Structural and Mechanics Stability of ~1D Nanowires and Nanotubes

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Interest to quasi-1D material structures due to variety of device applications stimulates studies of their atomic packing and stability. We investigate the fundamental differences between the bulk-like whiskers of silicon or dimond and the unique tubular structures of carbon, boron nitride, or fluorinated carbon. While the generalized Wulff-type analysis for the bulk-like wires involves a complex competition of the contributions in the Gibbs energy,

$$G - FL = G(\text{bulk}) + G(\text{surface}) + G(\text{edges}) + G(\text{defects}) \quad [1]$$

the tubular wires have all their constituent atoms in the identical energy states. This homogeneity is an important cause of their stability, in addition to more frequently discussed inherent strength of interatomic bonds.

We have investigated the ground state structure of pristine Si and diamond-C wires (1) and compared the different crystallographic orientations, surface reconstructions and the facet-matching at the edges. This allowed us to establish true ground states for Si, while also to observe spontaneous annealing of thin diamond-whisker in to a series of tubular motifs – carbon nanotubes.

For the family of nanotubes of C, BN and C_2F, their stability with respect to high temperature and mechanical load is determined by thermodynamics of the primary defects, achieved by a Stone-Wales bond rotation-switch. *Ab initio* calculations show that in spite of homo-polar (BB and NN) bond frustration, the energy of SW defect is still below the energy of possible larger dipole of 4/8/8/4 (2).

While relaxation at high temperature involves series of bond rotations, they are suppressed at room conditions (3) and the failure may rather occur through the direct bond-breaking states, “virtual defects”. Recent quantum mechanical calculations (4) allowed us to establish a series of metastable configurations, almost degenerate in energy, corresponding to b = 1, 2, 3, 4, *etc.* broken bonds, and serving as precursors of brittle Griffith crack, Fig. 1. If stabilized in a bent-tube configuration, these edges can permit a side-wall field emission similar to that from an open tube end.

Possibility of bond-rotation at either high temperature or under irradiations leads to understanding of welding mechanisms that can be viewed as a reversed failure. Indeed we have recently identified (5), through 2D-topology mapping and molecular simulations, the exact sequences for a variety of geometries. Fig. 2 shows one example of high-T welding.

Large distortions in monoatomic layers cause redistribution of electron charge density, a charge spill-out which results in a formation of local dipoles. Recent computations (6) confirmed this hypothesis, also consistent with the pyramidalization angle analysis. The magnitudes of the curvature-induced dipoles are quite substantial and directly proportional to the local curvature.

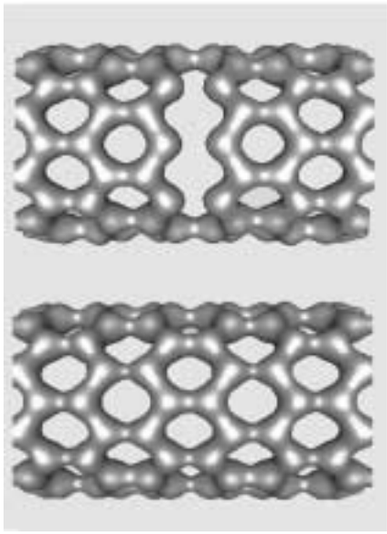

Fig. 1 Computed charge density deistribution for a still-intact and “bifurcated” SWNT, of nearly equal energies at large strain (6).

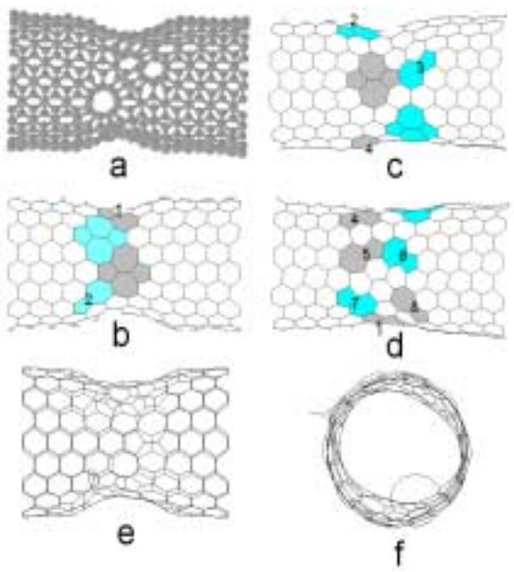

Fig. 2 Welding process for a pair of (10,10) SWNTs (5).

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