Chapter 17
Bundlet Model for Single–Wall Carbon Nanotubes, Nanocones and Nanohorns

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ABSTRACT

This paper discusses the existence of single-wall carbon nanocones (SWNCs), especially nanohorns (SWNHs), in organic solvents in the form of clusters. A theory is developed based on a bundlet model describing their distribution function by size. Phenomena have a unified explanation in bundlet model in which free energy of an SWNC, involved in a cluster, is combined from two components: a volume one, proportional to number of molecules n in a cluster, and a surface one proportional to $n^{1/2}$. Bundlet model enables describing distribution function of SWNC clusters by size. From purely geometrical differences, bundlet (SWNCs) and droplet (fullerene) models predict different behaviours. The SWNCs of various disclinations are investigated via energetic–structural analyses. Several SWNC's terminations are studied, which are different among one another because of type of closing structure and arrangement. The packing efficiencies and interaction-energy parameters of SWNCs/SWNHs are intermediate between fullerene and single-wall carbon nanotube (SWNT) clusters; an in-between behaviour is expected. However, the properties of SWNCs, especially SWNHs, are calculated close to SWNTs. The structural asymmetry in the different SWNCs, entirely characterized by their cone angle, distinguishes the properties of some, such as P2.

INTRODUCTION

Nanoparticles (NPs) interest arises from the shape-dependent physical properties of materials at nanoscale (Faraday, 1857; Murphy *et al*., 2010). The occurrence of single-wall carbon nanocones (SWNCs) was used to investigate the nucleation and growth of curved carbon structures, suggesting that pentagon presence performs a fundamental role. When a pentagonal defect is introduced into a graphitic sheet (graphene, GR), via the extraction of a 60º sector from this sheet, one forms a

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cone sheet. Pentagon presence in an SWNC apex is analogue of that in single-wall carbon nanotube (SWNT) tip topology. The SWNT terminations attracted interest once peculiar electronic states, related to topological defects in graphite lattice, were theoretically predicted (Tamura & Tsukada, 1995). The resonant picks in the density of states were observed in SWNTs (Kim *et al*., 1999) and multiple-wall carbon nanotubes (MWNTs) (Carroll *et al*., 1997). Table 1 shows SWNT–MWNT comparison.

The SWNCs with discrete opening angles (apices, θ) of 19º, 39º, 60º, 85º and 113º of cone were observed in a carbon sample generated by hydrocarbon pyrolysis (Krishnan *et al*., 1997). The observation was explained by a model of the cone wall composed of wrapped GR sheets, where geometrical requirement for seamless connection naturally accounted for the semi-discrete character and absolute values of cone angle. The total disclinations of all conic graphenic microstructures are multiples of 60º, corresponding to the presence of a given number ($P \geq 0$) of pentagons in SWNC apices. Considering GR sheet symmetry and Euler theorem, only five types of SWNCs (corresponding to the values of angle) can be obtained from a continue GR sheet, matching to P values in 1–5. Cone angle (θ) is given by $\sin(\theta/2) = 1 - P/6$ leading to reported values for SWNC angles, where flat discs and caped SWNTs correspond to $P = 0$ and $P = 6$. The SWNC with $P = 5$ pentagons ($\theta = 19º$) is called single-wall carbon nanohorn (SWNH). Several configurations exist for a given SWNC angle, depending on the form in which pentagons are arranged in conic tips. A 113º SWNC presents only one pentagon in the centre of the tip and only one configuration. The other structures show two or more isomers as the pentagons can be organized in various manners. According to the *isolated pentagon rule* (IPR) derived from the study of fullerenes (Kroto, 1987), the configurations containing isolated pentagons lead to isomers that are more stable than those containing grouped pentagons, for SWNCs. Additional simple rules were derived form *ab initio* calculations (Jan & Jaffe, 1998), performed to evaluate the stability of SWNCs containing isolated/grouped pentagons. Consideration of a curvature-producing pentagon as a defect, in a planar network of hexagons, results in that the arrangement of two pentagons in a hexagonal lattice can be specified by a hexagonal co-ordinate (a,b), with a pentagon in (a,b) and another in (0,0). The nearest-neighbouring pentagons are only (1,1)-co-ordinated in C_{60} (all pentagons are connected by a C–C bond), and are (1,1)- and (2,0)-co-ordinated in C_{70} (the latter corresponds to two pentagons separated by one hexagon). In accordance with density-functional-theory calculations, pentagons (1,1) lead to SWNC tip structures more stable than those of pentagons (2,0), which is attributed to the lower *stress* induced by each pair (1,1) in relation to pairs (2,0). The SWNCs present high asymmetry in geometry and are semiconductors. The SWNC insolubility in all solvents and their great tendency to agglomerate (micrometre-order) must be overcome, before considering practical technological applications. The SWNC covalent functionalization

Table 1. Comparison between SWNTs and MWNTs

SWNT	MWNT
Single layer of graphene	Multiple layer of graphene
Catalyst is required for synthesis	Can be produced without catalyst
Bulk synthesis is difficult as it requires proper control over growth and atmospheric condition	Bulk synthesis is easy
Purity is poor	Purity is high
A chance of defect is more during functionalization	A chance of defect is less but once occurred it is difficult to improve
Less accumulation in body	More accumulation in body
Characterization and evaluation is easy	It has complex structure
It can be easily twisted and are more pliable	It cannot be easily twisted