Transmission signatures of peapod-grown double-walled carbon nanotubes

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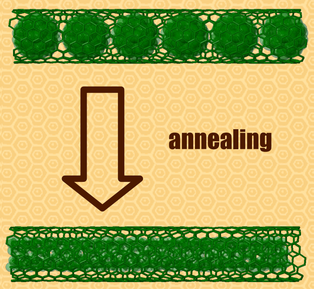
Motivation



Measurements on **peapod** grown double-walled carbon nanotubes show anomalies:

NMR - metallic spin relaxation for all inner tubes [1],

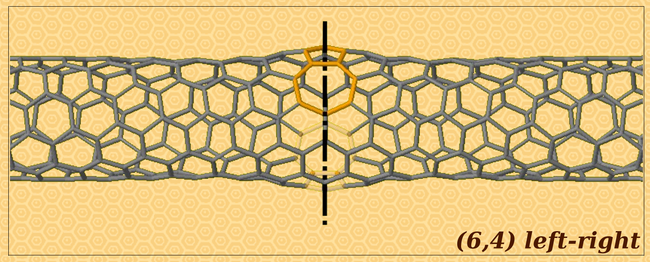
ESR - features reminiscent of localized states appear during annealing,

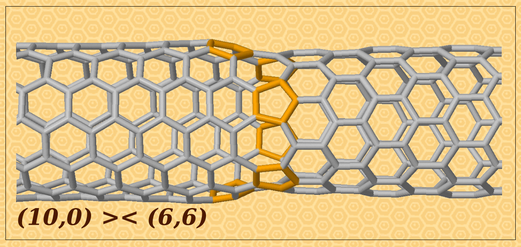
mechanically breakable – e.g. Raman signal of inner tubes disappears after grinding the samples.

What kind of essential difference will show **electronic transport** measurements on such structures by the state of annealing?

Introduction

- For a given outer tube more inner tubes are possible (selected by van der Waals distance)
- Inner tube growth can start at different places
- Connection of different chiralities form a defect (pentagon-heptagon pairs were considered so far)
- Simplest possibility: a junction of a left-handed and a right-handed chiral nanotube
- Nanobamboo: bamboo-like nanostructure (on the right)



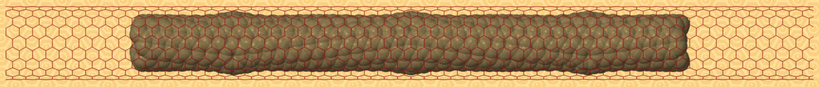


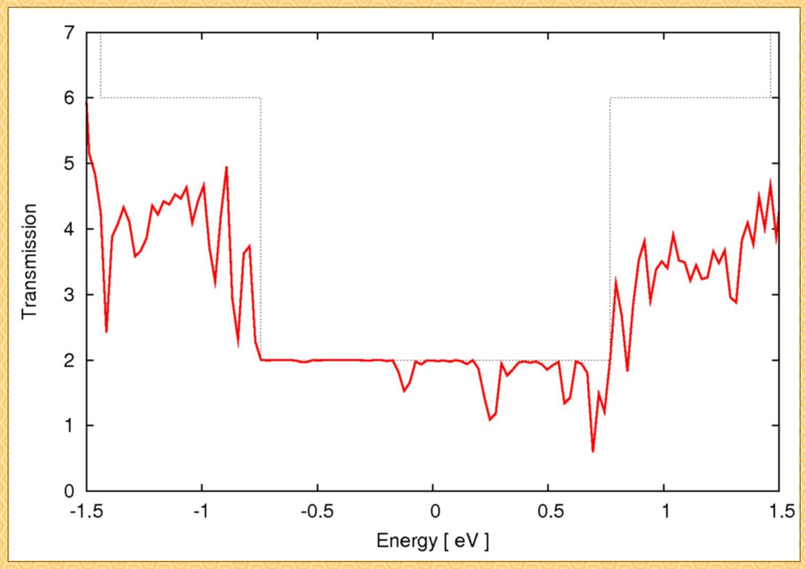
- with different chiralities metallic-semiconductor junction also possible (on the left)
- localized states were found around the Fermi level by DFT
- Find details of geometry fabrication and localized states of nanobamboo in *physica status solidi b*, **246**, 2671-2674, (2009)

