

Heuristic Model For Conical Carbon Nanofiber

John P. Dismukes^a, Xinglong Xu^a,
 Arunan Nadarajah^a, Muhammed U. Afzal^a
 Thomas W. Hughes^b, Thomas Wittberg^c
^aCollege of Engineering, University of Toledo
 Toledo, Ohio 43606-3390
^bApplied Sciences, Inc.
 Cedarville, Ohio 45314-0579
^cUniversity of Dayton Research Institute
 Dayton, OH 45469-0168

Although the growth of conical structured carbon nanofibers by decomposition of hydrocarbons on nanoscale metal particles dates to the 1970's, relatively fewer studies of the basic structure of these materials [1] have been reported than of carbon nanotube materials. Federal government funded research has demonstrated that relatively small additions of these materials to polymer matrices provide promising combinations of electrical and structural properties. Current manufacturing volume worldwide is several hundred thousand pounds per year at \$100/pound, and production at the million pound per year scale is forecast as prototype applications become accepted into products.

These 50-100 nm-diameter conical carbon nanofiber materials warrant systematic scientific and engineering study at this time, particularly from the point of view of the nature of the conical subunits making up the conical nanofiber substructure, the number and axial alignment of the graphene planes making up the conical subunits, the perfection of C-C bonding, and the chemical reactivity of the external surfaces with inorganic and organic or polymeric moieties. This knowledge is required as a basis for synthesis-process-structure-property relations, engineering economics and manufacturing design.

Initial research [1] on a heuristic model for carbon nanofiber built up from graphene planes, with no atomic defects, has provided a numerical basis for calculation of nanofiber density, the concentration of external surface carbon atoms, and the stoichiometry for organic functionalization of fibers oxidized to form carboxylic acid groups. The initial research has also stimulated interest in a cone-helix [2] substructure rather than a stacked-cup substructure [3] for conical nanofiber. The current paper describes a fundamental and applied effort to explore and assesses the two proposed conical nanofiber structures, on theoretical and practical grounds. This paper provides a comparative assessment of two models, including synthetic mechanism and mechanical and electrical properties inherent in the two different conical forms.

References

1. X. Xu et al., Hierarchical Model of Stacked Cup Carbon Nanofiber (SCCNF) Structure, SAMPE National Conference, Long Beach, CA, May 2004.
2. D. D. Double and A. Hellawell, "Cone-Helix Growth Forms of Graphite", *Acta Met.* Vol. 22, 481-487 (1974).
3. M. Endo et al., "Structural characterization of cup-stacked-type nanofibers with an entirely hollow core", *Applied Physics Letters*, Vol. 80, 1267-1269 (2002).

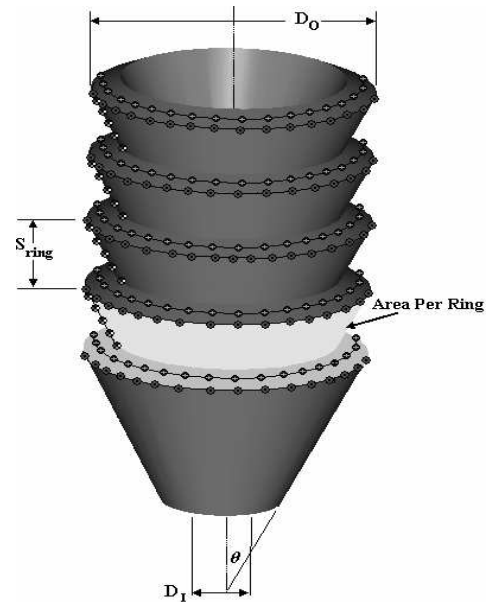


Fig. 1. Stacked-cup carbon nanofiber with two graphene layers in the conical substructure.

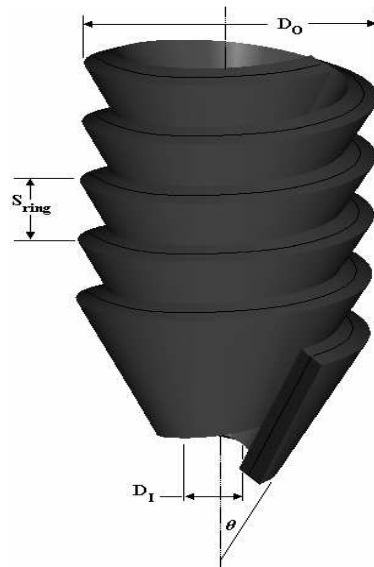


Fig. 2. Cone-helix carbon nanofiber with two graphene layers in the conical substructure.

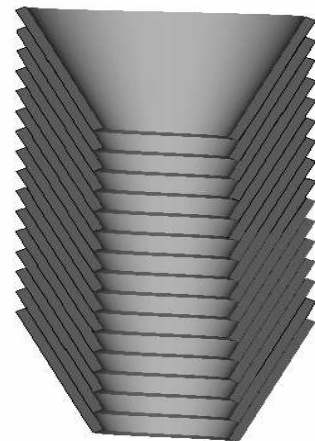


Fig. 3. Cross-sectional view of cone-helix carbon nanofiber