FROM NANODIAMOND TO NANOWIRES

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Recent advances in the fabrication and characterization of semiconductor and metallic nanowires are proving very successful in meeting the high expectations of nanotechnologists. It is not surprising that diamond-based nanomaterials have been proposed as ideal candidates for various nanoscale applications since they possess unique electronic, optoelectronic and structural properties such as high elastic modulus and strength-to-weight ratio. Still, although the nanoscience surrounding sp^2 bonded carbon nanotubes has continued to flourish over recent years the development of the sp^3 analogue, diamond nanowires, has been slow.

Observations of the transformation of nanodiamonds into carbon-onions (and vice versa) inevitably lead to the question of whether a similar transformation occurs in diamond nanowires. Are there fundamental reasons why diamond nanowires are thermodynamically or structurally unstable? Will diamond nanowires convert to multi-walled nanotubes structures, and if so, in which size regime? Few experimentalists have succeeded thus far in synthesizing diamond nanowires, but a number of theoretical models have been used to compare the structure and stability of diamond nanowires as a function of morphology and size.

Using ab initio techniques to study the structural relaxation of diamond nanowires, it has been found that the energetic and structural stability of a diamond nanowire is dependent on both the surface morphology and the crystallographic direction of the principal axis. Dodecahedral and cubo-dodecahedral morphologies have been found to retain the diamond structure and remain stable upon relaxation, although nanowires with the principal axis in the [110] direction appear less favorable. In contrast, diamond nanowires with octahedral surface facets (and trigonal cross-section) exhibited delamination of octahedral surfaces parallel to the nanowire axis; forming hybrid structures known as `bucky-wires'.

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