:
_Phys. Chem. Chem. Phys._

_____

http://www.swansea.ac.uk/library/researchsupport/ris-support/

# Resonance Raman and IR spectroscopy of Aligned Carbon Nanotube Arrays with Extremely Narrow Diameters Prepared with Molecular Catalysts on Steel Substrates

Sagar Motilal Jain[a,b], Federico Cesano[a], Domenica Scarano[a] and Tomas Edvinsson[c]*

[a]Department of Chemistry, NIS (Nanostructured Interfaces and Surfaces) Interdepartmental Centre and INSTM Centro di Riferimento, University of Torino, Via P. Giuria, 7, 10125 Torino, Italy  [b]SPECIFIC, College of Engineering Swansea University Bay Campus, Fabian Way, SA1 8EN Swansea, United Kingdom

[c]Department of Engineering Sciences, Solid State Physics, Uppsala University, Box 534, SE 751 21 Uppsala, Sweden.

## Electronic Supplementary Information (ESI)
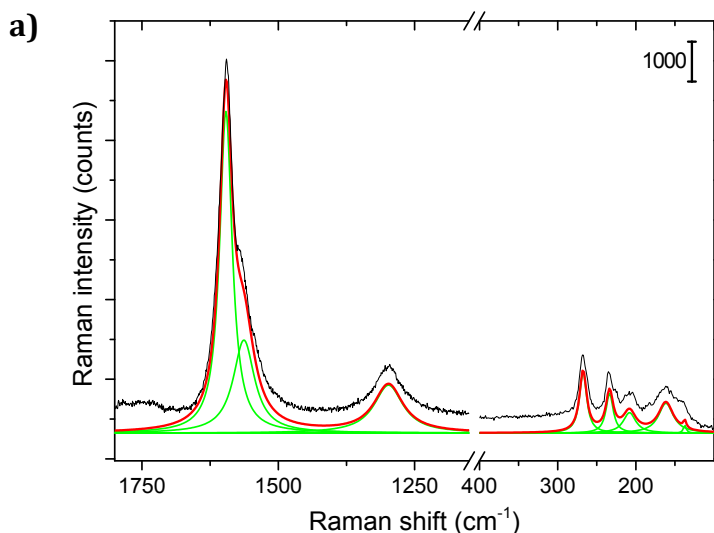
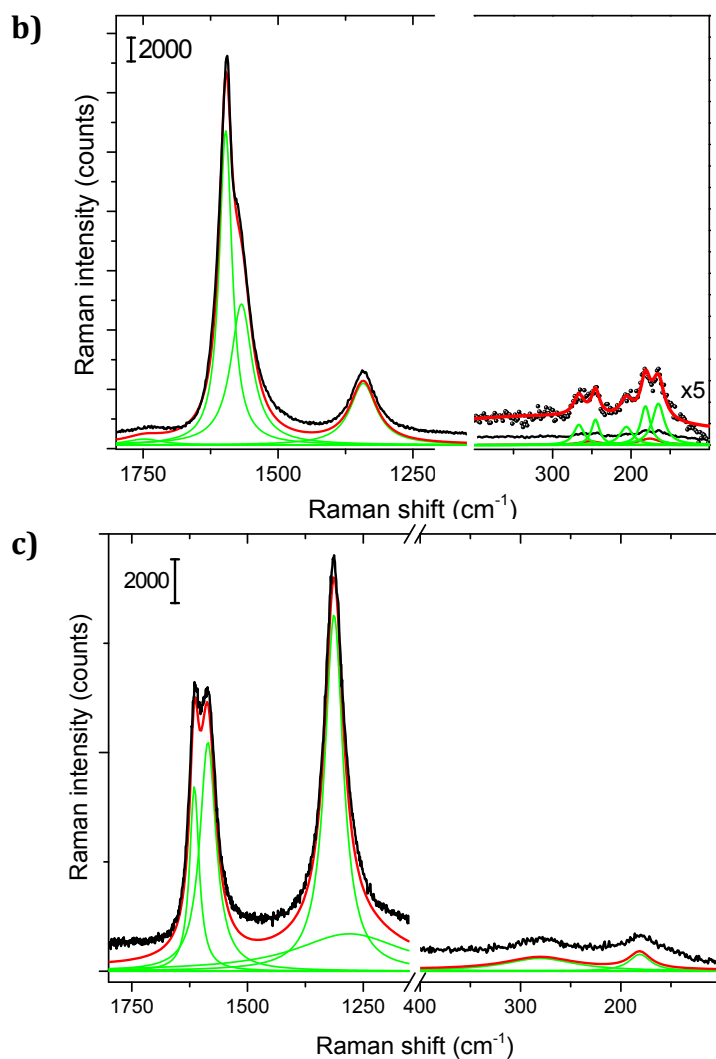**Fig. S1.** First-order and radial-breathing-mode (RBM) Raman spectra of SWCNTs: a) and b) commercial (Elicarb) excited under 785nm and 514 nm laser lines, respectively, as compared to the as c) grown sample, excited under 785 nm laser line. Fittings of the simulated contributions as sum (red curves) and individual bands (green curves) are shown where the fit under the $G^-$ peak is best performed using a Lorentzian shape.