Methods

- Density Functional Theory (DFT) based Vienna ab-initio Simulation Package [2], within the local density approximation (LDA) and projector augmented-wave method (PAW),
- DFT-optimized geometries (plane-wave cutoff energy of 500 *eV*), screw-axis symmetry was used to create longer geometries, if needed,
- transport calculations were carried out on (10,10) nanotube filled with C_{60} fullerenes, nanobamboo or pristine inner nanotube, with adding contacts only to the outer tubes,
- Inter molecular Hückel-type Hamiltionian (IMH, [3]) with a sufficiently large supercell of at least 5000 atoms,
- transport calculation with a recursive Green-function technique and Landauer-Büttiker formalism.

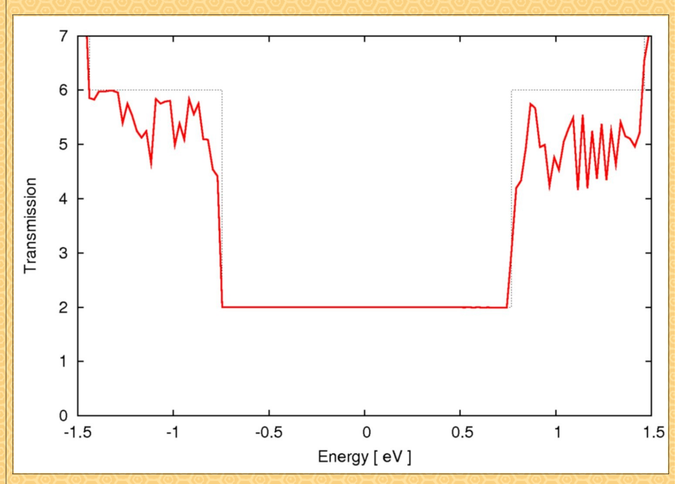
Nanobamboo





Calculated transmission probability against the energy for a 293.93 Å long (6,4) left-right nanobamboo with 9 bumps in (10-10) nanotube (*Fermi energy is shifted to 0*).

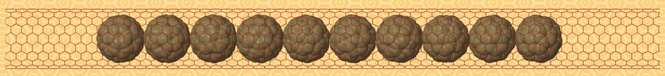
DWCNT

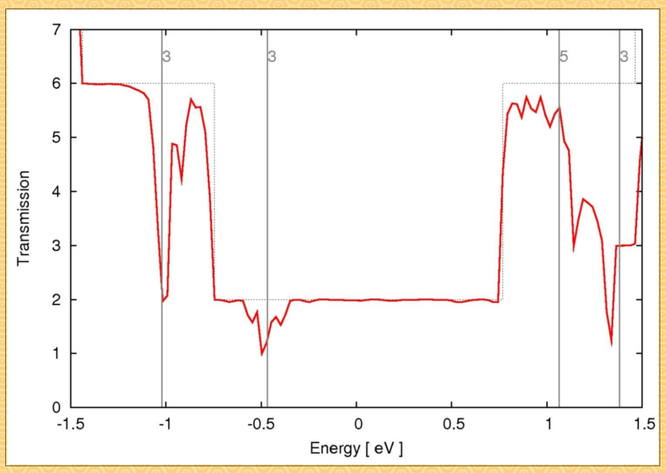


Calculated transmission probability against the energy for (6,4)@(10-10) double-walled carbon nanotube (*Fermi energy is shifted to 0*).

The dotted line depicts the number of open channel in the outer tube. The transmission is barely effected by the pristine inner tube.

