Relations between global and local topology in multiple nanotube junctions

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General topological rules determine the carbon ring structures in arbitrary sp^2-bonded structures, particularly nanotube junctions. [S0163-1829(98)09543-5]

The experimental observation[1] of junctions between multiple tubelike carbon nanostructures motivates a topological study of the constraints on the types of carbon rings comprising arbitrary sp^2-bonded structures, in particular junctions that incorporate three or more terminals[2–4] into carbon nanotube[5] devices.[4,6–8]

The results herein all follow directly from the generalized Euler rule for the polygons on the surface of a closed polyhedron of arbitrary genus (number of holes). The number of faces plus the number of vertices equals the number of edges plus 2 minus twice the genus, $F+V=E+2-2G$. For sp^2 carbon nanostructures, we refer to a purely hexagonal structure with admixtures of 4-, 5-, 7-, or 8-gons. The excess in the number of polygonal sides due to these nonhexagonal polygons is called the bond surplus. For example, an otherwise hexagonal structure containing two pentagons has a bond surplus of minus two (regardless of whether the pentagons are fused).

The large-scale topology of the overall sp^2 sheet constrains the small-scale topology of the constituent carbon rings. A simple quasispherical fullerene of genus zero satisfies $F+V=E+2$, which yields the familiar bond surplus of -12, e.g., the 12 pentagons in a C_{60}. An open-ended nanotube can be closed upon itself in a large-radius donut without disturbing the polygonal structures on the surface. This donut has $G=1$ and satisfies $F+V=E$, with zero bond surplus. Such a nanotube can contain all hexagons or equal numbers of pentagons and heptagons as described previously.[4,7–9]

The new, more topologically interesting cases arise from junctions of three or more half-tubes.[2,3] The bond surplus in an arbitrary closed sp^2-bonded structure is $6(E-F-V)=12(G-1)$. This formula follows directly from the cases of fullerenes ($G=0$) and closed nanotubes ($G=1$), since the bond surplus is linear in the genus. Two nanotube T or Y junctions can be mated into a closed surface of genus 2,

with a bond surplus of 12 shared between the two junctions. The bond surplus of six in each junction can be taken up, for example, by six heptatons or a combination of six octagons and six pentagons within a hexagonal framework. (This result can also be obtained by placing six-pentagon caps on each open end of a single junction and applying Euler's rule with $G=0$). Inclusion of pentagons allows junctions between tubes of arbitrary wrapping indices.

Similarly, two X junctions can be mated into a surface of genus 3,

with a total bond surplus of 12 per junction. In general, a junction or series of junctions comprising N half-tubes has a bond surplus of $12(N-2)$. In this picture a simple closed shell of genus zero is the special case of an $N=1$ half-tube.

The strongly directional carbon sp^2 covalent bonds guarantee structural metastability so long as extreme conformations such as multiple fused squares are avoided. Analogous topological rules also apply for other tubular structures (e.g., transition metal dichalcogenides[10]) with global and local topological constraints.

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[1] D. Zhou and S. Seraphin, Chem. Phys. Lett. **238**, 286 (1995).
[2] M. Menon and D. Srivastava, Phys. Rev. Lett. **79**, 4453 (1997).
[3] L. A. Chernozatonskii, Phys. Lett. A **172**, 173 (1992).
[4] L. Chico, V. H. Crespi, L. X. Benedict, S. G. Louie, and M. L. Cohen, Phys. Rev. Lett. **76**, 971 (1996).
[5] S. Iijima, Nature (London) **354**, 56 (1991).
[6] N. Hamada, S. I. Sawada, and A. Oshiyama, Phys. Rev. Lett. **68**, 1579 (1992); J. W. Mintmire, B. I. Dunlap, and C. T. White, *ibid.* **68**, 631 (1992); R. Saito, M. Fujita, G. Dresselhaus, and M. S. Dresselhaus, Appl. Phys. Lett. **60**, 2204 (1992).
[7] R. Saito, G. Dresselhaus, and M. S. Dresselhaus, Phys. Rev. B **53**, 2044 (1996); J. C. Charlier, T. W. Ebbesen and Ph. Lambin, *ibid.* **53**, 11 108 (1996); Ph. Lambin, A. Fonseca, J. Vigneron, J. B. Nagy, and A. A. Lucas, Chem. Phys. Lett. **245**, 85 (1995); B. I. Dunlap, Phys. Rev. B **49**, 5643 (1994).
[8] V. H. Crespi, M. L. Cohen, and A. Rubio, Phys. Rev. Lett. **79**, 2093 (1997).
[9] S. Iijima, T. Ichihashi, and Y. Ando, Nature (London) **356**, 776 (1992).
[10] Y. Feldman, E. Wasserman, D. J. Srolovitz, and R. Tenne, Science **267**, 222 (1995).