(9,2)    (7,5)

d=8,0±0,1 Å

(11,7)    (12,6)    (14,3)
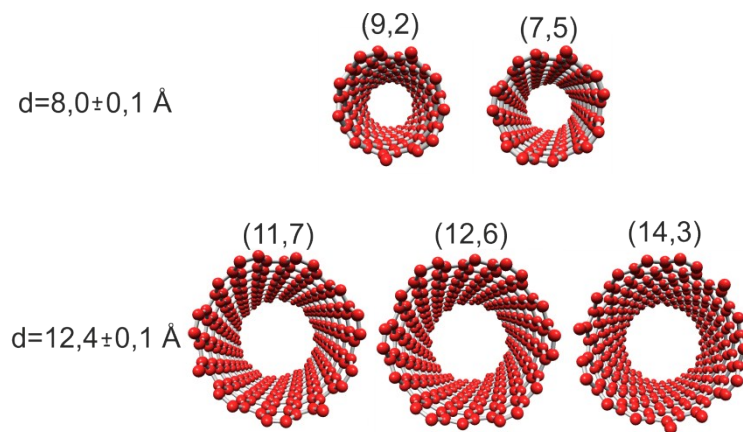
d=12,4±0,1 Å

**Fig. S2.** Models of semiconducting SWCNTs with d = 8,0 ⬚0,1 Å and d= 12,4 ⬚0,1 Å corresponding to the maxima observed in the RBM region of the Raman spectra for the CNT grown on the grid (279.4 cm$^{-1}$ and 180.4 cm$^{-1}$).
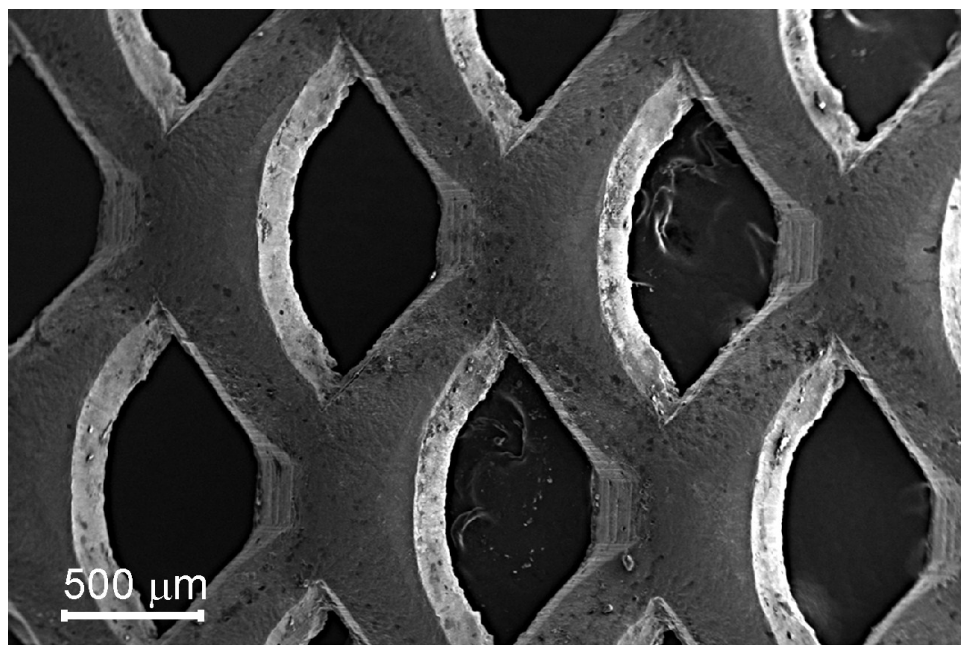
500 μm

**Fig. S3.** SEM image of the steel grid used as a support.

**Table S1.** Chiral vector ($C_k$), angle and diameter of the lowest and highest dimensional SWCNTs grown on the steel grids as extracted from analysis of the Raman spectra irrespectively of the G⁻ line shape analysis.

| CNT | $C_k$ (m,n) | Chiral angle[a], ⱷ (degrees) | Diameter (nm) | Metallicity[b] | Band gap[c] (eV) |
|---|---|---|---|---|---|
| SWCNT | (9,2) | 9.8 | 0.81 | S | 1.05 |
| | (7,5) | 24.5 | 0.83 | S | 1.02 |
| | (8,4) | 19.1 | 0.84 | S | 1.01 |
| | (10,1) | 8.4 | 0.84 | M | - |
| | (11,7) | 22.7 | 1.25 | S | 0.68 |
| | (14,3) | 9.5 | 1.25 | M | - |
| | (12,6) | 19.1 | 1.26 | S | 0.67 |

[a] *Chiral angle as defined from the deviation from the zigzag direction (n=0, Fig 1 (a))*

[b] *Semiconducting (S) and metallic (M)*

[c] *Estimated through the parametrized equation Eg=(0.85 eVnm)/diameter* and neglecting strain.

Table S2 Comparison of laboratory synthesis costs of CNTs and that from commercial companies.

| CNTs | Price ($/g) | Reference |
|---|---|---|
| SWCNTs | 110 | Thomas Swan Elicarb<br><br>http://www.thomas-swan.co.uk/ |
| MWCNTs | 80 | Mitsui<br><br>https://www.mitsui.com/eu/en/index.html |
| SWCNTs + MWCNTs | ~ 35 | This study |