

## **Nanotechnology with Carbon: Fullerenes, Nanotubes, Peapods**

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In view of their atomic-level perfection, the efficient formation of fullerenes, nanotubes, peapods and other sp<sup>2</sup> bonded carbon nanostructures raises questions about the role of defects and their elimination during the hierarchical self-assembly process. Combining ab initio calculations with molecular dynamics simulations, I will show that defects may assist in the efficient inter-conversion of nanostructures, such as multi-wall nanotubes and scrolls [1], and in the formation of new systems including foams and peapods [2,3]. The unusual stability of carbon nanostructures, both at high temperatures and under electronic excitations, stems from their ability to reduce the impact of defects such as atomic vacancies [4]. The efficiency of the self-healing mechanism increases with decreasing system size, with interesting implications for device application.

[1] J. Gerard Lavin, Shekhar Subramoney, Rodney S. Ruoff, Savas Berber, and David Tomanek, *Scrolls and Nested Tubes in Multiwall Carbon Nanotubes*, Carbon (2002).

[2] Savas Berber, Young-Kyun Kwon, and David Tomanek, *Microscopic Formation Mechanism of Nanotube Peapods* (submitted for publication).

[3] Young-Kyun Kwon, David Tomanek, and Sumio Iijima, "Bucky-Shuttle" Memory Device: Synthetic Approach and Molecular Dynamics Simulations, *Phys. Rev. Lett.* 82, 1470 (1999).

[4] Yoshiyuki Miyamoto, Savas Berber, Mina Yoon, Angel Rubio, and David Tomanek, *Onset of nanotube decay under extreme thermal and electronic excitations* (Proceedings of the CNT'10 Conference, Tsukuba, October 3-5, 2001).