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Carbon nanotubes

As if the excitement of the buckyballs was not enough, researchers in the area of carbon materials now have carbon nanotubes (buckytubes) and onions to play with. Truly a nanomaterial, the properties and possible applications of nanotubes are legion. Consider a structure comprised of concentric cylinders (of graphite in this case), about 20 nm in diameter and stiff and straight along a 1 μm length; perfectly (nano) crystalline throughout. Chemistry can offer no other material that fits this description. How strong are these fibres? What are their structural properties? Are these materials electrical conductors? From the electronic structure viewpoint, there are two ways in which nanotubes differ from graphite. First, there is the effect of reduced dimensionality. Nanotubes are, in effect, the holy grail of quasi-1D structures. Second is the effect of forcing the graphite sheets out of planarity, endowing them with curvature. This would result in an enhancement of the electron density in the outer lobe of the p_z orbital, the orbital responsible for conductivity in graphite. At present, there are more questions than answers. One of the problems is to study the properties of *single nanotubes*, and to distinguish these from the properties of bundles of nanotubes. The purity of these materials would be critical.

The article by Seshadri *et al.* (page 839) discusses some current problems in nanotube research, apart from presenting new results that point the direction to future work. One interesting feature of nanotubes is that the central void can be filled with metals and compounds. The properties of such encapsulated metals is an area of research by itself. Are metals encapsulated in nanometer cavities crystalline? What would their electronic, magnetic and superconducting properties be, and more importantly, how would these be measured? While many of these questions would require further work, involving the use of novel experimental techniques for even a partial resolution, the message that shines through is clear; that carbon nanotubes are a fertile new area of Materials Research, and will remain so for some time to come.

Prospecting amongst protein structures

The 'protein folding problem' or the process by which amino acid sequence information is translated into a specific three-dimensional architecture is one of the most active areas of research in structural biology. The flood of protein crystal structures (almost a deluge, now) threatens to drown those grappling with this problem, in a sea of information. Paradoxically, in science, too much data can

sometimes confound as much as illuminate. This wealth of three-dimensional information on protein structures provides, those who are bold enough to venture to do so, an opportunity to identify common threads in apparently diverse structures. There have been many attempts to analyse amino acid sidechain conformations (rotameric states) and the introduction of the concept of rotamer libraries has allowed the development of algorithms to identify sequences, which can be accommodated in specific three-dimensional folds. Are side-chain conformations and backbone structures correlated? Baranidharan and Murthy address this question in an analysis of 102 high resolution protein structures, reported on page 847. These authors rationalize the preference of specific residues to occur at the ends of helices in terms of individual backbone-sidechain interactions. Several residues appear to exert an asymmetrical influence at the N- and C-terminal ends of the polypeptide chain. Unfortunately, individual sidechains 'do not appear to have remarkably significant and predictable effects on the backbone geometry in the case of helices and sheets'. Clearly, the codes for protein folding are well hidden and the structural biologists treasure hunt will continue.

P. B.