Peapods

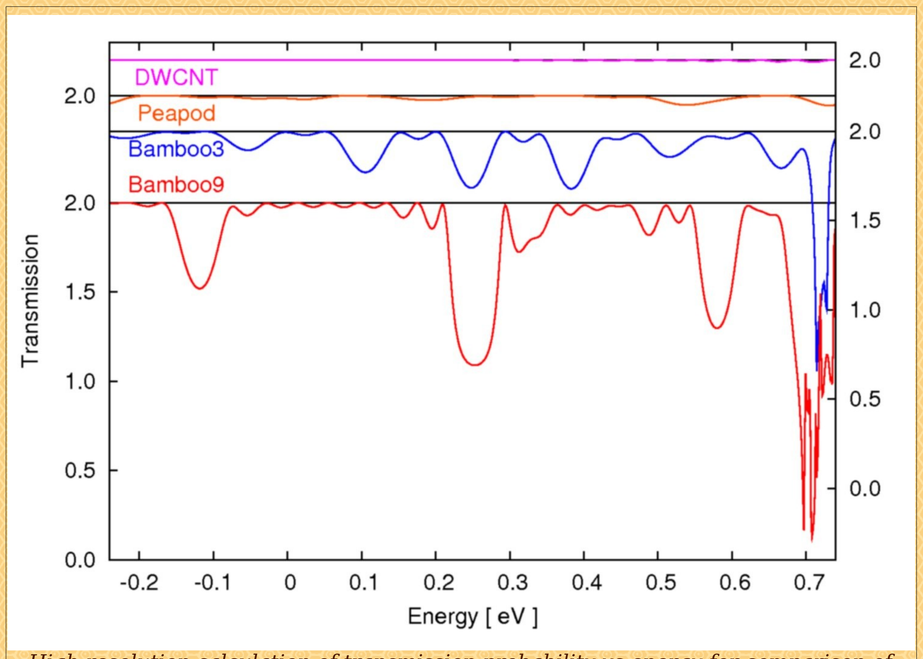




Calculated transmission probability against the energy for C_{60} filled (10-10) carbon nanotube (*Fermi energy is shifted to 0*).

Gray bars depict the energy levels of a separated fullerene computed with the same Hückel-type tight binding calculation. The gray numbers show the degeneracy of the levels. Splitting of the degenerate levels are expected because of the intershell interactions.

Comparison



High resolution calculation of transmission probability vs energy for comparison of key transport signatures. (Note that the curves are shifted vertically for better visibility).

Notation of the figure:

- DWCNT: (6,4)@(10,10)
- Peapod: C_{60}@(10,10), random orientation
- Bamboo3: (6,4) left-right in (10,10), 3 bumps, distance between successive bumbs: L_3=82.019 Å total length: 255.433 Å.
- Bamboo9: (6,4) left-right in (10,10), 3 bumps, distance between successive bumbs: L_9=32.533 Å, total length: 293.93 Å.

Structure of the peaks:

- main peak at 0.25 eV.
- satellite peaks at $\pm\Delta E_3$=0.13 eV, $\pm 2\Delta E_3$, for Bamboo3.
- satellite peaks at $\pm\Delta E_9$ =0.33 eV for Bamboo9.
- $\Delta E_3/\Delta E_9 = L_9/L_3$.
- n-2 small peaks equally spaced between satellite peaks (n=3 or 9).

Conclusions

- **transmission probabilities were calculated for nanotubes filled with C_{60}, nanobamboo and for double-walled carbon nanotubes,**
- **peaks near the Fermi energy are found for the bamboo-like structure, with a remarkable structure (Kronig-Penney model),**
- **more chiralities, random lengths, disorder should be investigated.**

References

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[3] Lázár A, Surján P, Paulsson M and Stafström S, Int. J. Quantum Chem. **84**, 216 (2002)

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