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Mathematical modelling of nanostructures

Duangkamon Baowan
University of Wollongong

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Baowan, Duangkamon, Mathematical modelling of nanostructures, PhD thesis, School of Mathematics and Applied Statistics, University of Wollongong, 2008. <http://ro.uow.edu.au/theses/51>

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Mathematical modelling of nanostructures

*A thesis submitted in fulfillment of the
requirements for the award of the degree of*

Doctor of Philosophy

from

University of Wollongong

by

Duangkamon Baowan

B.Math (Hons), Mahidol University

School of Mathematics and Applied Statistics

2008

CERTIFICATION

I, Duangkamon Baowan, declare that this thesis, submitted in fulfilment of the requirements for the award of Doctor of Philosophy, in the School of Mathematics and Applied Statistics, University of Wollongong, is wholly my own work unless otherwise referenced or acknowledged. The document has not been submitted for qualifications at any other academic institution.

Duangkamon Baowan

May, 2008

Acknowledgements

A journey is easier when you travel together. Interdependence is certainly more valuable than independence. This thesis is the result of three years of work whereby I have been accompanied and supported by many people. It is a pleasant aspect that I have now the opportunity to express my gratitude to all of them.

The first person I would like to thank is my supervisor, Professor Jim Hill. During these years I have known him as a sympathetic and principled person. His enthusiasm and his wide ranging view of research has made a deep impression on me. I owe him lots of gratitude for having shown me this approach to research and I am grateful that I have come to know Professor Jim Hill in my life.

I would like to acknowledge my co-supervisor Dr. Ngamta Thamwattana who has constantly kept an eye on the progress of my work and was always available when I needed her advice. Dr. Ngamta is not only my supervisor, but she is also my sister and my friend, who has taken care of me since the first day I arrived here in Australia.

The Nanomechanics Group also substantially contributed to the development of this work. Especially the extensive comments and the interactions with Dr. Barry Cox which have had a direct impact on the quality of this thesis. I would also like to thank my fellow PhD student Tamsyn Hilder for our many discussions and for providing me much sisterly advice.

This research has been supported by a Royal Thai Government Scholarship. I am grateful for their confidence in me. I am also grateful to the School of Mathematics and Applied Statistics at the University of Wollongong for providing me with an excellent working environment during the years of my study.

Last but not least, I wish to express my gratitude to the people who never failed to support me throughout my journey, my father, my mother and my brother.

Abstract

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 utilised to examine three specific areas in nanotechnology.

Firstly, the Lennard-Jones potential function for the non-bonded 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 nano-bearings and nano-oscillators. This thesis examines issues regarding nano-oscillators 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.

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 minimisation 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 is to determine the perpendicular joining structures for carbon nanotubes and flat graphene 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 generalise those for isotropic materials. Further, 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,
- Elastic model for the deformations of double-walled carbon nanotubes.

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