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# Coalescence of single-wall carbon nanotubes and nano-peapods

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For various applications in nanotechnology, electronic devices and strong nano-mechanical systems need the establishment of molecular connections among single-walled nanotubes (SWNTs). Coalescence of SWNTs has been observed in-situ under electron irradiation at high temperature in a transmission electron microscope [1]. The merging process is investigated at the atomic level using molecular dynamics simulations. Vacancies induce coalescence via a zipper-like mechanism, imposing a continuous reorganization of atoms on individual tube lattices along adjacent tubes. Other topological defects induce the polymerization of tubes.

However, it is also imperative to join and connect nanotubes in a controllable way. Here, we demonstrate for the first time, that electron beam exposure at elevated temperatures, can be used as an effective tool to covalently weld crossed SWNTs in order to create molecular junctions of various geometries. Stable ”X“-, ”Y“-, or ”T“-like junctions have been created in-situ in a transmission electron microscope [2]. Electron beam exposure at high temperatures induces structural defects, which promote the joining of tubes via cross-linking of dangling bonds. The observations of the merging are supported by molecular dynamics simulations, which show that the creation of vacancies and interstitials induces the formation of junctions involving seven- or eight-membered carbon rings at the surface interface between the tubes. Electronic properties of junction models, resembling those observed in the experiments, are also predicted. We envisage that our results will pave the way towards controlled fabrication of nanotube based molecular circuits and network architectures exhibiting exciting electronic and mechanical behaviour.

A number of different potentials have been used to perform molecular dynamics and Monte Carlo calculations at various temperatures [3] in order to elucidate the electron irradiation and thermal annealing driven coalescence mechanism of fullerenes inside single-walled carbon nanotubes (SWNTs). Experimentally, various sequences of fullerene coalescence have been observed *in situ* by electron irradiation inside a transmission electron microscope (TEM). Both theoretical and experimental results indicate that the fullerene merging results in stable corrugated SWNTs. The so-obtained new tubular form of carbon contains heptagonal and hexagonal rings, and exhibits diameters ranging from 5 to 7 Å. This process occurs via polymerization of $C_{60}$ molecules followed by surface reconstruction, which can be triggered either by the formation of vacancies (created under electron irradiation) or by surface energy minimization activated by thermal annealing. The electronic properties and electron conductance of these novel tubules are investigated, and possible applications of the materials are discussed.

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[2]. M. Terrones, F. Banhart, N. Grobert, J.-C. Charlier, H. Terrones, and P.M. Ajayan, Physical Review Letters 89, 075505 (2002)
[3]. E. Hernandez, V. Meunier, B.W. Smith, R. Rurali, H. Terrones, M.B. Nardelli, M. Terrones, D.E. Luzzi, and J.-C. Charlier, submitted for publication (2002)

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