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MATHEMATICAL MODELLING OF NANOSTRUCTURES

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Worldwide nanotechnology is a major focus in science and technology, and most research in this area deals with chemical, physical and biological issues or a combination of these areas, but to date very little work has been undertaken on mathematical modelling. Rather than employing large-scale computations using molecular dynamics simulation, in this thesis elementary mechanical principles and classical applied mathematical modelling procedures are utilized to examine three specific areas in nanotechnology.

Firstly, the Lennard-Jones potential function for the nonbonded interaction potential energy between two molecules and the continuum approximation, which assumes that the interatomic interactions can be modelled by smearing the atoms uniformly across surfaces, are undertaken to investigate the mechanical properties of certain nanostructures, namely double-walled carbon nanotubes, nanopeapods, nanocones and carbon onions. Owing to their special mechanical, electrical and thermal properties, these nanostructures promise many applications for future nanoscale devices, such as nanobearings and nanooscillators. This thesis examines issues regarding nanooscillators constructed from these nanostructures. In particular, the van der Waals interaction energy, the suction energy, the offset location and the oscillatory behaviour are determined. Analytical expressions are obtained as a function of the radii and the lengths of the structures. In addition, all the predicted mechanical properties derived here are in excellent agreement with results from molecular dynamics simulations.

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The second area is the joining of nanostructures by invoking the principle that the atoms arrange themselves in such a way that the total squared deviation of the distance between atoms at the junction and some ideal bond length is a minimum. Initially, toroidal molecules are described, which are formed from three distinct carbon nanotube sections, through minimization of the total squared deviation of the distance between two carbon atoms at the junction from the ideal physical bond length. Representative formulae for the mean generating toroidal radius and tube radius of the tori are determined. Following this, the perpendicular joining structures for carbon nanotubes and flat graphene are determined by two least squares approaches, which are the variation in bond length and the variation in bond angle. Such a combined structure might constitute a transmission platform for ultra small computer chips. Given that the corresponding boron nitride nanostructures are also good semiconductors, the corresponding combined structures are also determined. However, the essential mathematical ideas for combining boron nitride structures are quite different to those required for connecting the corresponding carbon structures, since only rings with an even number of sides are energetically favourable.

The third area in this thesis involves the elastic model of carbon nanotubes. Here, carbon nanotubes are assumed to be modelled as transversely isotropic linearly elastic materials which have the same properties in one plane, but vary in the normal direction to this plane. The equilibrium equations are derived and they can be shown to generalize those for isotropic materials. Furthermore, wave-like deformations on the outer-most surface of the oscillating carbon nanotubes are investigated. On neglecting any frictional effects and assuming that the inner surface atoms of the outer tube and those located on the outer surface of the inner tube dominate the van der Waals force, expressions for displacements in the r- and z-directions are obtained.

The major contribution of this thesis is the use of conventional applied mathematical modelling techniques to formulate analytical expressions for nanostructures. Broadly three mechanical issues are studied, including (i) van der Waals interaction energy and oscillatory behaviour for nanostructures, (ii) geometry of combining two nanostructures and (iii) deformation of carbon nanotubes as transversely isotropic materials. However, many of the theoretical structures proposed here have yet to be confirmed either experimentally or by molecular dynamics simulations, and as such the work might be considered as a first step to settling some of the important physical principles in nanotechnology. In summary, the new elements of the thesis comprise:

- analytical expressions to determine the equilibrium locations, force distributions and oscillatory behaviours for nested nanostructures;
- simple least squares methods to connect two nanostructures;
- an elastic model for the deformations of double-walled carbon nanotubes.

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